Factors that Influence Energies of Simple Hydrocarbons

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Although several models have been proposed to account for the varying stabilities of alkanes, the ability of these models to fit experimental data remains controversial. The work presented here focuses on evaluating the abilities of three models to describe the energy differences of alkanes, thereby providing insight into the factors that are the most consequential to hydrocarbons' relative stabilities and leading to the proposal of the vicinal interactions model (VIM). In contrast to older models that generally lack theoretical support, the VIM is justified by natural bond orbital (NBO) analysis confirming that vicinal, antiperiplanar bond-bond and bond-antibond interactions are the most consequential. The VIM is a fairly simple additivity scheme based on bond enthalpies and vicinal, antiperiplanar bond pair interactions. The VIM was compared to the localized bond model (LBM) and geminal interactions model (GIM). Energy parameters for each model were fitted to best represent the atomization enthalpies (AE) of the C1-C6 alkanes, calculated by the Gaussian electronic structure program. Parameter fittings yielded chi squared values for the LBM, GIM, and VIM of 15.26, 12.04, 7.68 respectively. As anticipated, the LBM failed to account for differing AEs as it attributed no significance to any factors other than CC and CH bond enthalpies. The GIM, although exhibiting an improvement over the LBM, failed to describe the AEs of alkane conformers. The proposed VIM, on the other hand, generated unique AEs for each C1-C6 alkanes. The results of this study strongly support the VIM as a new model for understanding the differing stabilities of alkanes.

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