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Quantum Computing using Molecular Vibrational and Rotational Modes of the Open-shell $^{14}N^{16}O$ Molecule[1] KENJI MISHIMA, KOICHI YAMASHITA, The University of Tokyo, JST-CREST — We demonstrate the possibility of using internal molecular vibrational and rotational modes of an open-shell molecule for one of the most important quantum algorithms: the Deutsch-Jozsa algorithm. The molecular system of interest is one of the representative open-shell molecules: $^{14}N^{16}O$. The gate pulses are constructed by utilizing multi-target optimal control theory (MTOCT). The gate fidelities of each quantum gate are more than 95.23%. Upon implementing the Deutsch-Jozsa algorithm combining these elementary gates, we obtained fidelity of at least 94.76%. This indicates that vibrational and rotational qubits of the open-shell $^{14}N^{16}O$ molecule are about as promising for processing quantum algorithms as those of the closed-shell molecule $^{12}C^{16}O$ that we studied earlier.

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