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 ($^2\text{A}''$) and linear upper ($^2\text{A}'$) Renner-Teller components of HCCO: a) $^2\text{A}''$: $r_e$ (CH) = 1.0709 Å, $R_{1e}$ (CC) = 1.2975 Å, $R_{2e}$ (CO) = 1.1710 Å, $\alpha_e$ (HCC) = 134.1°, and $\beta_e$ (CCO) = 169.3°; b) $^2\text{A}'$ ($^2\Sigma$): $r_e$ = 1.0604 Å, $R_{1e}$ = 1.2600 Å, and $R_{2e}$ = 1.1834 Å. The barrier height to linearity of the $^2\text{A}''$ component is predicted to be 637 cm$^{-1}$. 