Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Accurate Determination of Pyridine – Poly (Amidoamine) Dendrimer Absolute Binding Constants with the OPLS-AA Force Field and Direct Integration of Radial Distribution Functions YONG PENG, GEORGE KAMINSKI — OPLS-AA force field and direct integration of intermolecular radial distribution functions (RDF) were employed to calculate absolute binding constants of pyridine molecules to NH_2 and amide group hydrogen atoms in 0th and 1st generation poly (amidoamine) dendrimers in chloroform. The average errors in the absolute and relative association constants, as predicted with the calculations, are 14.1% and 10.8%, respectively, which translate into ca. 0.08 kcal/mol and 0.06 kcal/mol errors in the absolute and relative binding free energies. We believe that this level of accuracy proves the applicability of the OPLS-AA, force field, in combination with the direct RDF integration, to reproducing and predicting absolute intermolecular association constants of low magnitudes (ca. 0.2 – 2.0 range).

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Date submitted: 13 Dec 2005 Electronic form version 1.4