HIGH-SPIN ELECTRONIC STATES OF MOLECULAR OXYGEN

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As a by-product of an ongoing rather comprehensive study of the electronic structure of the lowest valence and Rydberg states of O_2, chiefly singlets and triples, in this contribution we focus on high-spin electronic states, namely, quintets and septets. Although these latter states may be thought of as of pure academic interest, the current calculations show interesting features of their potential energy curves (PECs) which have not been studied and are actually unknown for most diatomics made up of first-row atoms (plus hydrogen and helium). Experimentally, there is essentially no information whatsoever, aside from some indirect evidence of the possible involvement of high-spin species in the spectroscopy or photodissociation processes. Theoretically, there are a few studies, but they are usually issued from early and modest calculations, so the accuracy is not good enough.

We report in this contribution an insight into the quintet and septet electronic states of molecular oxygen. Their PECs display a rich and complex structure, and interactions among states which could not be anticipated. We report PECs of valence, Rydberg and ion-pair quintet states as well as of various Rydberg septet states. Most PECs are repulsive, as expected, yet, a few of the high-spin states are bound. Excitation energies are tabulated for all states. Spectroscopic constants are given for the bound states. A case is also presented of a bound sextet state of O_2^+, along with potential curves of several sextet repulsive states of the cation.