Abstract Submitted
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Neural Network and Least Squares Predictions for 43 "new" s and p Electron Diatomics RAY HEFFERLIN, Southern Adventist University — We combine least-squares and neural-network forecasts for vibration frequencies of diatomic molecules with 10 to 12 atomic valence electrons. We start with 108 least-squares forecasts based on CRC 2009 data,* and 1001 neural network forecasts based on Huber and Herzberg 1979 data,** and then insist that the standard-deviation bounds of one forecast overlap the bounds of the other; this requirement leaves 68 molecules, for 43 of which we find no tabulated data. The 68 composite predictions average 2.2% on either side of the composite standard deviations. We find 41 literature values, for 22 molecules (none of which were in the set of 43) useable as tests; of them, 33 (80%) fall within the 4.4% composite standard deviation of the predictions. The 43 molecules are AlTe, AsI, AsSb, AsSn, AsTe, BeAt, BeBr, BeSe, BeTe, BPo, CAs, CBi, CPb, CSn, CTe, CaTe, GaTe, GeSb, GeSn, InS, LiSe, LiTe, MgTe, NAt, NGe, NI, NPb, NPo, NSn, NTe, NaSe, PSn, SbBr, SbCl, SbI, SbS, SbSe, SbTe, SiSb, SiSn, SnSb, SrSe, and TlO. *Hefferlin, R., Davis W.B., J. Ileto, *J. Chem. Inf. Comp. Sci.* 43, 622-628, 2003. **Ms. Amy Beard assisted in the least-squares analysis.

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