

Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Large scale valence-bond calculations on diatomic molecules: Aspects of spectral compression PETER W. LANGHOFF, MICHAL BEN-NUN, UCSD, JEFFREY MILLS, AFRL, KYLE ROLLIN, MICHAEL BROMLEY, SDSU, JERRY BOATZ, AFRL, GORDON GALLUP, UNL — Progress is reported in performing large scale valence-bond calculations of the ground and electronically excited Born-Oppenheimer eigenstates of diatomic molecules. A code suite for this purpose has been devised which combines spin-free methods in enumerating electronic configurations in terms of the standard tableau functions devised by one of us (GG - Crunch Code) with an efficient Slater-orbital-based integrals package (Smiles Code) modified for present purposes. Slater orbitals are employed in the forms of standard valence basis sets supplemented with diffuse terms, Sturmian sets with high powers of the radial coordinate, and even-tempered sets with low radial powers. Previously devised (Stieltjes) methods are employed to compress the resulting large SCF spectra to obtain reduced numbers of configurations which can nevertheless describe the complexities of Rydberg-valence mixing and avoided crossings common in excited diatomic eigenstates. The calculated results are of spectroscopic interest and also form the basis of a recently devised exact-pair atomic spectral method for *ab initio* calculations of polyatomic molecules, the implementation of which is facilitated by the use of a valence-bond description of the interacting atomic pairs.

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Date submitted: 22 Jan 2010

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