Inter-molecular potentials in complexes of the Nitrogen Monoxide (NO) calculated by *ab initio* methods

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The Nitrogen monoxide properties, have been and continue being of great concern in several research areas, both from the fundamental and applicative point of view. In this work we present several intermolecular potentials for the complexes of NO calculated using ***ab initio*** methods by our research group.

The main features of the intermolecular potential of: I.the first Rydberg state (A) of the NO-Ne system [1], II. the ground state of the NO-NO system [2] and III. NO − H_2 system in the ground and first Rydberg state(A) [3], are shown.

The inter-molecular potentials shown, have been used successfully in several molecular dynamics research, for example in the references [4] and [5].

References

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