EXTENSION OF AN ATOMIC-IONS-IN-MOLECULE ELECTRONIC STRUCTURE MODEL FROM CALCIUM MONOXIDE TO SCANDIUM MONOXIDE

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The electronic spectrum of CaO is so complicated that it had been dismissed as uninterpretable random fragments from a polyatomic molecule. An atomic-ions-in-molecule model, which employs foundational concepts from Inorganic Chemistry, provides the "why" as well as the "what." There are two oxidation states, $Ca^{2+}O^{2-}$ and $Ca^{+}O^{-}$, the latter manifest in O^- 2pπ-hole (π^{-1}) and 2pσ-hole (σ^{-1}) "hard/soft" forms. These three families of electronic structure states are co-present in the low-energy region, and their large differences in molecular structure (R_e and ω_e) result in a dense web of perturbations. But all is now understood. Going from CaO to ScO, the addition of a single valence electron awakens the sleeping giant of complexity, bellowing "you ain't seen nothin' yet." The number of low-lying electronic states in each of the three families increases significantly. Can an atomic-ions-in-molecule model guide the interpretation of the ScO spectrum?

New Laser Induced Fluorescence (LIF), Dispersed LIF, and lifetime-gated LIF spectra offer insights into the electronic structure of ScO. These spectra sample the ScO $A^2\Pi$, $C^2\Pi$ and $D^2\Sigma^+$ states over a wide range of vibrational levels. Of special importance is the A(v=6) C(v=16) perturbation and two previously unobserved, closely-spaced, long-lived, Ω=1/2 states that lie near, and are probably made visible by their interaction with the $C^2\Pi_{1/2}$(v=6) and $A^2\Pi_{3/2}$(v=16) states.

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