

AB INITIO CALCULATIONS OF THE GROUND ELECTRONIC STATES OF THE C₃-Ar AND C₃-Ne COMPLEXES

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The C₃Ar and C₃Ne complexes have four large amplitude vibrations. These are the in- and out-of-plane C₃ bending motions, and the two van der Waals vibrations. Assignment of the spectra of the complexes is therefore challenging. The ab initio potential energies of their ground electronic states have been calculated at the CCSD(T)/pVQZ level. 46620 points have been computed to describe the four-dimensional potential of C₃Ar: $\angle C - C - C = 112-179.5^\circ$, $r(\text{C-C bond length}) = 1.298 \text{ \AA}$, $R(\text{C}_3\text{-Ar}) = 3.4-6.0 \text{ \AA}$, ϕ (azimuth angle between Ar and the principal axis of C₃) = 0-180°, and θ (colatitude angle) = 0-180°. For C₃Ne, 69190 points have been computed: $\angle C - C - C = 106-179.5^\circ$, $r(\text{C-C}) = 1.298 \text{ \AA}$, $R(\text{C}_3\text{-Ne}) = 3.0-7.0 \text{ \AA}$, $\phi = 0-180^\circ$, $\theta = 0-180^\circ$. Basis set superposition errors have been corrected in the C₃-Ne potential energy calculations. Morse type functions and power series were used to fit the calculated points.