A COUPLED CLUSTER STUDY OF LINEAR C_7: NO EVIDENCE OF FLOPPINESS

PETER BOTSCHWINA, *Institut für Physikalische Chemie, Universität Göttingen, Tammanstraße 6, D-37077 Göttingen, Germany*.

Linear C_7 has been studied by means of coupled cluster calculations including connected triple substitutions (variant CCSD(T)) and a large basis set of 385 contracted Gaussian type orbitals. The calculations indicate that linear C_7 is a fairly normal semi-rigid molecule with no sign of floppiness. In particular, excitation of the bending vibration with lowest wavenumber (ν_{11}) produces only a 0.2% change in the rotational constant. The results of the present calculations are at variance with an experimental study by Heath and Saykally[a]. A renewed analysis of the experimental data and possible remeasurement is strongly recommended. Rovibrational transitions within the ν_{11} band of linear C_7 are predicted around 70 cm^{-1} and thus rather close to transitions within the ν_2 band of non-rigid C_3, but with very different spacing.

[a] J. R. Heath and R. J. Saykally , *J. Chem. Phys.* **94**(1724), 1991.