Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Comparison of vibrational and electronic contributions to van der Waals interactions MARK R. PEDERSON, Naval Research Laboratory, KYUNGWHA PARK, Virginia Polytechnic Institute, AMY Y. LIU, Georgetown University — The van der Waals interaction can be caused by either ionic vibrations or instantaneous electronic motion relative to the atomic center. In this study, the vibrational contribution to the van der Waals interaction is formulated by considering the interaction between induced dipoles caused by the infrared-active normal modes of a neutral molecule. Using the derived formula, the contribution is quantified, within the density-functional theory formalism, using a screened, i.e., self-consistent, vibrational polarizability. Applications for several neutral nonpolar dimers are presented. It is found that the vibrational contributions for the dimers are substantially smaller than their electronic contributions. The ratio of the vibrational to electronic contributions depends strongly on the ratio of the screened vibrational to electronic polarizabilities and on the ratio of the frequency of the strongest infrared-active mode to an ionization energy.

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Date submitted: 27 Nov 2007 Electronic form version 1.4