

Addition/Correction

Probing Excitation Delocalization in Supramolecular Chiral Stacks by Means of Circularly Polarized Light: Experiment and Modeling [*J. Am. Chem. Soc.* 2007, 129, 7044–7054].

Frank C. Spano, Stefan C. J. Meskers, Emanuelle Hennebicq, and David Beljonne

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Probing Excitation Delocalization in Supramolecular Chiral Stacks by Means of Circularly Polarized Light: Experiment and Modeling [J. Am. Chem. Soc. 2007, 129, 7044–7054]. Frank C. Spano,* Stefan C. J. Meskers, Emanuelle Hennebicq, David Beljonne

A sign error in the fortran code used to evaluate $g_{abs}(\omega)$ and $g_{lum}(\omega)$ has been discovered. Since $g_{abs}(\omega)$ and $g_{lum}(\omega)$ change sign when the helical pitch angle ϕ changes sign, the values for ϕ reported for all calculations need to be negated. With these corrected values of ϕ all figures remain unchanged. We therefore obtain good agreement with the measured $g_{abs}(\omega)$ and $g_{lum}(\omega)$ for a pitch angle of $+14^\circ$ (left-handed helix) and not -14° (right-handed helix) as originally reported.

Additional support for the left-handed helix was obtained from molecular dynamics calculations. We started with a 12-molecule MOPV4 stack built from enantiomerically pure MOPV4 molecules bearing exclusively (*S*)-2-methylbutoxy side chains. Two structures were generated with intermolecular angles (ϕ) along the stack direction of either 20° or -20° . A molecular dynamics simulation of 50 ps at 300 K (within the NVT ensemble, Dreiding force field,¹ Gasteiger charges²) was then performed for both the left-handed and right-handed helices. The most stable structures generated from the MD run were subsequently optimized at 0 K using the same force field. In the optimized structures, the rotation angle is reduced to an average value of $\sim 15^\circ$ (left) and $\sim -13^\circ$ (right). The calculations indicate that the left-handed helix is more stable by ~ 3 kcal/mol per molecule than its right-handed counterpart and that the energy difference arises primarily from less favorable van der Waals interactions.

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Synthesis of Monoalkoxide Monopyrrolyl Complexes Mo(NR)(CHR')(OR'')(pyrrolyl): Enyne Metathesis with High Oxidation State Catalysts [J. Am. Chem. Soc. 2007, 129, 12654–12655] Rojendra Singh, Richard R. Schrock,* Peter Müller, and Amir H. Hoveyda

Page 126555. In ref 4 “Blanc, R.” should be “Blanc, F.”

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