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Data Article

Helical push-pull systems for solar cells: Electrochemical, computational, photovoltaic and NMR data

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A R T I C L E I N F O

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A B S T R A C T

The data presented in this article are related to the research article entitled “An unconventional helical push-pull system for solar cells” (Dova et al., 2019). This article provides: a) the cyclic voltammogram plots in solution of helical push-pull sensitizers and the corresponding precursors; b) the visualization of the leading natural transition orbital (NTO) pairs obtained by theoretical calculation of frontiers orbitals; c) *J*/*V* curves of dye-sensitized solar cells (DSSC) sensitized by the dyes, without 3a,7a-dihydroxy-5b-cholic acid (CDCA) as co-adsorbent agent; d) ^{1}H and ^{13}C NMR spectra of dyes.

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Specifications table

Subject area	Chemistry
More specific subject area	Organic dyes, solar cells, helicenes
Type of data	Synthetic scheme, figures, tables, and graphs
How data was acquired	Cyclic voltammograms (AUTOLAB PGSTAT potentiostat, EcoChemie, The Netherlands). Computational data (Gaussian 09 Rev. D.01 program package). Photovoltaic measurements (Keithley digital source meter). NMR spectra (Bruker AC-300, Bruker Avance III 400 MHz, Bruker AMX-500 MHz and Bruker Avance 600 MHz).
Data format	Analyzed
Experimental factors	CV scan of dyes and their precursors in solution. Computational data. Current density-voltage (J/V) scans of dye-sensitized solar cell stained with sensitizers without co-adsorbent agent. ^{1}H and ^{13}C NMR spectra of dyes.
Experimental features	Electrochemical studies in solution, computational data, and J/V scan of dye-sensitized solar cell
Data source location	University of Milano and University of Milano-Bicocca Milano, Italy. Heidelberg University, Heidelberg, Germany
Data accessibility	Data is with this article
Related research article	Dova D, Cauteruccio S, Manfredi N, Prager S, Dreuw A, Arnaboldi S, et al. An unconventional helical push-pull system for solar cells. Dyes Pigm. 2019, 161, 382–388. [1]

Value of the data

- The CV patterns of helical push-pull sensitizers can be used by other researches to compare the redox properties of this helical-based dyes with other push-pull systems.
- Photovoltaic performances of DSSCs sensitized with the two dyes without CDCA could give important information about the efficacy of the helical structure in suppressing the aggregation compared to the data reported in Ref. [1].
- NMR spectra can be used to evaluate the variation of the chemical shift of the helical structure with different substituents.

1. Data

The dataset of this article affords information on the redox properties, photovoltaic performances and NMR spectra of two helical-based push-pull sensitizers. Figs. 1 and 2 show CV patterns of dyes and their corresponding precursors, respectively. Table 1 displays the visualization of the leading NTO pairs. Fig. 3 shows photovoltaic performances of DSSCs sensitized obtained with the two dyes without CDCA. Figs. 4–13 are related to the ^{1}H-NMR and ^{13}C-NMR spectra of the dyes.

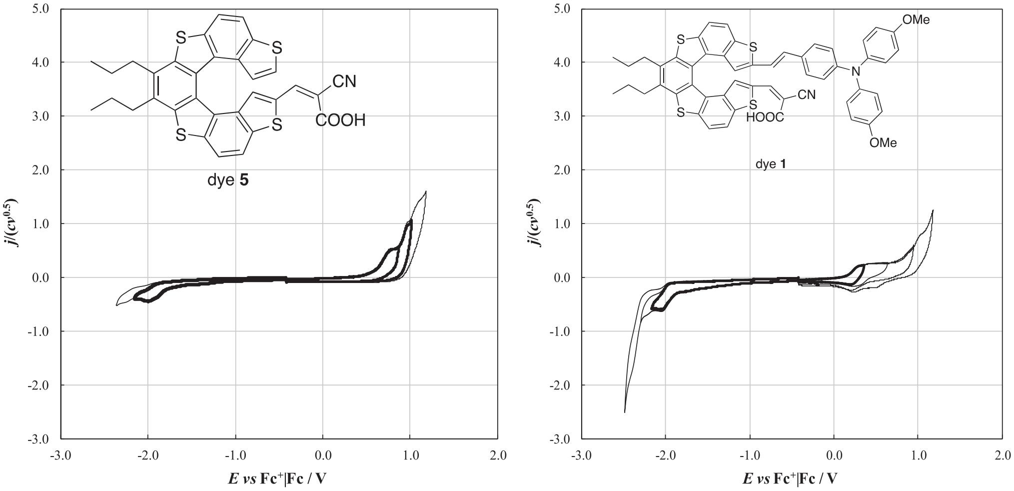


Fig. 1. CV patterns of dye **5** (on the left) and dye **1** (on the right) recorded at 0.2 V s^{-1} potential scan rate, on GC electrode in ACN + TBAP 0.1 M.

