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High-fidelity transformations of the vibrational qubits in thiophosgene molecule DMYTRO SHYSHLOV, DMITRI BABIKOV, Marquette University — In this computational work, we study how to use shaped picosecond laser pulses for controlling state-to-state transitions in thiophosgene molecule ($CSCl_2$) with the goal of encoding quantum information into molecular vibrational eigenstates and implementing quantum gates with high fidelity. State-to-state transitions are induced indirectly through the excitation of a gateway state within the excited electronic state so that a UV/vis laser can be employed for control. We optimize shape of the laser pulse using optimal control theory (OCT) and numerical propagation of laser-driven vibrational wavepackets. This optimization was performed for two-qubit gate CNOT and we were able to optimize laser pulses with fidelity exceeding 0.9999. We analyze the high-fidelity pulse in the frequency domain and explore its robustness by reducing the number of available frequency channels. We also intentionally introduce systematic and random errors to the pulse in the frequency domain by modifying the values of amplitudes and of phases for different frequency components. We conclude that the accurate control of the vibrational two-qubit system can still be achieved with a very limited number of frequency channels and in the presence of some amplitude and phase errors.

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