

Supporting Information

**Predicting the Initial Thermal Decomposition Path of Nitrobenzene
Caused by Mode Vibration at Moderate-Low Temperatures:
Temperature-Dependent Anti-Stokes Raman Spectra Experiments
and First-Principals Calculations**

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IRC determination for the transition state of isomerization

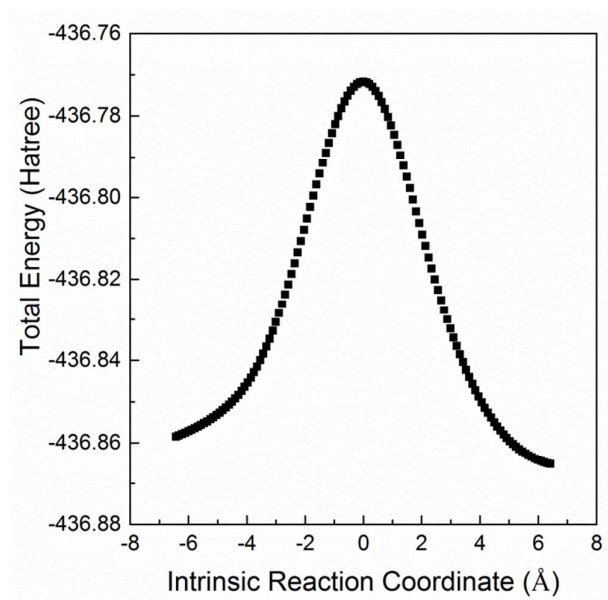


Figure S1. The IRC path of the transition state leading the nitrobenzene to the isomer phenyl nitrite.