RAS Scientific Council on chemical kinetics and structure
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Yaroslav the Wise State University of Novgorod the Great
Division for Computational Chemistry at the D.I. Mendeleev Chemical Society of Russia
A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS
Independent University of Moscow

17-th V.A.Fock Meeting on Quantum, Theoretical and Computational Chemistry.
23-27.08.2021, Novgorod, Russia

BOOK OF ABSTRACTS
of the 17-th V.A. Fock Meeting on Theoretical, Quantum and Computational Chemistry

A.L. Tchougréeff — Editor

Novgorod the Great

2021

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Calculation of CO molecule ground state using quantum computing

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Practical challenges in simulating quantum systems on modern classical computers are well known in the quantum chemistry community. None of the currently existing algorithms can provide high accuracy and acceptable computational speed at the same time.

The rapidly developing quantum computing science can be of great help for the quantum chemistry problems[1]. Significant advances in development of algorithms[2-4] and hardware[5-7] for quantum calculations have been made in the past two decades.

In this work, we have demonstrated the possibility of calculating the potential energy curve of a CO molecule in the STO-3G basis set using a quantum computer emulator. A qubit representation of the Hamiltonian was constructed using the Jordan-Wigner transformation in the second quantization formalism. The calculation was carried out using the qubit coupled clusters method[8], the obtained results were compared with those calculated using classical coupled clusters method and full CI method.

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