Theoretical study of the $^{29}Si^{16}O^{+}$ cation

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An experiment aimed at detecting nuclear spin-dependent parity-violating effects in the $^{29}Si^{16}O^{+}$ cation [1] is currently being prepared by an international collaboration of scientists based at the Massachusetts Institute of Technology. A clear understanding of the electronic structure of this molecule is required for both setting up the experiment and interpreting its results. This topic has been addressed in several publications [2–8], but none of them employ the coupled-cluster method, which is currently considered the standard of accuracy. The accuracy of results is not analyzed in these works.

In the present study, the $^{29}Si^{16}O^{+}$ cation is investigated within multielectron approaches at the level of relativistic coupled-cluster theory. Scalar-relativistic potential energy curves are calculated near the equilibrium bond length for both the ground and excited electronic states, as well as the spin-orbit coupling curve between them. The excitation energy from the ground to the excited state is reported along with an estimate of its accuracy, enabled by systematic variation of basis sets and the level of electron correlation. The influence of spin-orbit interaction on the lowest vibrational levels of both the ground and excited electronic states is also evaluated.

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References

1. J. Karthein *et al.*, Phys. Rev. Lett. **133**, 033003 (2024).
2. Z.-L. Cai, J. P. François, Chem. Phys. **234**, 59–68 (1998).
3. Z.-L. Cai, J. P. François, Chem. Phys. Lett. **282**, 29–38 (1998).
4. Z.-L. Cai, J. P. François, J. Mol. Spectrosc. **197**, 12–18 (1999).
5. S. Chattopadhyaya *et al.*, THEOCHEM. **639**, 177–185 (2003).
6. D. Shi *et al.*, Comput. Theor. Chem. **980**, 73–84 (2012).
7. R. Li *et al.*, Chem. Phys. **525**, 110412 (2019).
8. R. Li *et al.*, Chin. Phys. B. **28(4)**, 043102 (2019).