ACCURATE EQUILIBRIUM STRUCTURES AND PREDICTIONS OF SPECTROSCOPIC PROPERTIES FOR LINEAR CARBON-SILICON CLUSTERS.

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On the basis of large-scale coupled cluster calculations including connected triple substitutions and experimental ground-state rotational constants for seven different isotopomers of C₂Si, accurate equilibrium geometries have been established for linear C₄Si, C₅Si₂, C₆Si, C₅Si₂, C₅Si and C₇Si₂ in their electronic ground-states. The calculated harmonic vibrational wavenumbers for C₄Si and C₅Si₂ should be accurate to a few cm⁻¹ and a full set of vibration-rotation coupling constants has been calculated for both species which appear to be rather well-behaved semi-rigid molecules.