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Karnamohit Ranka, Ajith Perera, Rodney J. Bartlett

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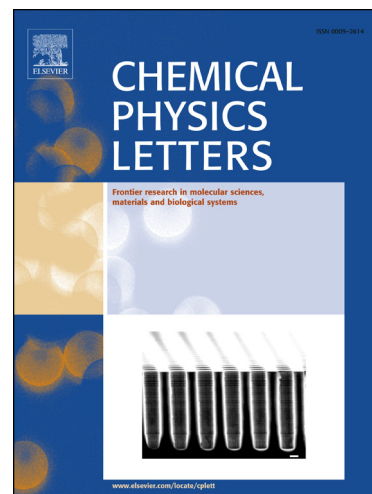
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Elementary reaction profile and chemical kinetics study of $[C(^1D)/(^3P) + SiH_4]$ with the CCSD(T) method

Karnamohit Ranka^{§,1}, Ajith Perera[§], Rodney J. Bartlett[§]

[§]Quantum Theory Project, University of Florida, Gainesville, FL 32611, USA

Abstract

Carbon and silicon-based molecules are omnipresent in the fields of combustion, atmospheric, semiconductor, and astronomical chemistry, amongst others. This paper reports the underlying elementary reactions for the $[C(^1D) + SiH_4]$ and $[C(^3P) + SiH_4]$ reaction profiles, optimized geometries of the intermediates, transition states (at the CCSD(T) level), RRKM and TST rate constants, and the corresponding branching ratios. Previously unreported van der Waals complex intermediates have been found for both reactions.

Keywords: atomic carbon, silane, reaction profile, chemical kinetics, van der Waals complex

¹ Electronic mail: kmrk24@ufl.edu

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