Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Explicitly correlated six-dimensional potential energy surface for the SiCSi+H_2 complex (Supplementary materials)

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3.1.2 Features of the surface

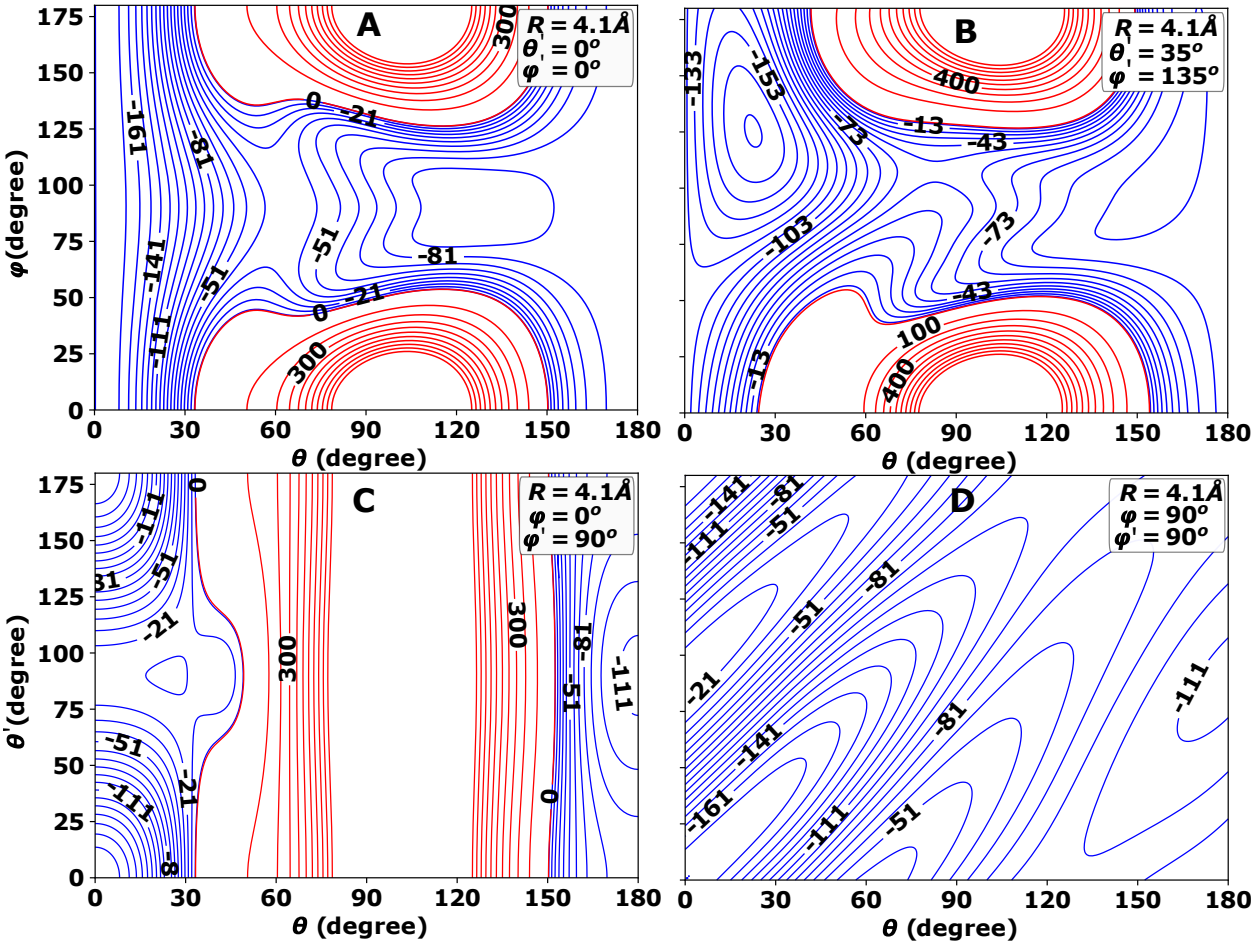

Figure 1: Contour plots of the PES at different angular configurations for $\gamma = \gamma_e$. Negative (blue lines) and positive (red lines) energies are separated in steps of 10 cm^{-1} and 100 cm^{-1}, respectively.

