عنوان مقاله:

+Ab initio potential energy curves and transition dipole moments for the low-lying singlet states of SiH

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 2

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خلاصه مقاله:

The SiH+ ion was observed in the laboratory for the first time by Douglas and Lutz in 1970and it was detected in a solar photospheric spectrum in the same year from the emission ofthe SiH+ A1Π - X1Σ+ transition. Because of its astrophysical importance, it has been thesubject of several experimental, theoretical and astronomical investigations [1-4]. We reportab initio calculations on five singlet states of SiH+ using the multi-reference configurationinteraction (MRCI) method with large active space and basis sets. We have computedpotential energy curves, dipole moments .+and transition dipole moments for the X1Σ+, 11Π,11Δ, 21Σ+ and 21Π states of SiH

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا: