A QUANTUM CHEMICAL EXPLORATION OF THE SF_nO SERIES ($n = 1 - 5$): AN ATOM-BY-ATOM APPROACH

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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, transition states, bonding and bond energies of the SF_nO series ($n = 1-5$). Oxygen is capable of participating in covalent, recoupled pair, and dative bonding and, unlike monovalent ligands, forms both σ and π bonds. This study explores the effect of oxygen in order to anticipate its impact on trends in bond energy and other properties similar to those observed in previous SF_n ($n = 1 - 6$) recoupled pair bonding studies. 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.