

COUPLED CLUSTER CALCULATIONS FOR MOLECULES IN TRIPLET GROUND STATES

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On the basis of large-scale open-shell coupled cluster calculations accurate equilibrium structures are established for a number of molecules in triplet ground states. Among these are species of type HC_{2n}N ($n = 1-3$), C_{2n}S ($n = 1-3$), SiC_{2n+1} ($n = 1-3$) and $\text{SiC}_{2n-1}\text{S}$ ($n = 1-4$). The equilibrium structure of HC_2N is definitely non-linear with a barrier height to linearity close to 300 cm^{-1} . On the other hand, triplet HC_4N has a linear equilibrium structure and this probably also holds for the larger members of the series. Various spectroscopic properties calculated for the above mentioned molecules are discussed.