SPECTROSCOPIC COMPARISONS OF HELIUM-DIHALOGEN COMPLEXES: WHAT DICTATES THE SPECTRAL STRUCTURE?

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The electronic spectra resulting from the $(\tilde{B} - \tilde{X})$ transitions in He-I_2 have been investigated. Comparisons were made between previously reported He-Br_2 spectra and the He-I_2 spectra.[a] Differences in the higher energy spectral feature in both the experimental and calculated spectra led us to question the origin of its structure. To investigate this difference, we calculated the He-Br_2 spectrum using the parameters from the He-I_2 $\tilde{B}$-state potential surface.[bc] The resulting spectrum more closely resembles the form of the He-Br_2 spectrum rather than the He-I_2 spectrum. The results from calculating the He-I_2 spectrum using the $\tilde{B}$-state potential parameters of He-Br_2 resemble the initial He-I_2 spectrum.[d] This leads us to believe the features within the spectra reflect the rotational structure of the I_2/Br_2 rather than the anisotropies in the potential surface.

We further tested this theory by approximating the He-I_2 $\tilde{B}$-state surface by an elliptical potential, where the potential energy is a function of the sum of the distance of the helium atom from the two focal points used to describe the ellipse. The results show good qualitative agreement with the initial He-I_2 spectral features. This further demonstrates that the spectral structure of these systems, initially believed to be very complex,[e] can be described with simple models that are relatively insensitive to the details of the potential surface.

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