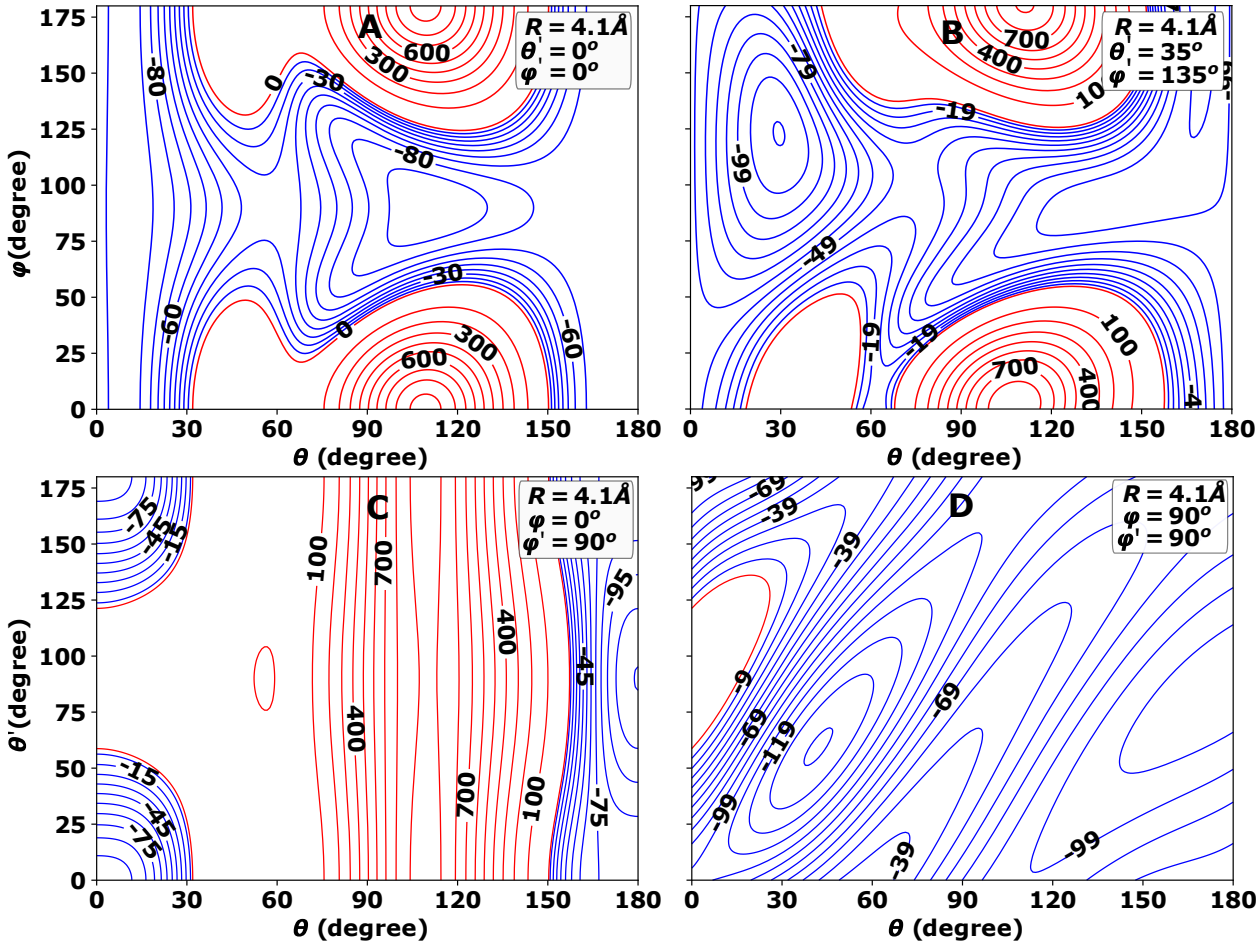

Figure 2: Same as Fig. 1 but for $\gamma = 80°$.

