Physics > Chemical Physics

Weak intermolecular interactions in gas-phase NMR

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Gas-phase NMR spectra demonstrating the effect of weak intermolecular forces on the NMR shielding constants of the interacting species are reported. We analyse the interaction of the molecular hydrogen isotopomers with He, Ne, and Ar, and the interaction in the He-CO_2 dimer. The same effects are studied for all these systems in the ab initio calculations. The comparison of the experimental and computed shielding constants is shown to depend strongly on the treatment of the bulk susceptibility effects, which determine in practice the pressure dependence of the experimental values. Best agreement of the results is obtained when the bulk susceptibility correction in rare gas solvents is evaluated from the analysis of the He-rare gas interactions, and when the shielding of deuterium in D_2-rare gas systems is considered.

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