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Theoretical Investigation of the Singlet and Triplet Electronic States of ^{90}ZrS Molecules

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Abstract : The electronic structure of 90ZrS has been investigated using Ab-initio methods based on Complete Active Space Self Consistent Field and Multi-reference Configuration Interaction (CASSCF/MRCI). The number of predicted states has been extended to 14 singlet and 12 triplet lowest-lying states situated below 36000cm-1. The equilibrium energies of these 26 lowest-lying electronic states have been calculated in the 2S+1Λ(±) representation. The potential energy curves have been plotted in function of the inter-nuclear distances in a range of 1.5 to 4.5Å. Spectroscopic constants, permanent electric dipole moments and transition dipole moments between the different electronic states have also been determined. A discrepancy error of utmost 5% for the majority of values shows a good agreement with available experimental data. The ground state is found to be of symmetry X1Σ+ with an equilibrium inter-nuclear distance Re= 2.16Å. However, the (1)3Δ is the closest state to X1Σ+ and is situated at 514 cm-1. To the best of our knowledge, this is the first time that the spin-orbit coupling has been investigated for all the predicted states of ZrS. 52 electronic components in the Ω(±) representation have been predicted. The energies of these components, the spectroscopic constants ωe, ωeχe, βe and the equilibrium inter-nuclear distances have been also obtained. The percentage composition of the Ω state wave-functions in terms of S-Λ states was calculated to identify their corresponding main parents. These (SOC) calculations have determined the shift between (1)3Δ1 and X1Σ+ states and confirmed the ground state type being 1Σ+.

Keywords : CASSCF/MRCI, electronic structure, spin-orbit effect, zirconium monosulfide
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