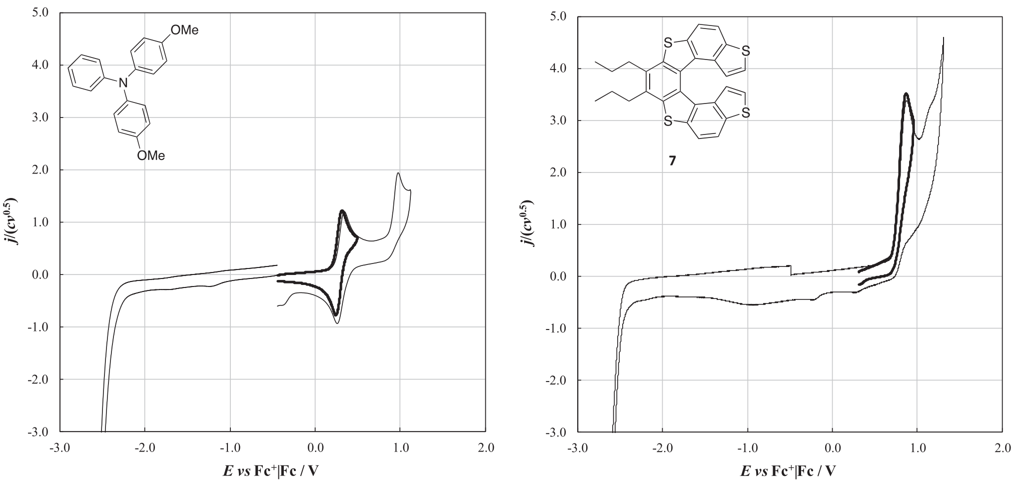


Fig. 2. CV patterns of bis(paramethoxyphenyl)phenylamine (on the left) and tetrathiahelicene **7** (on the right) recorded at 0.2 V s^{-1} potential scan rate, on GC electrode in ACN + TBAP 0.1 M.

2. Experimental design, materials and methods

All information about the data obtained in electrochemical measurements, computational studies, photovoltaic measurements, and NMR spectra are reported in reference [1].

Table 1
Visualization of the leading NTO pairs with contributions of at least 80% of the total excitation. NTO of the hole (left) describing the origin of the excitation and of the electron (right) describing the target. The NTOs are labeled as HONTO and LUNTO for highest occupied natural transition orbital and lowest unoccupied natural transition orbital, respectively. These labels are chosen in analogy to the molecular orbital labelling scheme although it is not fully correct in the case of NTOs.

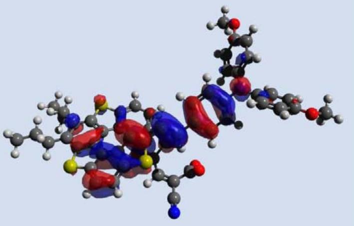
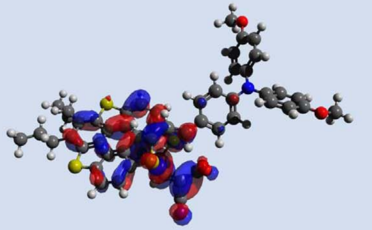
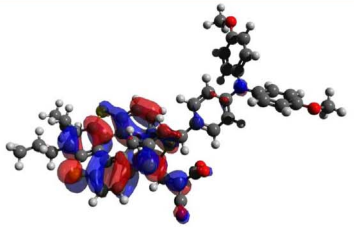
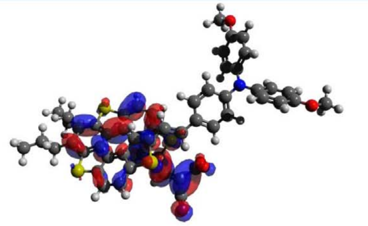
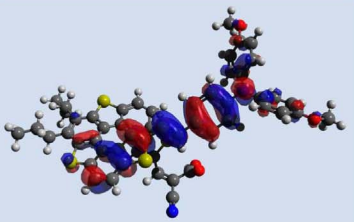
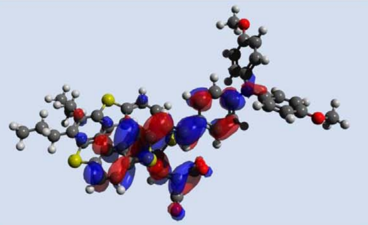
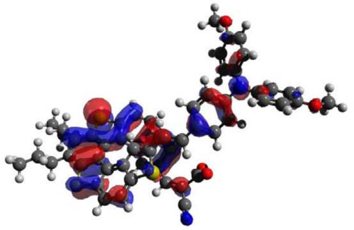
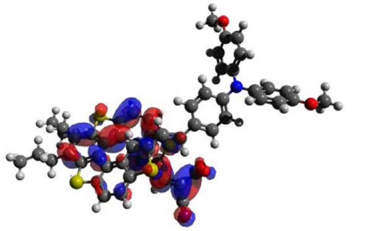
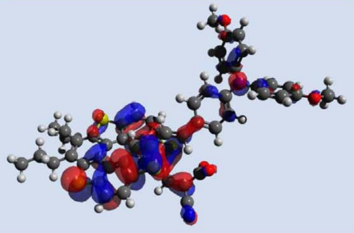
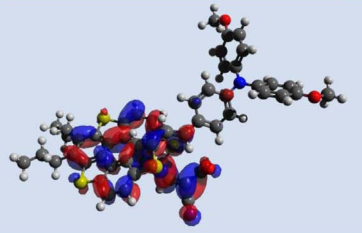
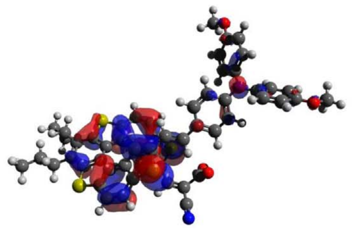
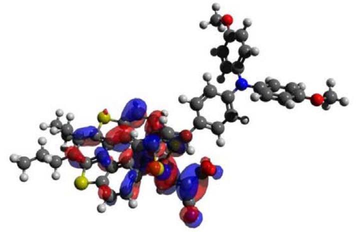
Excited state	Transition from (HONTO):	To (LUNTO):
S_1		
S_2		
S_3		
S_4		

