LARGE-SCALE COUPLED CLUSTER CALCULATIONS FOR THE TWO RENNER-TELLER COMPONENTS OF HCCO

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CCSD(T) calculations with basis sets of up to 282 contracted Gaussian-type orbitals have been carried out in order to establish accurate equilibrium structures for the trans-bent lower (^{2}A'') and linear upper (^{2}A') Renner-Teller components of HCCO: a): ^{2}A'': r_e (CH) = 1.0709 Å, R_{1e} (CC) = 1.2975 Å, R_{2e} (CO) = 1.1710 Å, α_e (HCC) = 134.1°, and β_e (CCO) = 169.3°; b) ^{2}A' ($^2\Pi$): r_e = 1.0604 Å, R_{1e} = 1.2600 Å, and R_{2e} = 1.1834 Å. The barrier height to linearity of the ^{2}A'' component is predicted to be 637 cm^{-1}.