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The ionic states of iodobenzene studied by photoionization and *ab initio* configuration interaction and DFT computations

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Streszczenie

New valence electron photoelectron spectra of iodobenzene obtained using synchrotron radiation have been recorded. Ionization energies (IEs) determined using multi-configuration SCF calculation (MCSCF) procedures confirmed the adiabatic IE order as: $X^2B_1<A^2A_2<B^2B_2<C^2B_1$. Although it is convenient to retain C_{2v} labelling, there is an evidence that minor distortion to C_S symmetry occurs at the MCSCF level for the C state. The fifth ionization process shown to be D^2A_1 exhibits dissociation to $C_6H_5^+$ + I both in the experimental and theoretical studies. The calculated Franck-Condon vibrational spectral envelopes, including hot band contributions, for the first four ionic states reproduce the observed peak positions and intensities with reasonable accuracy. In order to simulate the observed spectra, different bandwidths are required for different states. The increase in the required bandwidths for the A^2A_2 and B^2B_2 states is attributed to internal conversion to lower-lying states. The presence of relatively high intensity sequence bands leads to asymmetry of each of the X^2B_1 state bands.

Słowa kluczowe

Unrestricted Hartree-Fock, Ab initio configuration interaction, Rydberg states, Vacuum ultraviolet radiation, Synchrotron radiation, Photoionization, Ions and properties, Absorption spectroscopy, Photoelectron spectroscopy, Resonance-enhanced multiphoton ionization

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