Table 1 (*continued*)

S_5		
S_6		

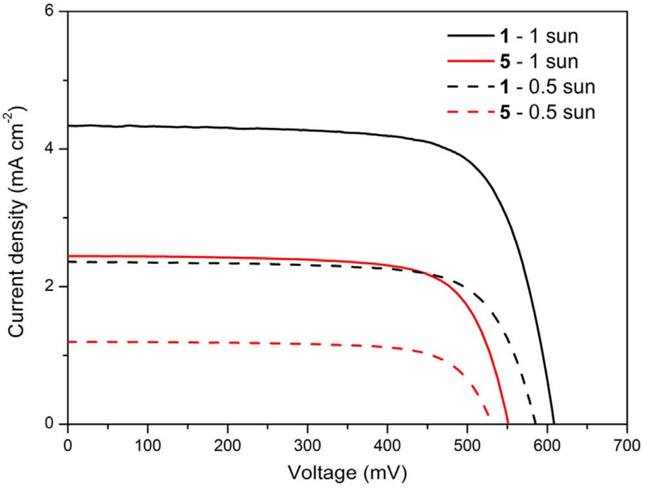


Fig. 3. *J*/*V* curves of DSSC sensitized by dyes **1** and **5**, with different solar intensities.

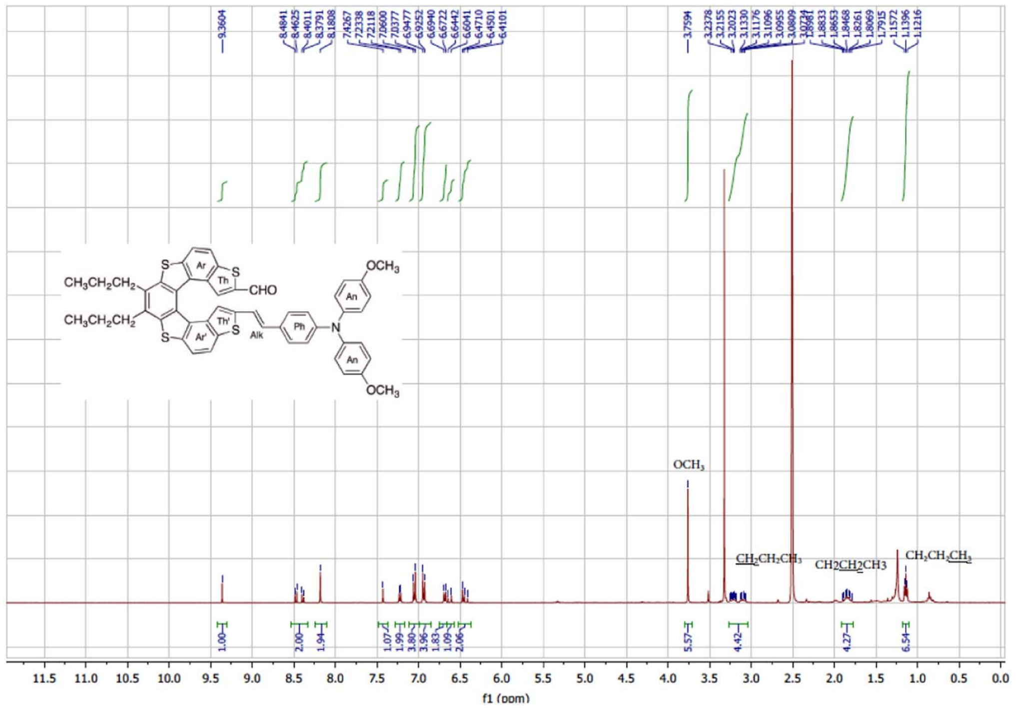


Fig. 4. [1]H NMR (400 MHz, $(CD_3)_2SO$) of the precursor of dye **1**.

