APPLICATION OF THE RECOUPLED PAIR BONDING MODEL TO BOUND DOUBLET AND QUARTET STATES OF HSO, SOH, OSF AND SOF

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The recoupled pair bonding model and high level *ab initio* calculations [MRCI, RCCSD(T)] with correlation consistent basis sets were used to examine the optimized structures, bonding behavior and bond energies of bound HSO, SOH, OSF and SOF doublet and quartet states. This was done by the systematic addition of H or F to the $^3\Sigma^-$, $^1\Delta$ and $^3\Pi$ states of SO or by adding O(^{3}P,^{1}D) to the $^2\Pi$ and $^4\Sigma^-$ states of SF. Of particular interest are those states that are either formed as a result of decoupling a pair of electrons or by further addition to a molecule that has already undergone the decoupling process. One of the goals of these studies is to explore the effect of ligand properties such as electronegativity or electron affinity in order to anticipate their impact on trends in bond energy and other properties similar to those observed in previous SF_n (n=1–6) recoupled pair bonding studies. This study marks the first exploration of the behavior of a divalent ligand in hypervalent bonding under the recoupled pair bonding model.