

Metastability of the low-lying electronic states of CBr^{2+} : A CASSCF/MRCI Study

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Abstract: Spectroscopic data for the low-lying electronic states of the doubly ionized cation, CBr^{2+} , are scarce due to the inherent difficulties related to the preparation and detection of this highly reactive ion. To the best of our knowledge, the only experimental evidence of this dication was reported in 1982 by Proctor et al. [1], who demonstrated by charge stripping mass spectrometry the existence of this species. In this context, the aim of this work is to present a reliable characterization of the metastability, structure, and spectroscopy of the low-lying electronic states of CBr^{2+} thus extending our present knowledge of the halocarbon dications. For this purpose, the low-lying electronic states of CBr^{2+} correlating with the two lowest dissociation channels was investigated at a high level theoretical approach, SA-CASSCF/MRCI. Spin-orbit interaction changes substantially the profile of the potential energy curves, specially for the ground ($X\ ^2\Sigma^+$) and first excited ($1\ ^2\Pi$) states. The second adiabatic ionization energies are also determined and show an excellent agreement with the experimental derived values. Tunneling widths computed for the Ω bound states show that the lowest vibrational levels of components 1/2 are stable against tunneling.

Key-words: Spectroscopic, Metastability, MRCI

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References:

[1] C. Proctor, C. Porter, T. Ast, J. Beynon Int. J. Mass Spectrom. 41, 251 (1982).