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Electronic Circular Dichroism of Gamma-valerolactone dimers extracted from Monte Carlo liquid phase simulation.

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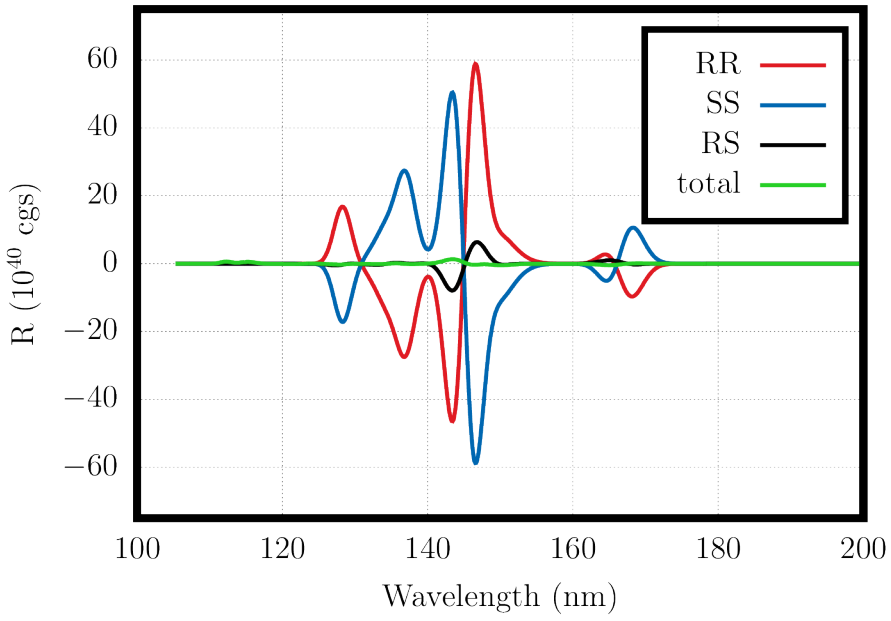
Abstract: Gamma-valerolactone (GVL) is a chiral green solvent which gained high importance in the past decade due to its environmental-friendly properties[1]. The presence of an asymmetric carbon within its structure gives rise to two enantiomers, RGVL and SGVL, leading to different interactions between GVL molecules in the racemic mixture: homochiral interactions (those between equal enantiomers: RR and SS) and heterochiral interactions (those between different enantiomers: RS). From a Monte Carlo NpT ensemble simulation (T = 25 ºC, p = 1 atm) the most stable RR, SS and RS dimers from racemic mixture were sampled within a 10k configurations inteverval and 8000 uncorrelated structures were obtained for each pair. Electronic Circular Dichroism (ECD) calculations were performed for all structures using the semiempirical ZINDO/S hamiltonian. Only single excitations were calculated and the first 20th low excited states were analyzed. The average spectra for RR, SS and RS dimers ensembles and also the total average are shown below:



One observes symmetric curves from RR and SS contributions. The results from RS dimers presents low amplitudes which is consistent with the opposite contributions from each chiral structure. The total average shows a very low amplitude as expected from a racemic mixture.

Key-words: Gamma-valerolactone, Monte Carlo, Dimers, Electronic Circular Dichroism, chirality.

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References:

[1] J. M. Tukacs, B. Fridrich, G. Dibó, E. Székely, L. T. Mika. Green Chem. 17, 5189 (2015).