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Calculation of molecular vibrational spectra on a quantum annealer[1] ALEXANDER TEPLUKHIN, BRIAN KENDRICK, Los Alamos National Laboratory, DMITRI BABIKOV, Marquette University — Conventional computers have been used to study molecular spectra theoretically for a long time. In recent years, quantum computing hardware has become available to theoreticians, and recently the electronic spectrum of a molecule was computed on a quantum simulator. In this paper, a new methodology is presented to calculate the vibrational spectrum of a molecule on a quantum annealer. The method is based on a mapping of the the ground state variational problem onto an Ising or quadratic unconstrained binary optimization (QUBO) problem by expressing the expansion coefficients using spins or qubits. The algorithm is applied to two chemically important molecules O_2 (oxygen) and O_3 (ozone). The lowest two vibrational states of these molecules are computed using both a hardware quantum annealer and a software based classical annealer. Noise simulation studies demonstrate that the accuracy of the method is largely affected by the hardware noise. The algorithm is general and represents a new revolutionary approach for solving the real symmetric eigenvalue problem on a quantum annealer.

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