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Abstract Submitted
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Harmonic Vibrational Frequencies: Approximate Global Scaling Factors for TPSS, M06, and M11 functional families using several common basis sets.¹ D. O. KASHINSKI, R. G. NELSON, G. M. CHASE, O. E. DINALLO, United States Military Academy, E. F. C. BYRD, Army Research Laboratory — We propose new approximate global multiplicative scaling factors for the DFT calculation of harmonic vibrational frequencies using functionals from the 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. A total of 99 harmonic frequencies are being calculated for 26 gas phase organic and non-organic molecules typically found in detonated solid propellant residue. The approximate multiplicative scaling factors and associated uncertainties are being determined using a least squares approach comparing the computed harmonic frequencies to experimental counterparts well established in the scientific literature. A comparison of our work to previously published global scaling factors will be made to verify method reliability and the applicability of our molecular test set. An update on the progress of this work will be given at the meeting.

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