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X-ray excited photoelectron spectra of free molecules containing oxygen

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Abstract

High resolution X-ray excited photoelectron spectra (XPS) of carbonyl- and hydroxyl-containing compounds are presented and discussed in terms of electronic structure theory. The results presented comprise O1s binding energy shifts, core hole shake-up/shake-off, inner-valence and outer-valence spectra. New features are analyzed by means of computational data, and various examples are given where XPS valence spectra aid a molecular orbital analysis. Emphasis is put on similarities and differences between spectra within series of compounds containing identical, hydroxyl or carbonyl, functional groups. Characteristic structures that fingerprint these compounds have been unravelled. The spectra have been investigated in terms of a simple scheme for XPS analysis. The spectra are divided into five regions, which are described within a hierarchy of approximation levels. Following this scheme, basic similarities and differences in theoretical XPS analysis of the different energy regions are identified, e.g. the character of wave functions, the roles of relaxation and electron correlation, the dominant factors in the intensity analysis and the role of orbital interpretations. Particular emphasis has been put on the analysis of the O1s shake-up spectra of the carbonyl-containing compounds. Some of these display strong shake-up peaks due to charge-transfer excitations. Analysis of these features has been carried out by means of MCSCF calculations as well as by a simple orbital model. The energetics and character of shake-up transitions involving acceptor and donor groups are established by the model, and have been further verified by the MCSCF calculations. Except for the carbonyl spectra, a few of the spectra presented have been selected for a more detailed analysis. These are the valence spectra of carbon monoxide and benzaldehyde and the core electron shake-up spectrum of water.

¹ Also at Institute of Quantum Chemistry.

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