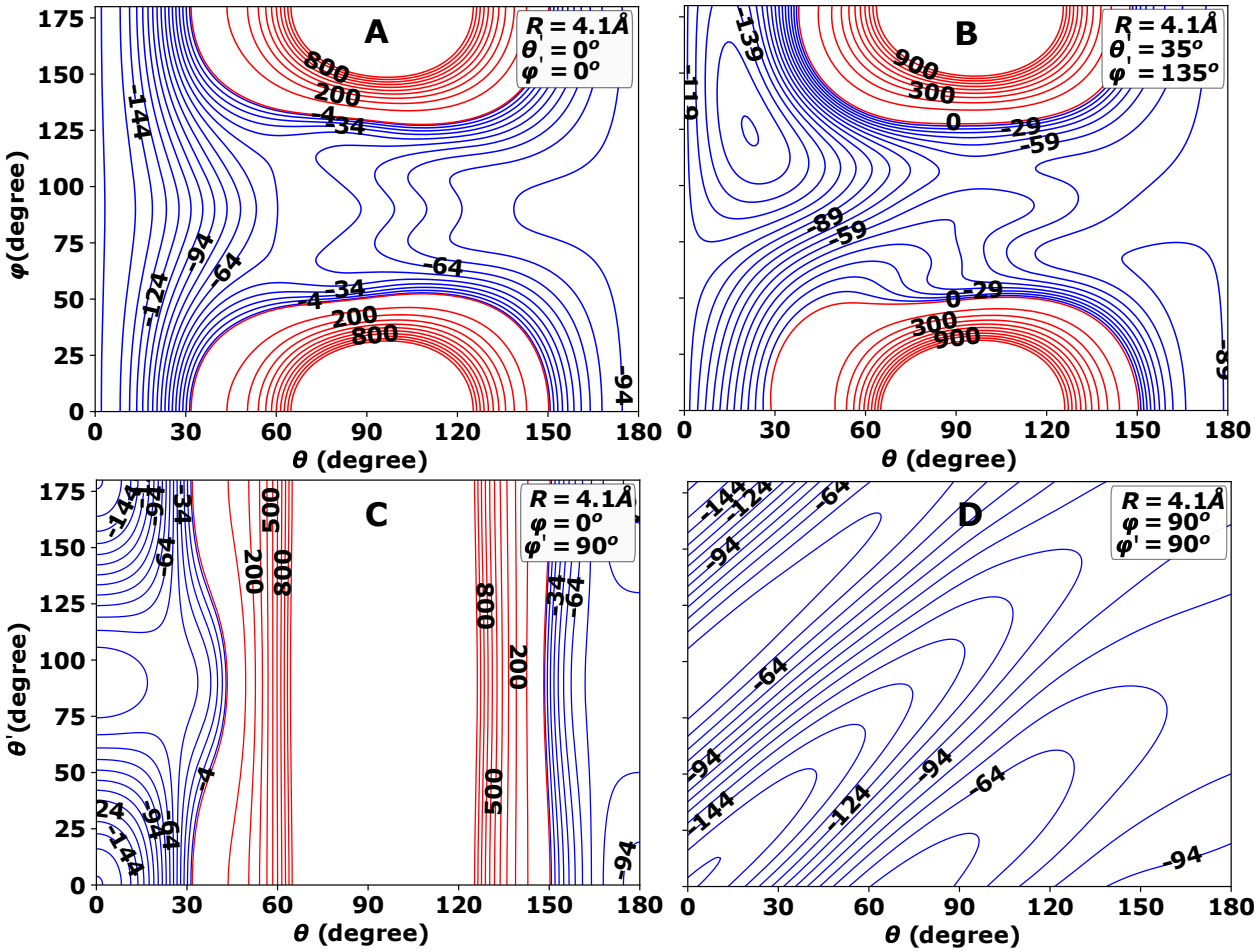

Figure 3: Same as Fig. 1 but for $\gamma = 150°$.

3.1.3 Long range behavior

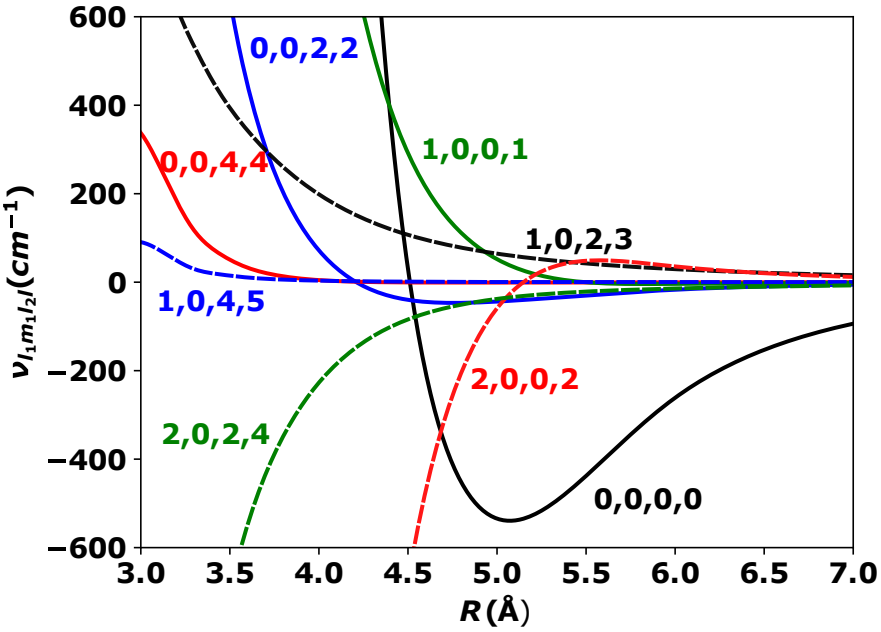

Figure 4: First $v_{l_1m_1l_2l}(\gamma_e, R)$ radial coefficients of the SiCSi-H2 PES.

