ATTEMPTS TO SOLVE O_2-CONTAINING VAN DER WAALS INTERACTIONS USING SPFIT AND SPCAT WITH MICROWAVE MEASUREMENT PRECISION: PROBLEMS, PITFALLS, AND SUCCESSES.

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Although there is a vast amount of van der Waals complexes containing small molecular species, there have only been a small number of studies containing an O_2 binding partner. Within this grouping, only five are known to have been attempted using high-resolution microwave techniques with only two- O_2-HF[a] and O_2-H_2O[b]- appearing in the literature. This void is presumably due to the $^3\Sigma$ ground state of O_2 and how this coupling complicates spectral assignment. However, these sorts of couplings determined from high-resolution analysis add rich and important information useful in complex structure determination. Until now, the only analyses of such complexes have been done utilizing Hund's case *a* asymmetric models[c,d] or Hund's case *b* linear Hamiltonians. However, further study either resulted in inaccurate predictions of close transitions (O_2-H_2O) or difficult adjustments to similar systems due to extra complexity (O_2-HCl from O_2-HF). This made a more standardized approach, such as using the ubiquitous program suite of SPFIT/SPCAT by Pickett[e] seem like a more flexible solution. However, SPFIT/SPCAT uses a Hund's case *b* approach which needed to be sorted out and the problems and pitfalls of these analyses will be discussed. This talk will include how to be predictive using O_2-H_2O and O_2-HF as examples as well as discuss work currently being pursued on the molecules O_2-HCl and O_2-OCS to extend the analyses. Structural parameters from these newly determined parameters and their interpretations will also be discussed.

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