VIBRATIONAL CORRECTIONS TO MOLECULAR PROPERTIES:
SECOND-ORDER VIBRATIONAL PERTURBATION THEORY VS VARIATIONAL COMPUTATIONS

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For a small set of linear and non-linear molecules, a detailed comparison of two different procedures for predicting vibrationally averaged molecular properties, i.e., second-order vibrational perturbation theory (VPT2) and a variational approach, is carried out. Results for vibrational corrections to dipole and quadrupole moments, nuclear quadrupole moments, static electric-dipole polarizabilities, NMR chemical shielding tensors, nuclear spin-rotation tensors, magnetizabilities, and rotational g-tensors are reported.