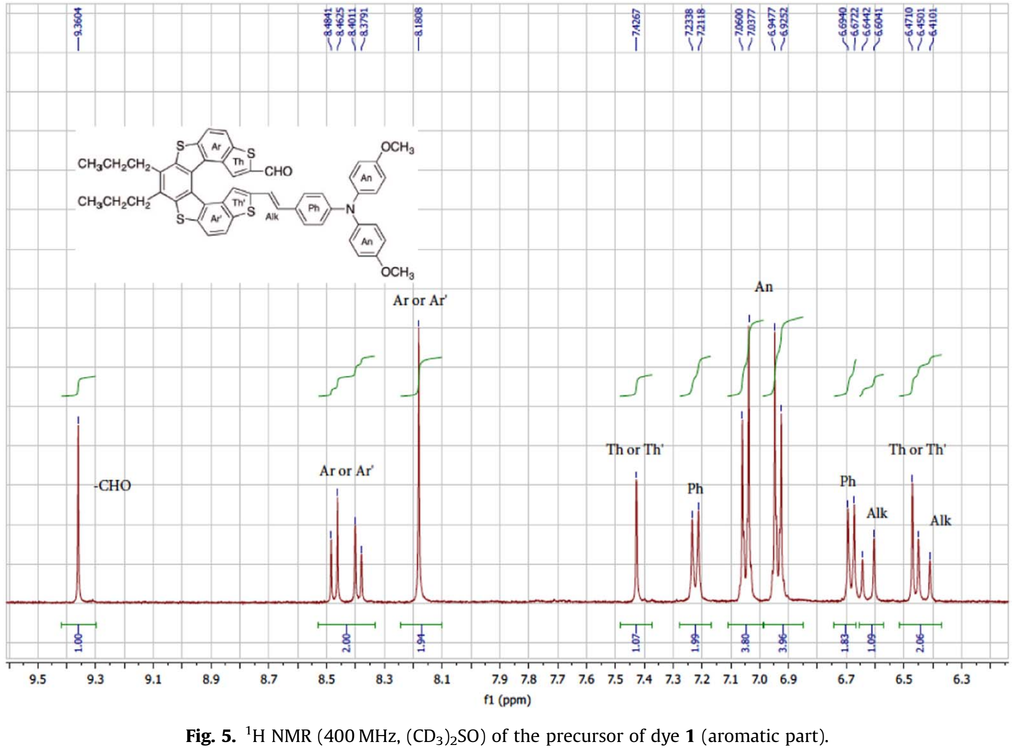


Fig. 5. [1]H NMR (400 MHz, $(CD_3)_2SO$) of the precursor of dye **1** (aromatic part).

