

THEORETICAL PREDICTION OF THE SPECTROSCOPIC CONSTANTS OF FeS: AN *AB INITIO* MOLECULAR ORBITAL STUDY

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Energy levels of nearly degenerated ${}^5\Delta$ and ${}^5\Sigma$ states have been studied by the MR-SDCI + Q/ Roos-ANO (or various combinations of other basis sets) method with Breit-Pauli Hamiltonian for relativistic effects and spin-orbit coupling interaction corrections. The ${}^5\Sigma$ state has been predicted to be situated between ${}^5\Delta_2$ and ${}^5\Delta_1$ substates, and hence the ground state is ${}^5\Delta_i$. Spectroscopic constants for ${}^5\Delta$ state (and those for ${}^5\Sigma$ state) are predicted as follows: $r_e = 2.0247$ (1.9963) Å; $B_0 = 6043.2$ (6217.1) MHz; $D_0 = 3.80$ (3.64) kHz; $\nu = 510.4$ (543.9) cm^{-1} ; $\mu_e = 5.92$ (4.88) D.