Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Structure Calculations and Quantum Dynamics of Rotational Deexcitation of CNNC by He

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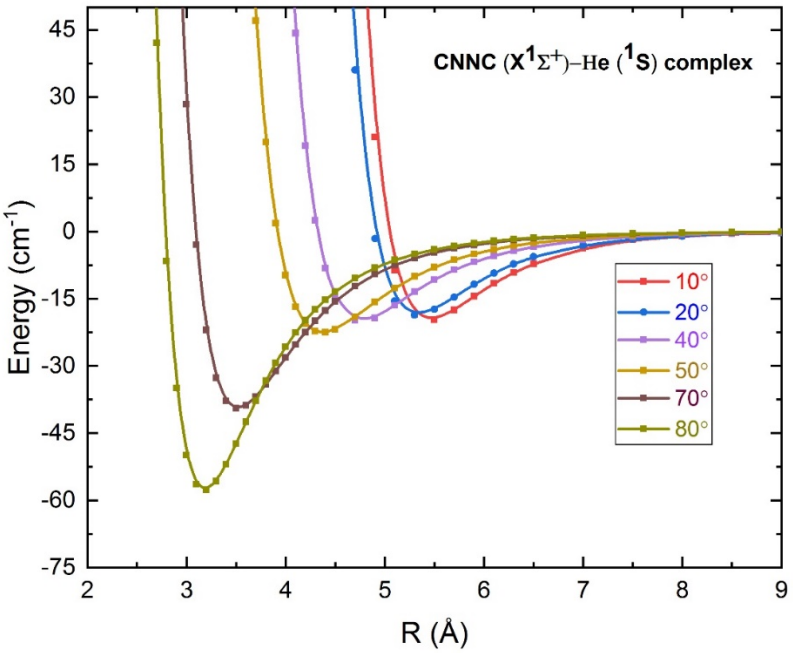

Figure S1: Ab initio potential energy curves for θ = 10°, 20°, 40°, 50°, 70° and 80°.

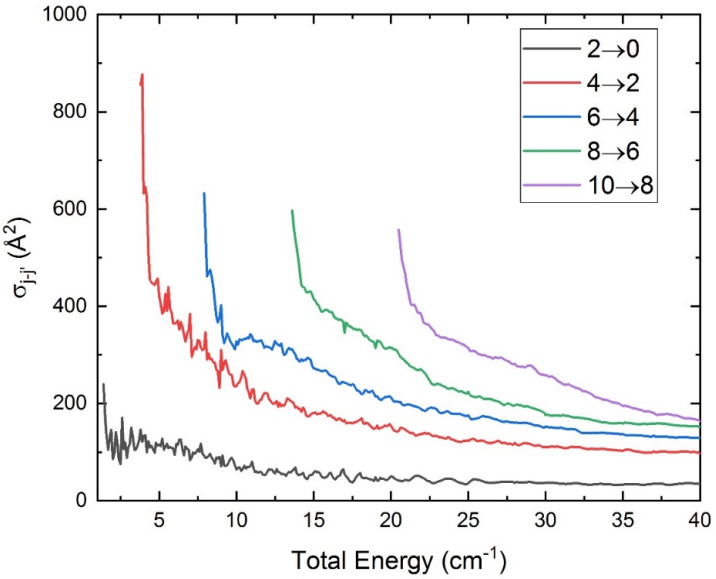

Figure S2: Cross sections as a function of total energy ranging from 0.5 to 40 cm^{-1} for transitions $j \rightarrow j'$.

