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Satellite bands in the rotational spectrum of doped helium clusters TATJANA SKRBIC, SAVERIO MORONI, STEFANO BARONI, INFM-DEMOCRITOS and SISSA, Trieste, Italy — Recent measurements of infrared spectra of Carbon dioxide molecules embedded in Helium droplets reveal a weak satellite band (SB) accompanying a sharp R(0) rovibrational line. By re-analyzing previous quantum Monte Carlo calculations of the rotational dynamics of various dopant molecules in Helium clusters, we find indeed evidence for rotational excitations with energies and spectral weights close to the measured values of the SB. We present new simulations, in which specifically devised imaginary-time correlation functions are introduced for an explicit theoretical characterization of individual excitations, as well as for enhanced computational efficiency in the calculation of weak spectral features. The proposed assigment of the SB to a coupled rotational state of the molecule and a ring of Helium atoms is discussed.

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