THE EMISSION SPECTRA OF THE Å STATE OF THE C₃-Xe VAN DER WAALS COMPLEX

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Emission bands of the C₃-Xe van der Waals complex near the 2₁̃₂, 2₁̃₂, and 2₄⁎ bands of the Å—X system of C₃ have been recorded, but as yet definitive spectral assignments could not be made. Unlike those of the C₃-Ar and C₃-Kr complexes, the observed C₃-bending vibrational progressions of the Xe-complex could not be fitted to a simple dipole-induced dipole model potential. Ab initio calculations of the Ar- and Xe-complexes have been carried out using the CCSD(T) method at the cc-pVQZ level. Tentative vibrational assignments of the Xe-complex based upon the ab initio calculation will be discussed.