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Computer Simulations of Quantum Computational Operations Performed on the Vibrational Energy Levels of Small Molecules DANIEL WEIDINGER, University of Illinois, MARTIN GRUEBELE[1], University of Illinois — The vibrational energy levels of a molecule can be regarded as a register for quantum information. An applied electric field (provided by a shaped laser pulse) will transform the state vector of the molecule in a manner that can be regarded as a quantum computational operation. Optimization algorithms have been developed and computer simulations have been run to determine the optimum laser pulses to act as specific operators. Simulations of 1-, 2-, 3-, and 4-qubit gates have been run using 2-, 4-, 8-, and 16-level tracts of vibrational energy levels, respectively. Simulations have been generated to model a realistic experiment using available technology. In the case of thiophosgene ($SCCl_2$), vibrational levels on the ground electronic state may be coupled via one or several energy levels on an excited electronic state. The coupling is provided by a single femtosecond laser pulse, which is shaped according to parameters consistent with available pulse shapers. Within these parameters, pulses have been simulated that perform gates such as the CNOT (4 levels) and Hadamard (2 levels) with fidelities over 95 %. The limiting factors for efficacy of the shaped pulse in performing the gate—such as the number of ground state vibrational levels involved—have been explored.

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