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 $SiC_{2n-1}S$ (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 HC4N 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.