THEORETICAL STUDY OF GROUP 14 $M^+(^2P_J)$ -RG COMPLEXES ($M^+ = C^+$, Si⁺; RG = He - Ar)

<u>WILLIAM DUNCAN TUTTLE</u>, REBECCA L. THORINGTON, TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, Nottingham, United Kingdom; LARRY A. VIEHLAND, Science Department, Chatham University, Pittsburgh, USA.

The light group 14 cations are found in a wide variety of environments, with, for example, C⁺ ions thought to play a key role in the chemistry of the interstellar medium,^a while Si⁺ ions are an important component of the upper atmosphere of the Earth due to their presence in meteoroids.^b

We calculate accurate interatomic potentials for a singly charged carbon cation^c, ^d and a singly charged silicon cation^e interacting with the rare gas atoms helium, neon and argon. The RCCSD(T) method is employed, with basis sets of quadruple- ζ and quintuple- ζ quality, and the energies counterpoise corrected and extrapolated to the basis set limit at each point. In all cases, we consider the lowest electronic states of the M⁺ atom, (2P_J), interacting with the ground electronic state of the RG atom, (1S_0), and compute potentials corresponding to the molecular terms, $^2\Pi$ and $^2\Sigma^+$, as well as the spin-orbit levels which arise: $^2\Pi_{3/2}$, $^2\Pi_{1/2}$ and $^2\Sigma_{1/2}^+$. The potentials are employed to calculated spectroscopic constants and ion transport properties.

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^bJ. M. C. Plane, J. C. Gómez-Martin, W. Feng, and D. Janches, J. Geophys. Res. Atmos. 121, 3718 (2016).

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 $[^]d$ W. D. Tuttle, R. L. Thorington, L. A. Viehland and T. G. Wright (in preparation).

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