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Localized Charge Distributions. III. Transferability and Trends of Carbon-Hydrogen Moments and Energies in Acyclic Hydrocarbons

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Abstract
The localized charge distributions defined previously are used to calculate INDO bond moments and energies of a variety of CH bonds in acyclic hydrocarbons. The polarity of all bonds discussed is c+H-. It is found that each basic type of CH bond (primary, vinyl, ethynyl) has an overflow of electron density (a "tail") out of the bond region which resides on and is characteristic of those atoms trans and coplanar to the bond. It is demonstrated that, since these tails are virtually independent of each other, the basic bond moments can be used to construct a model which predicts all calculated bond moments and orientations to a high degree of accuracy. While the total energies of the bonds ei (where the molecular energy E = ~iei) are not very transferable, the intra bond and interference energies can be predicted rather well using a similar model. The trends in the bond moments are discussed in terms of the point charge and polarization contributions, and the interference energies are shown to correlate well with the trends in experimental CH bond energies. The trends in both properties are principally determined by the loss of interference density within the bond due to the presence of overflow atoms.

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