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Analysis of van der Waals Interaction Energies from Quantum Chemistry: Aromatic Clusters and Rare Gas Dimers STEPHEN GARRISON[1], National Institute of Standards and Technology, NIST Center for Theoretical and Computational Nanosciences, INEZ GONZALEZ, University of Akron, Department of Chemistry, CARLOS GONZALEZ, National Institute of Standards and Technology, NIST Center for Theoretical and Computational Nanosciences, MANUEL MARQUEZ, Philip Morris USA Research Center, EDWARD LIM, University of Akron, Department of Chemistry — The weak van der Waals (vdW) interactions in aromatic clusters and rare gas systems are studied using ab initio quantum chemistry and the Hartree-Fock Dispersion (HFD) method. The results, extrapolated to the complete basis set limit and along with comparisons to experiment, are used to understand and explain a fortuitous cancellation of errors in the benzene interaction calculations. Additionally, interesting results are found for the all-electron calculations for argon.

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