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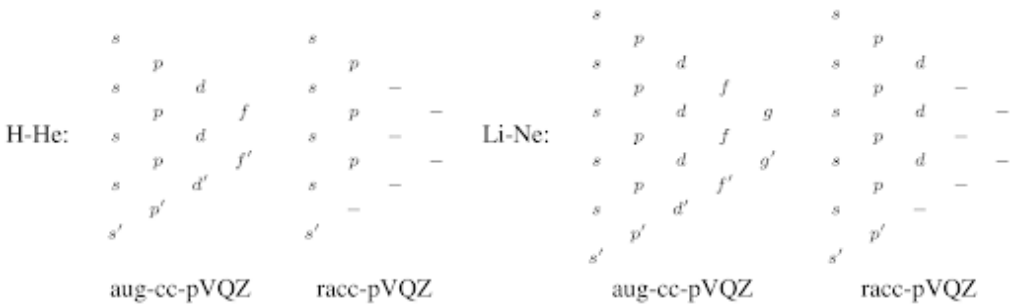
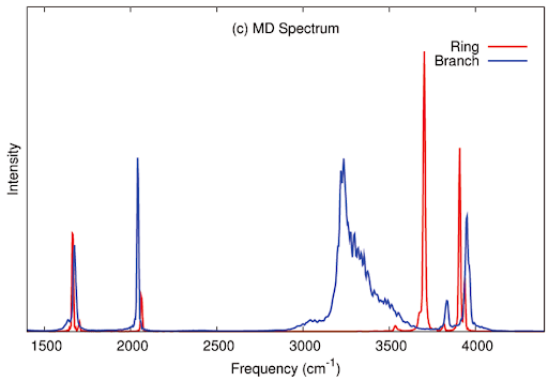
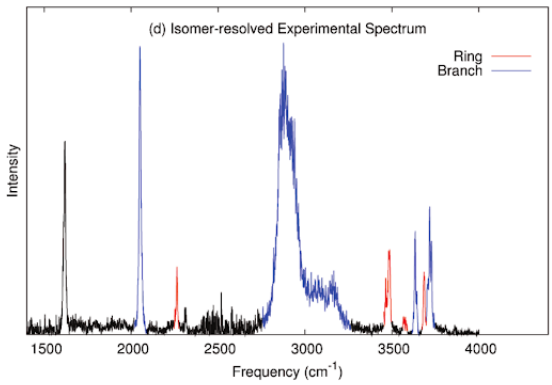
Dual-Basis SCF and MP2 Methods



- SCF and correlation calculations with large basis set with many polarized and diffuse functions are necessary to achieve chemical accuracy, which leads to high computational cost and slow SCF convergence.
- Dual basis methods : 1) An SCF calculation with a relatively small basis set is done; 2) The density matrix in the small basis set is projected onto the large basis set; 3) A single Fock-matrix build step in the large basis set is taken and the total energy is improved; 4) The obtained MOs in the large basis set can be used to evaluated the correlation energy at the MP2 level of theory.
- Analytic energy gradients are available for dual-basis SCF and MP2, so that geometry optimization and AIMD calculations with large basis sets can be done with very high efficiency.



(a) Calculated vibrational absorption spectra for two isomers of the $NO^+(H_2O)_3$ complex from BOMD with DB-RI-MP2/6-31++G**



(b) The corresponding experimental vibrational absorption spectra

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