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Binding energy spectra of methoxyphenols: Theory and experiment

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Methoxyphenols (MPs) are antioxidants play an important role in degenerative diseases & cancers. Methoxyphenols are found in many food products however, the molecular details of methoxyphenols are limitedly known. o-methoxyphenol (oMP), m-methoxyphenol (mMP) and p-methoxyphenol (pMP) are positional isomers of one another. The electronic structures, properties and spectra of oMP, mMP & pMP were studied quantum mechanically. The impacts that the methoxy and hydroxy functional groups have on the structure and properties of the MPs were revealed in gas phase. The geometries, ionization energies, ionization spectra & molecular orbitals were investigated and validated against synchrotron sourced experiments completed at the Elettra Sincrotrone. The electronic structure and properties of oMP, mMP and pMP were revealed by systematic studies on the functional groups in gas phase. The results presented indicate that the inner shell of each MP is dominated by the relative functional group positioning and the phenyl aromatic ring buffers the changes induced by the functional groups which stabilizes the MPs in gas phase. It has been established that the valence ionization spectra have conformation dependent changes in the energy range from 12.5eV to 20eV that can differentiate between each isomer. The HOMO-2 electron density distribution changes significantly between each MP. Ionization energy of the MPs all exhibit functional group dependent peaks in C1s and O1s spectra. It will be shown that as the frontier orbitals and outer valence space of the MPs show signature orbital configurations, the frontier orbitals can be used as fingerprint markers for each MP.

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Summary

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