**Ab initio** molecular orbital study of structures and energetics of Si$_3$H$_3$ neutral and anion

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The geometric structures and isomeric stabilities of various stationary points in Si$_3$H$_3$ neutral and its anion are investigated at the coupled-cluster singles, doubles (triples) [CCSD(T)] level of theory. For geometrical surveys, the basis sets used are of the Dunning's correlation consistent basis sets of triple-zeta quality (cc-pVTZ) for the neutral. To the anions, the Dunning's correlation consistent basis sets of double-zeta quality with diffuse functions (aug-cc-pVDZ) are applied. For the three lower-lying anion isomers, the Dunning's correlation consistent basis sets of triple-zeta quality with diffuse functions (aug-cc-pVTZ) are also used. The final energies for the optimized stationary
points are calculated at the CCSD(T) level of theory with the aug-cc-pVTZ basis sets. The basis sets of 6-311++G(3df,2pd) were also used for the lower-lying anion isomers. The Gaussian-2 (G2) method was performed only for the lower-lying anion isomers to clarify the relative stabilities. The global minimum neutral 1 (C₄v; 2A) has an unsymmetrical hydrogen-bridged bond; the conformer 2 in C₄v symmetry is a saddle point connecting the two equivalent isomers 1. Two lower lying isomers (3 and 4) are also predicted within the energy range of 20 kJ/mol. In the anion, however, the conformer 4 (C₃v; 1A') with 5 formal valence electrons is a global minimum. Two more isomers (2 and 3) lie within 20 kJ/mol as in the neutral; the conformer 1 converts to the isomer 2. The quartets for the neutrals and diradical triplets for the anions were further studied; lower lying quartets and triplets, competing with the corresponding doublet and singlet, respectively, were not found in the present systems. The vertical and adiabatic electron affinities of the global minimum neutral 1, producing the second lowest lying anion isomer 2, amount to 2.18 and 2.35 eV, respectively, at the CCSD(T)/aug-cc-pVTZ level of theory. The electron addition to the third lowest lying neutral isomer 4 produces the largest vertical electron affinities of 2.48 eV. The D₃h structure, being the global minimum in the corresponding Si₃H₃⁺ cation (trisilacycloprenyl cation), converts to the isomer 8 (C₄v) or 11 (C₂v) due to the Jahn-Teller effect in the Si₃H₃ neutral.

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