Infrared and Raman Spectra of a Well–Barrier–Well 1,2-Di(α,α′-Bithienyl)Vinylene

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Abstract

We have studied the FT-IR and FT-Raman spectra of a neutral thiophene-based oligomer in relation to the effective conjugation length of the π-electrons. The compound has a well–barrier–well structure, where the well parts are two bithienyl end-moieties and the barrier part is a vinylene fragment with a larger energy gap. Characteristic features are correlated with vibrational data of one-dimensional unsubstituted α-oligothiophenes and α,α′-dimethyl end-capped oligothiophenes.

Keywords: (Infrared and Raman spectroscopy, polythiophene and derivatives)

We have investigated the Raman spectrum of a thiophene-based oligomer having a well-barrier-well structure in quasi one-dimensional backbone chains, where the well part are two thiophene end-moieties and the barrier part is a vinylene fragment with larger energy gap (referred to as T2VT2 hereforth). This class of oligomers is attracting attention for their potential applications in light-emitting devices [1]. The details on the synthesis are described elsewhere [2]. The Raman spectrum was recorded for the solid compound on a Bruker FRA/106 FT-Raman spectrometer, with a 1064 nm exciting laser line. The obtained spectrum is displayed in Figure 1.

![Fig. 1. FT–Raman spectrum of neutral T2VT2 in the solid state.](image)

The Raman spectrum is characterized by three main bands at 1601, 1539 and 1433 cm⁻¹. The former band has to be assigned to the stretching of the trans-vinylene bridge, being downshifted by 17 cm⁻¹ with respect to the 1,2 bis(thienylene)vinylene compound [3] as a direct consequence of the increase of π-conjugation. The other bands are characteristic of the oligothienyl backbone [4]: i) that at 1539 cm⁻¹ corresponds to a C=C stretching mostly localized on the outer rings, and ii) that at 1433 cm⁻¹ is due to the collective in-phase stretching vibration of the C=C bonds, being probably spreaded over the whole molecule.

Acknowledgements

This research was financially supported by Dirección General de Enseñanza Superior (DGES, MEC, Spain) through the research project PB96-0682. We are also indebted to Junta de Andalucía (Spain), funding for our research group (FQM-0159).

References