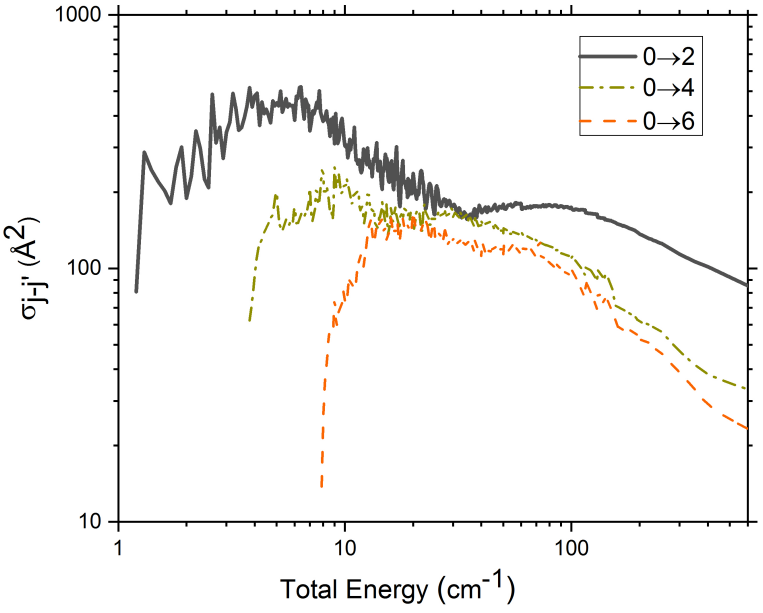

Figure S3: Excitation cross-sections of CNNC-He complex for transitions j=0→j'.

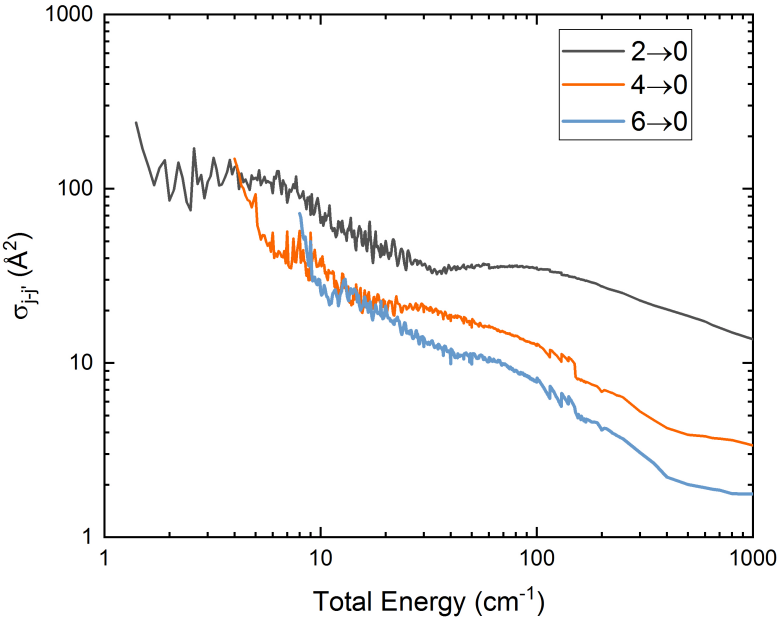

Figure S4: Deexcitation cross-sections of CNNC-He complex for transitions $j \rightarrow j' = 0$.

