A CANONICAL APPROACH TO MULTI-DIMENSIONAL VAN DER WAALS, HYDROGEN-BONDED, AND HALOGEN-BONDED POTENTIALS

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A canonical approach is used to investigate prototypical multi-dimensional intermolecular interaction potentials characteristic of categories in van der Waals, hydrogen-bonded, and halogen-bonded intermolecular potential energy functions. It is demonstrated that well-characterized potentials in Ar-HI, OC-HI, OC-HF, and OC-BrCl, can be canonically transformed to a common dimensionless potential with relative error less than 0.010. The results indicate common intrinsic bonding properties despite other varied characteristics in the systems investigated. The results of these studies are discussed in the context of the previous statement made by J. C. Slater [J. Chem. Phys. 57 (1972) 2389] concerning fundamental bonding properties in the categories of interatomic interactions analyzed.