Accurate *ab initio* based DMBE potential energy surface for the ground electronic state of N_2H_2

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Streszczenie

A global single-sheeted double many-body expansion potential energy surface is reported for the ground electronic state of N2H2. Starting from an approximate cluster expansion of the molecular potential that utilizes previously reported functions of the same family for the triatomic fragments, four-body energy terms have been calibrated from extensive accurate *ab initio* data so as to reproduce the main features of the title system. The switching function formalism previously suggested for three-body systems [A. J. C. Varandas and L. Poveda, Theor. Chem. Acc. 116, 404 (2006)] has been generalized to approximate the true multisheeted nature N_2H_2 of potential energy surface, thus allowing the correct behavior at the $N(^2D)+NH_2(^2A'')$ and $N(^4S)+NH_2(^4A'')$ dissociation limits. The resulting fully six-dimensional potential energy function reproduces the correct symmetry under permutation of identical atoms and predicts the main stationary points of the molecule in the valence and long-range regions in good agreement with available experimental and theoretical data on the diazene molecule.

Adres publiczny

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