Accurate MRCI study of ground-state N_2H_2 potential energy surface

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Streszczenie

Extensive ab initio calculations have been performed to determine the energy, geometry and vibrational frequencies of all stationary points of the N_2H_2 ground-state potential energy surface. The geometries of *trans*-, *cis*- and *iso*-minima as well as transition states are reported at the MCSCF/aug-cc-pVQZ level, while the relative energetics is established by single point MRCI/aug-cc-pVQZ calculations including the Davidson size-consistency correction. The data is useful for modeling a single-sheeted global potential energy surface for the title system.

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