

**$\pi$ -Stacking Behavior of Selected Nitrogen-Containing PAHs.** Tran, Fabien; Alameddine, Bassam; Jenny, Titus A.; Wesolowski, Tomasz A. Department of Physical Chemistry, University of Geneva, Geneva, Switz Journal of Physical Chemistry A (2004), 108(42), 9155-9160.

### **Abstract**

The packing preferences of dimers formed by nitrogen-contg. planar polycyclic arom. hydrocarbons ((C<sub>30</sub>H<sub>15</sub>N)<sub>2</sub> and (C<sub>36</sub>H<sub>15</sub>N)<sub>2</sub>) were studied by means of theor. calcns. Potential energy curves corresponding to various relative motions of the monomers (vertical displacement, rotating, slipping, and combinations of them) were derived. It was found that the monomers in such  $\pi$ -stacked dimers are rather strongly held together (the interaction energy is about -9 kcal/mol) in an off-centered arrangement. It emerges as a general picture that the aligned structures are less stable than the ones where the nitrogen atoms, as the centers of the considered monomers, are not on top of each other but offset by 1.8-2.7 Å. Displacing the centers further results in a rapid redn. of the interaction energy. Within these relatively large relative motions (up to about 3 Å) of the monomers, however, no significant loss of stability of the dimers is noted. In the case of C<sub>30</sub>H<sub>15</sub>N, changing the orientation of the enantiotopic faces in the dimer formation leads to two nonequivalent min. energy structures of similar energies but notably different geometries. The most stable structure of both dimers studied resembles that of two adjacent layers of graphite. We conclude, therefore, that the studied mols. could be considered as good building block candidates for the fabrication of columnar org. conductors.