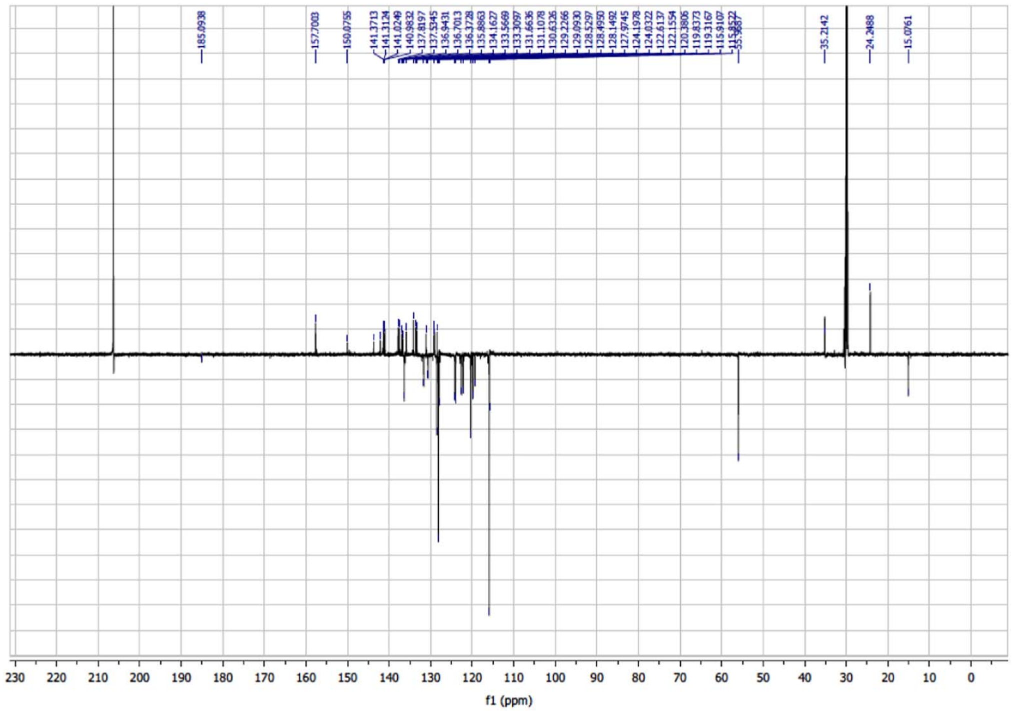


Fig. 6. ^{13}C NMR (150 MHz, $(CD_3)_2CO$) of the precursor of dye **1**.

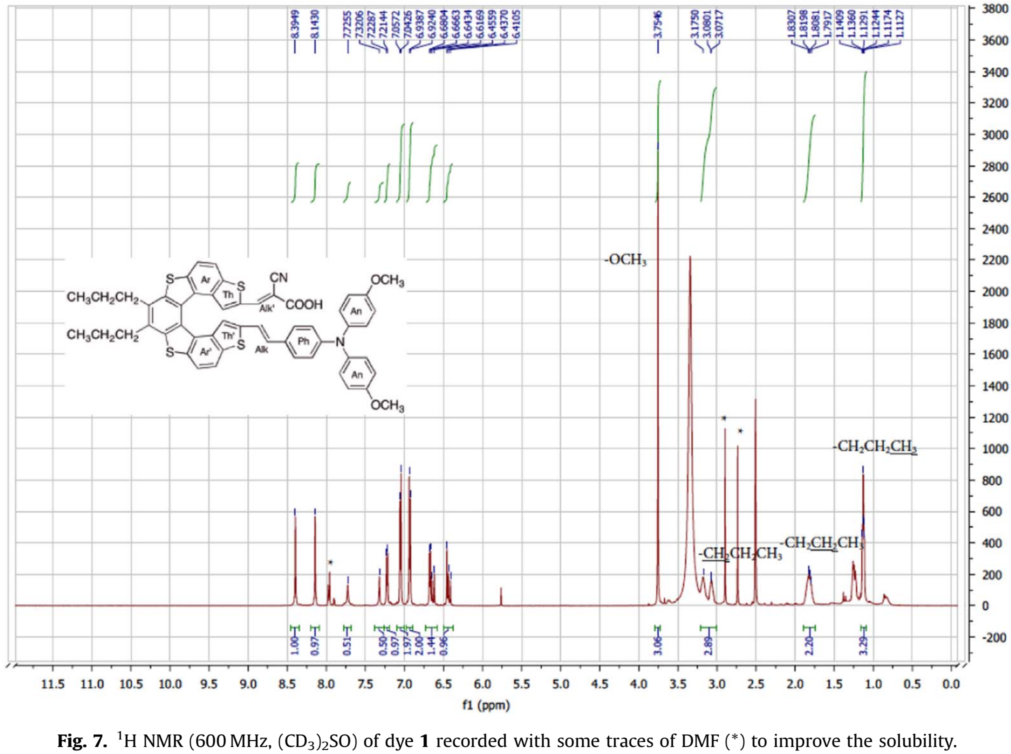


Fig. 7. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) of dye **1** recorded with some traces of DMF (*) to improve the solubility.