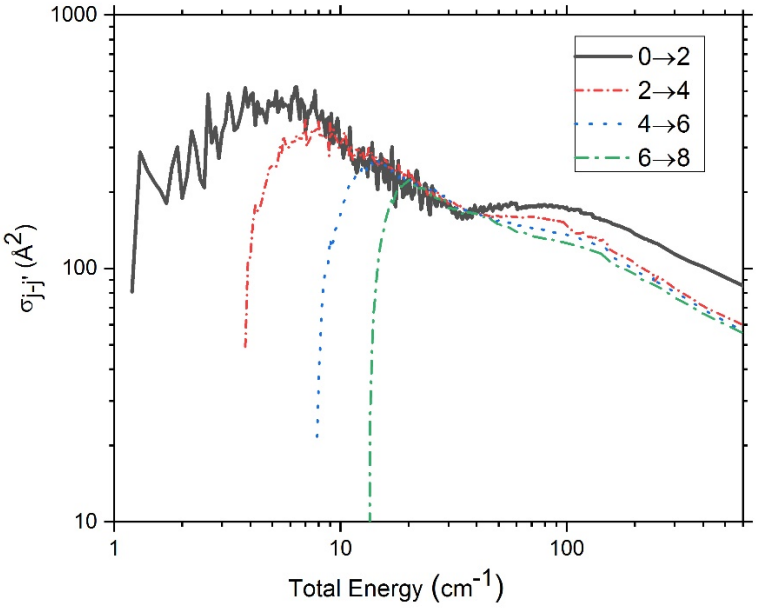

Figure S5: Variation of rotational excitation inelastic cross sections with total energy up to 650 cm^{-1} with Δj=2 for even j values.

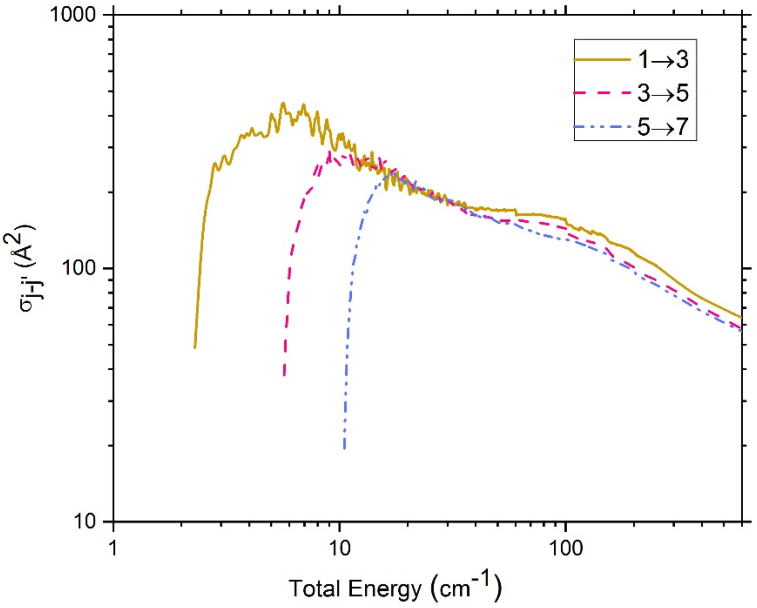

Figure S6: Variation of rotational excitation inelastic cross sections with total energy up to 650 cm^{-1} with Δj=2 for odd j values.

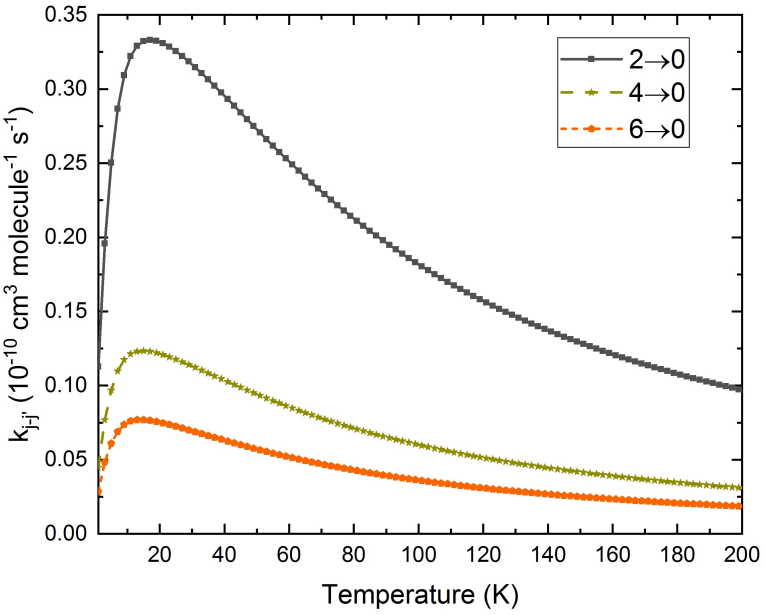

Figure S7: Rate coefficients of CNNC-He complex for $j \rightarrow j' = 0$ for up to 200 K.