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10 4 Photoelectron Spectroscopy Chemistry LibreTexts

When extensive vibrational structure is resolved in a PES molecular orbital, then the removal of an electron from that molecular orbital induces a significant change in the bonding (in this case an increase in the bond length since the bond order has been reduced).

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Probing Electron Density of H Bonding between Cation Anion

Attenuated total reflection infrared spectroscopy and density functional theory calculation have been employed to study the spectral properties of imidazolium-based ionic liquids (ILs) with different anions.

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Pseudopotential calculations for hydrogen centers in ionic

Pseudopotential cluster calculations have been performed for hydrogen centers H 0 i, H 0 a, H 0 c in XF and XCl ionic crystals (X = Li, Na, K, Rb). Results are given for interatomic potentials, for frequencies of localized vibration modes and for activation energies for diffusion of the hydrogen centers.

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