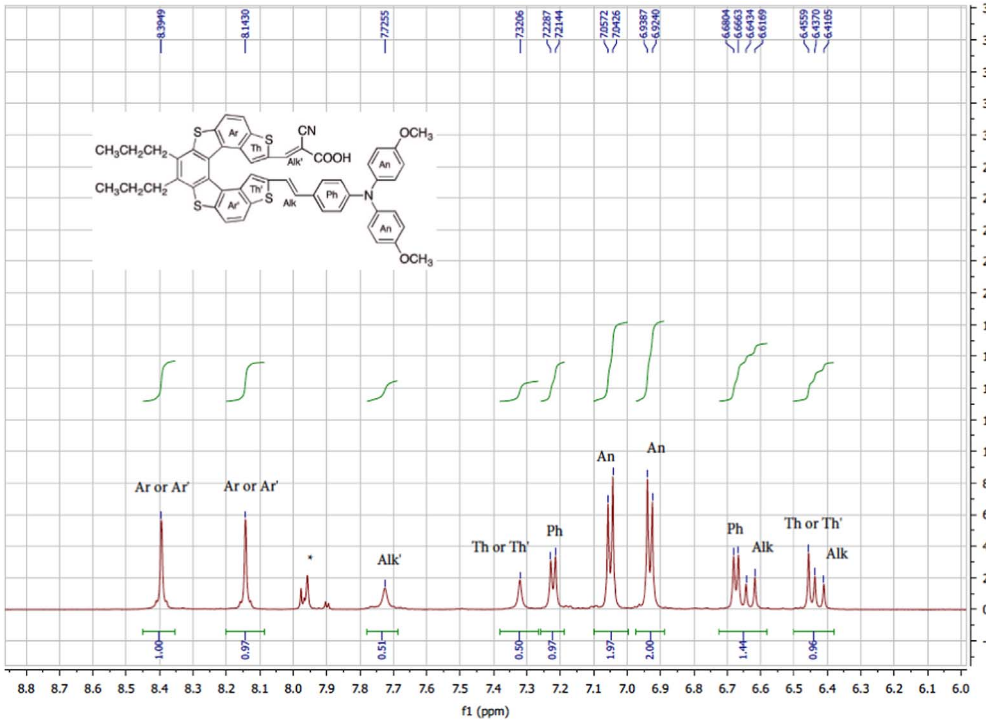


Fig. 8. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) of dye **1** (aromatic part).

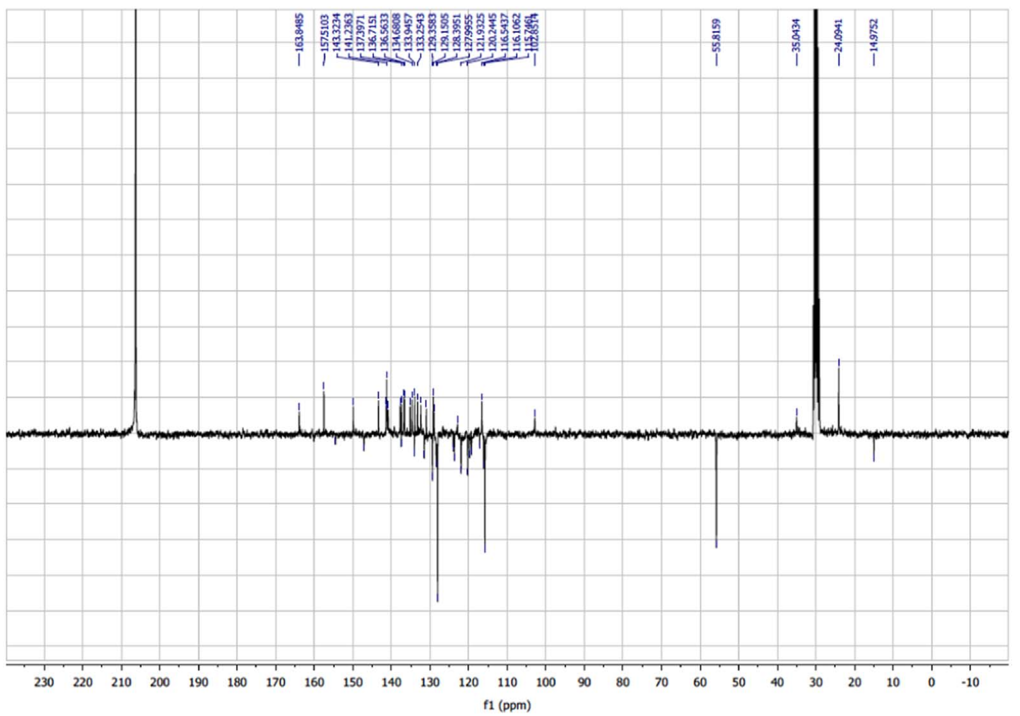


Fig. 9. ^{13}C NMR (75 MHz, $(CD_3)_2CO$) of dye **1**.

