**Supporting Information**

**to**

**Double-proton transfer triggering mechanism of nitromethane caused by intermolecular hydrogen bonding at low temperature**

Yajing Penga,\*, Weina Liua, Bowen Maa, Jinshun Zhanga,Yuhui Liua, Yan Sub, Yanqiang Yangc,\*

a*Department of Physics, Bohai University, Jinzhou 121013, China*

b*State Key Laboratory of Structural Analysis, Optimization and CAE Software for Industrial Equipment (Dalian University of Technology), Ministry of Education, Dalian 116024, China.*

c*Institute of Fluid Physics, China Academy of Engineering Physics, Chengdu 610000, China*.

\*Corresponding authors: pengyajing@126.com; yqyang@hit.edu.cn

S1 The Comparison of Raman spectrum of bimolecular nitromethane calculated using CPMD method with that using quantum chemistry method..........................................2

S2 The experimental anti-stocks Raman spectra............................................................3

S3 IRC path of the transition states leading the intermolecular double-proton transfer reaction of nitromethane.................................................................................................4

S1 The Comparison of Raman spectrum of bimolecular nitromethane calculated using CPMD method with that using quantum chemistry method



*Figure S1 The Comparison of Raman spectrum of bimolecular nitromethane calculated using CPMD method with that using quantum chemistry method. The main peaks are basically consistent except for the difference of several peak sites.*

S2 The experimental anti-stocks Raman spectra



*Figure S2 The experimental anti-stocks Raman spectra.*

S3 IRC path of the transition states leading the intermolecular double-proton transfer reaction of nitromethane



*Figure S3 IRC path of the transition states leading the intermolecular double-proton transfer reaction of nitromethane*.