Naphthalene-rare gas interaction: intermolecular potential energy surfaces and clusters' structures

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The noncovalent intermolecular interaction of naphthalene with Helium, Neon and Argon is investigated for selected dimer configurations by means of high level electronic structure calculations and exploiting complete basis set extrapolation techniques. The main features of the intermolecular potential have been identified, with two equivalent global minima (for each side of the naphthalene molecular plane) connected by a low barrier (of the order of 1 meV) which decreases with the size of the involved rare gas (Rg). An analytical formulation of the global potentials, based on simple and efficient atom-atom expressions, is also provided by optimizing few and physically meaningful parameters on the calculated interaction energies. The proper representation of the interaction covers the full range of relative configurations of the involved partners and it has been exploited to predict and analyze energies and structures of the low-lying minima in naphthalene-Rg_N (N=1-8) clusters by using Basin-Hopping and Diffusion Monte Carlo approaches.