Accurate (ro)vibrational energy levels of the C_2 molecule

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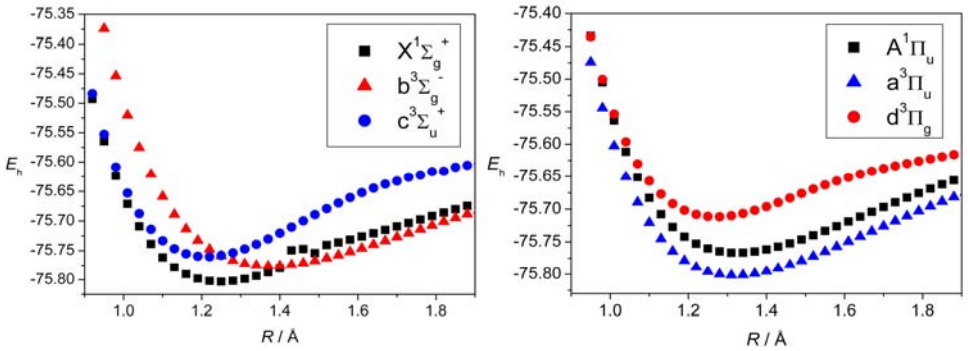

C_2 is one of the fundamental radicals which is abundant in flames, combustion sources and hydrocarbon discharges. It has been also observed in extraterrestrial sources, such as carbon stars, comets and protoplanetary nebulae. Theoretical computations are crucial for the interpretation of its experimental spectra, and the simulation of interstellar media. [1,2,3] In order to obtain the spectra of C_2 ab initio electronic structure and nuclear motion computations were performed within the Born-Oppenheimer approximation.

Potential energy curves (PEC) were calculated for six electronic states of C_2 over the internuclear separation region from 0.08 nm to 0.21 nm using the full valence complete active space self-consistent field (CASSCF) method followed by the valence internally contracted multireference configuration interaction (MR-CI) approach in combination with the aug-cc-pV5Z correlation-consistent basis set. The PEC calculations were caried out with MOLPRO 2009.1 program package. [4] Excellent agreement has been found between the PECs obtained in this study and previous reported results.

With the numerical PECs obtained (ro)vibrational energy levels were calculated using the LEVEL 8.0 program. [5] The Einstein coefficients related to the six ro-vibronic transitions (Phillips, Swan, Ballik-Ramsay, Duck, Bernath) were computed with the program Level 8.0, employing the untangled transition dipole curves computed using MRCI method in conjunction with the aug-cc-pV6Z basis set including the core and core-valence correlations and scalar relativistic energy corrections as implemented in the MOLPRO. The computed energy levels and intensities are going to be compared with the results obtained with the extended version of program Duo.

The calculated (ro)vibrational energy levels are in very good agreement with experimentally derived values for all investigated states.

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