

# Energetic, Structural, and Vibrational Properties of 4,4'-Methylenediphenyl Diisocyanate with Relevance for Adhesion

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© 2016 American Chemical Society. Through a polymerization process, the monomer 4,4'-methylenediphenyl diisocyanate can participate in glueing, whereby strong covalent bonds between the monomer and the substrates that will be glued have to be formed. In the present work, we use density functional theory (DFT) calculations to study a group of properties that are important for the initial steps of this process and for its experimental characterization. We focus on energetic and structural properties of a single monomer of 4,4'-methylenediphenyl diisocyanate as obtained using different theoretical approaches. We demonstrate that the molecule is chiral and that for each chirality, three different structures, differing in the orientations of the isocyanate groups, can be identified. The molecule is soft against certain geometry transformations and can, accordingly, easily take a structure that is optimal for the formation of covalent bonds with a substrate. Infrared spectroscopy may be used