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Molecular Orbital Calculations on the Adsorption Mode of n-Hexane above a Graphite Surface. Commensurate Binding is Not a Critical Factor THOMAS BAKER, RONALD SEE, Indiana University of Pennsylvania — Molecular orbital calculations were preformed to investigate the binding of n-hexane physisorbed on a graphite surface. In the model proposed by Groszek the binding mode of the alkyl chain is commensurate with the graphite surface. However, for the alkane to be perfectly commensurate with the graphite surface, the equilibrium length of the alkane must be distorted. Calculations were preformed to compare the binding of n-hexane constrained in the graphite-commensurate geometry to the binding of n-hexane in its equilibrium geometry. In each computational protocol used, the optimum hexane-surface distance was found to be 4.2 Angstroms for both the constrained and geometry-optimized molecules. The cost of constraining n-hexane to the graphite-commensurate geometry was calculated to be 18 kJ/mol, but the energetic advantage for perfectly commensurate binding, over binding of undistorted n-hexane, is much smaller; ranging from 4.6-12.2 kJ/mol. Therefore, the hexane-surface systems containing undistorted n-hexane are always favored over the graphite-commensurate hexane, with an advantage of 13.9 kJ/mol in the B3LYP/6-31G* calculation.

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