

**Investigation of the charge distribution of free and bound 1,1-dicyanoethylene-2,2-dithiolate. An ab initio HF-MO and XPS study.** Hummel, Hans U.; Foerner, W.; Krogmann, K.

**Abstract**

Ab initio Hartree-Fock-MO calcns. on  $S_2C:C(CN)_2^-$  revealed that the neg. charge is located to nearly equal amts. on the terminal S and N atoms. Influences on the electron binding energy of the S 2p and N 1s level of Coulomb effects in ionic crystals and substitution effects in derivs. of  $S_2C_4N_2^-$  were studied qual. using XPS.