

MODELING PHOTODETACHMENT FROM HO_2^- USING THE pd CASE OF THE GENERALIZED MIXED CHARACTER MOLECULAR ORBITAL MODEL

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Using the generalized model for photodetachment of electrons from mixed-character molecular orbitals, we gain insight into the nature of the HOMO of HO_2^- by treating it as a coherent superposition of one p- and one d-type atomic orbital. Fitting the pd model function to the ab initio calculated HOMO of HO_2^- yields a fractional d-character, γ_p , of 0.979. The modeled curve of the anisotropy parameter, β , as a function of electron kinetic energy for a pd-type mixed character orbital is matched to the experimental data.