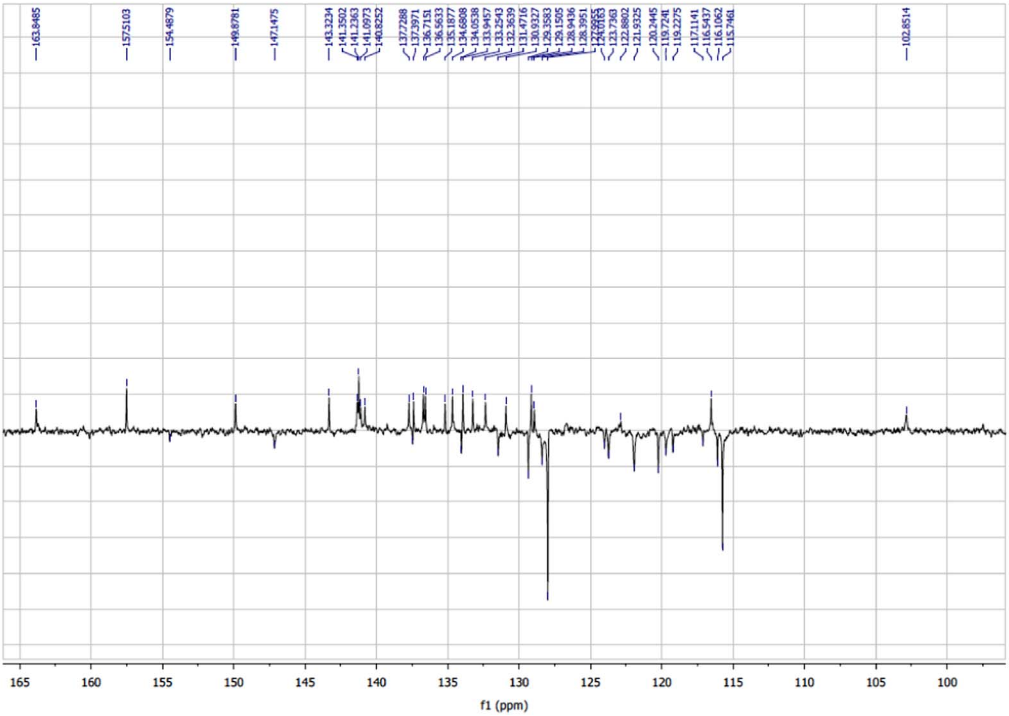


Fig. 10. ^{13}C NMR (75 MHz, $(CD_3)_2CO$) of dye **1** (aromatic part).

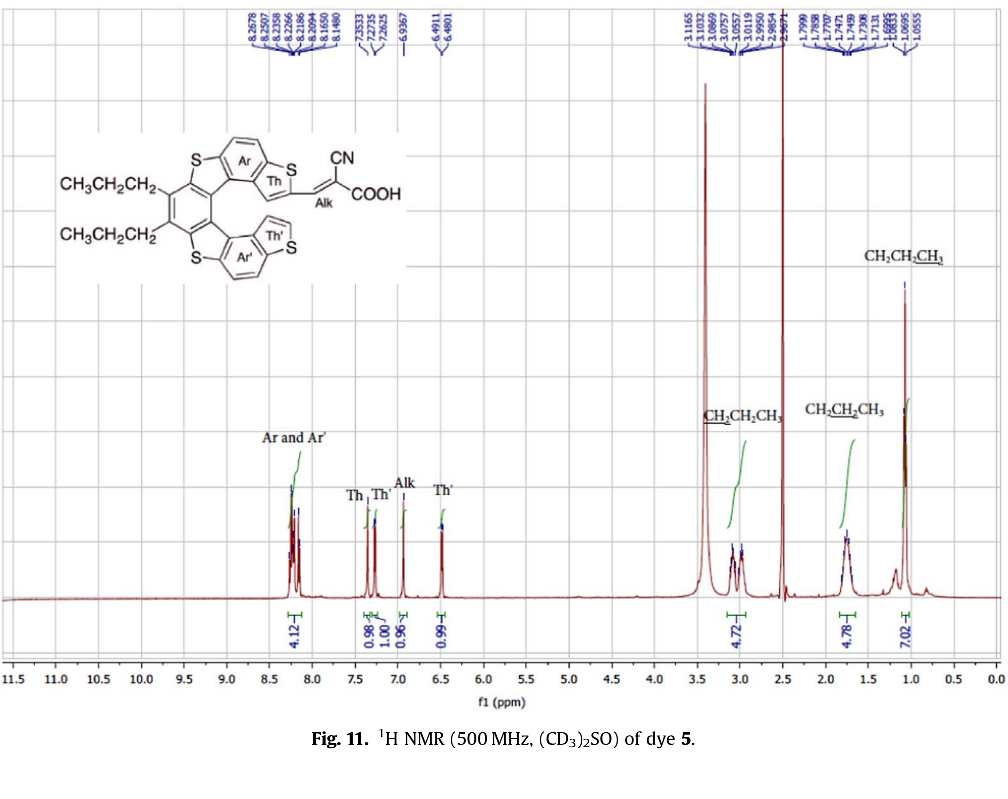


Fig. 11. ^{1}H NMR (500 MHz, $(CD_3)_2SO$) of dye **5**.

