# Calculation of Vibrational Energy Levels of Molecules Using a Tensor Method that Avoids Storing Large Vectors and Matrices

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Standard techniques for calculating vibrational spectra of polyatomic molecules suffer from so-called curse of dimensionality: the exponential increase of the cost of the calculation with the size of the molecule. We are developing a method that avoids the need to store large vectors and matrices. We use a tensor format called canonical polyadic (CP) format to represent vectors. As a result, the memory cost scales linearly with the dimensionality of the molecule. In CP format a vector is represented as a sum of terms. The vibrational calculations are done using a modified filter diagonalization technique. An alternating least squares (ALS) approach is used to do the filtering so that the number of terms in the CP vectors is constant. The usefulness of these ideas are tested by computing vibrational spectra of a 64-D bilinearly coupled model Hamiltonian and acetonitrile(12-D).