Abstract Submitted
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DFT Calculation of the Renner Coefficient for the Renner-Teller Splitting in the NCO radical: Assessing the accuracy of several common functional families and basis sets[1] D. O. KASHINSKI[2], M. G. SUAREZ, C. C. STEPHENS, United States Military Academy, E. F. C. BYRD, Army Research Laboratory — The "out of box" DFT calculation of the Renner coefficient for the Renner-Teller splitting in the NCO radical using functionals from the B3LYP, PBE, TPSS, M06, and M11 functional families with standard Correlation Consistent cc-pVxZ and aug-cc-pVxZ (x = D, T and Q), 6-311G split valence family, as well as Sadlej, and Sapporo polarized triple-ζ basis sets is being completed. Quantum chemistry calculations are being completed using the GAUSSIAN16 suite on DoD-HPCs. A comparison of our results to previously published theoretical and experimental results has been tabulated to assess the accuracy of the functional and basis set combination. The impact of functional and basis set choices on the resulting coefficients is being characterized. An update on the progress of this work will be given at the meeting. Early work on other linear triatomics will also be presented.

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