An explicitly correlated six-dimensional potential energy surface for the SiCSi + H2 complex

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Abstract

The first six-dimensional potential energy surface (PES) for the SiCSi + H_2 complex is presented in this work. This surface is developed from a large number of ab initio energies computed at the explicitly correlated coupled-cluster level of theory together with the augmented correlation-consistent polarized valence triple zeta basis set (CCSD(T)-F12/aug-cc-pVTZ). These energies are fitted to an analytical function through a procedure that combines spline, least-squares, and kernel-based methods. Two minimums of similar depths were found at the equilibrium geometry of the SiCSi molecule. The dependence of the PES on the bending angle is analyzed. Furthermore, a reduced four-dimensional PES averaged over the H_2 orientation is presented. Finally, the six-dimensional PES is used for computing the second virial coefficient of the SiCSi + H_2 pair using classical and semi-classical methods. © 2023 The Royal Society of Chemistry.