New insights into the ground and excited states properties of ThO and ThS from 4-component theories

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We present a comprehensive relativistic coupled cluster study of the electronic structures of the ThO and ThS molecules in the spinor basis. Specifically, we use the single-reference coupled cluster and the multi-reference Fock Space Coupled Cluster (FSCC) methods to model their ground and electronically-excited states [1]. Two variants of the FSCC method have been investigated: (a) one where the electronic spectrum is obtained from sector (1,1) of the Fock space, and (b) another where the excited states come from the doubly attached electronic states to the doubly charged systems (ThO^{2+} and ThS^{2+}), that is, from sector (0,2) of the Fock space. Our study provides a reliable set of spectroscopic parameters such as bond lengths, excitation energies, and vibrational frequencies, as well as a detailed analysis of the electron correlation effects in the ThO and ThS molecules [2].

References

1. L. Visscher, E. Eliav, and U. Kaldor,*J. Chem. Phys.* **115** (2001), 9720.
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