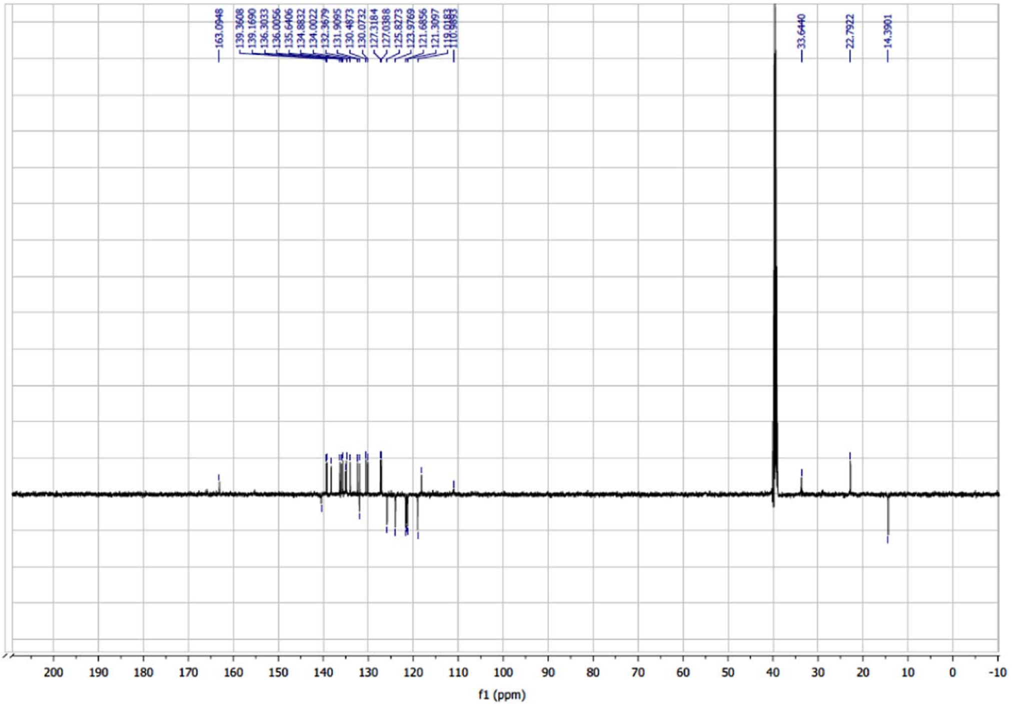


Fig. 12. ^{13}C NMR (125 MHz, $(CD_3)_2SO$) of dye **5**.

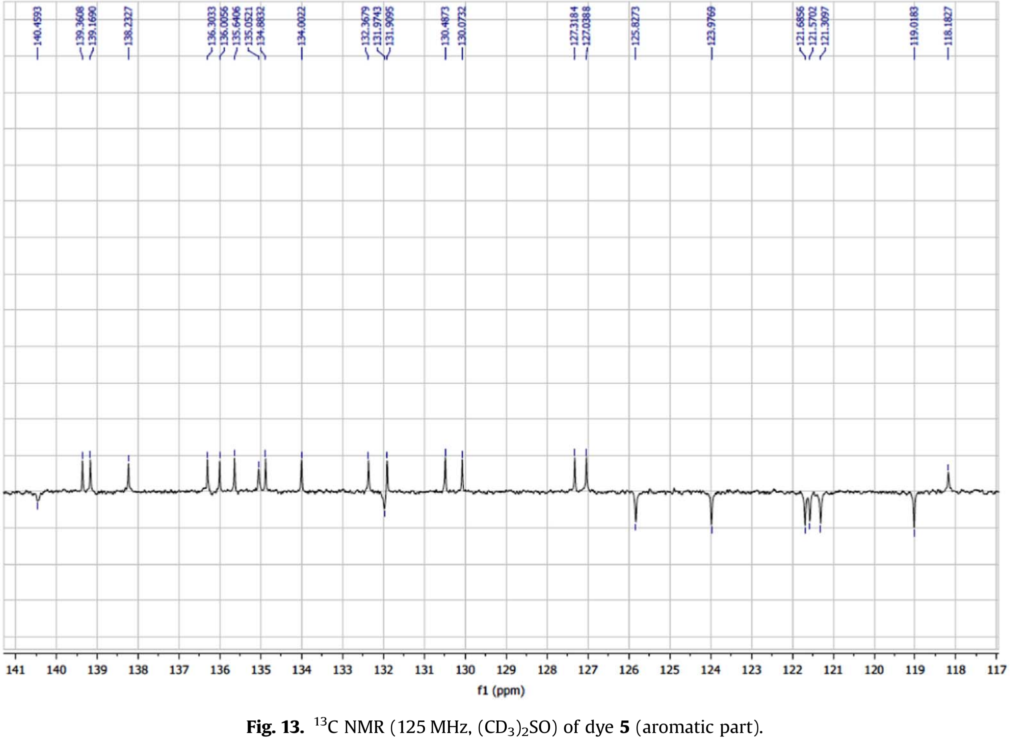


Fig. 13. ^{13}C NMR (125 MHz, $(CD_3)_2SO$) of dye **5** (aromatic part).

Acknowledgements

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.074.

Reference

[1] D. Dova, S. Cauteruccio, N. Manfredi, S. Prager, A. Dreuw, S. Arnaboldi, P.R. Mussini, E. Licandro, A. Abbotto, An unconventional helical push-pull system for solar cells, Dyes Pigm. 161 (2019) 382–388.