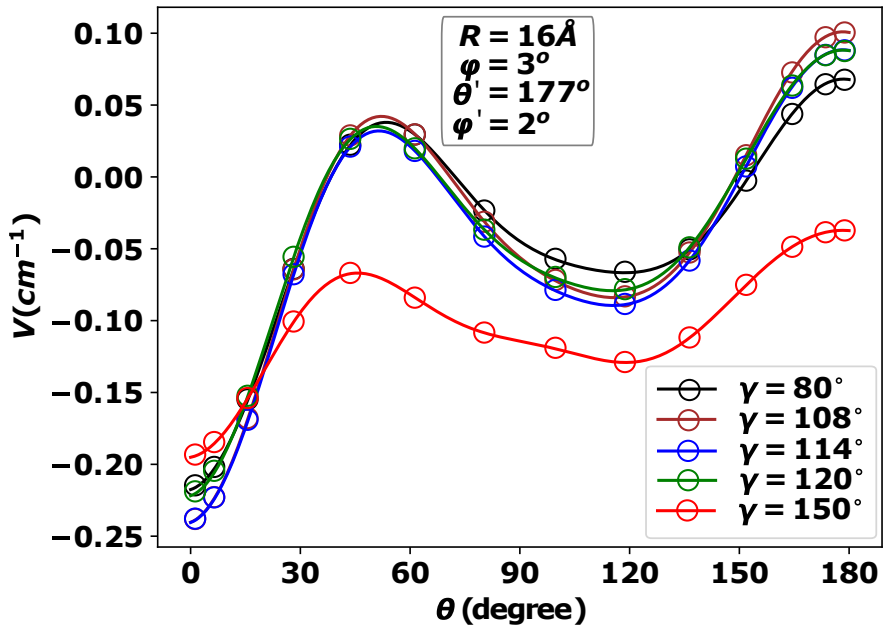

Figure 5: Analytical (lines) and *ab initio* (points) energies of the SiCSi-H_2 complex at $R = 16$ Å for several values of γ, at a fixed configuration of φ, θ' and φ'. These *ab initio* energies were not included in the fitting procedure.

3.2 Averaged four-dimensional PES

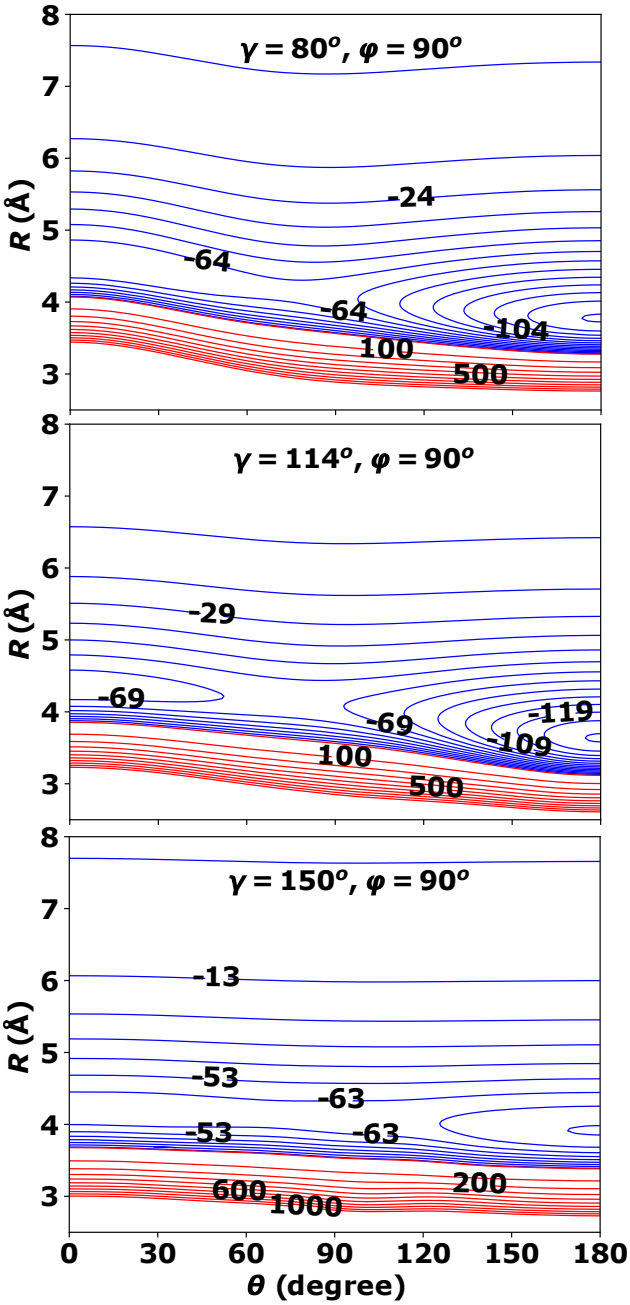

Figure 6: Contour plots of the PES of SiCSi-H_2 averaged over the H_2 orientation for $\varphi = 90°$ at several values of γ. Negative (blue lines) and positive (red lines) energies are separated in steps of 6 cm^{-1} and 50 cm^{-1}, respectively.