Simulating Infrared spectrum of *N*-MethylAcetamide dimer by Quantum Vibration Perturbation method

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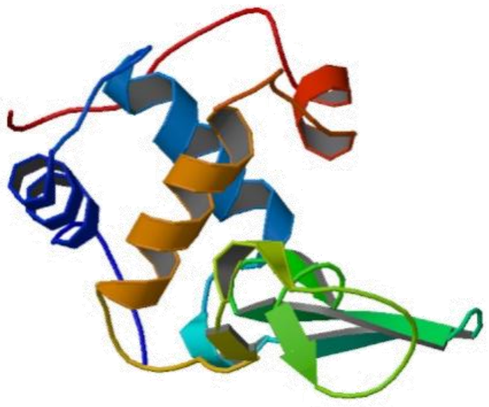
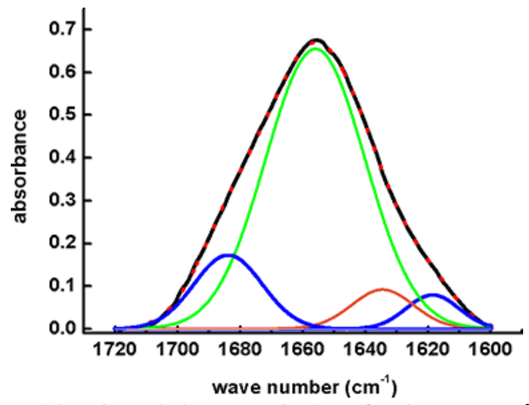
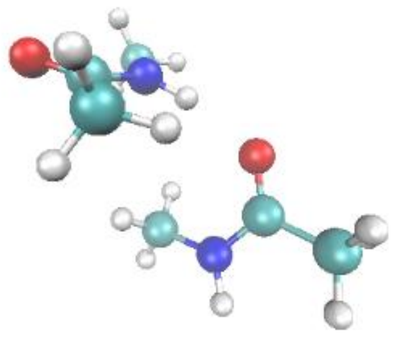
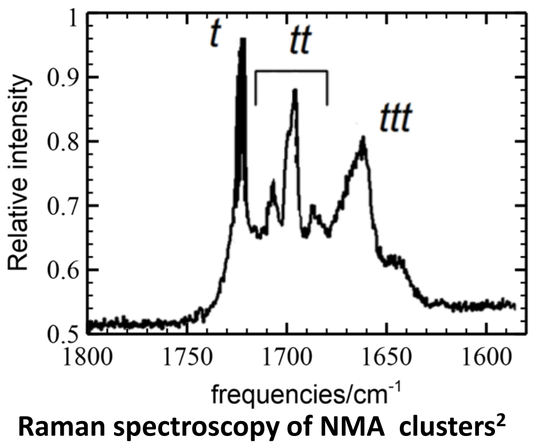
1 Introduction





Amide I band deconvolution for lysozyme[1]

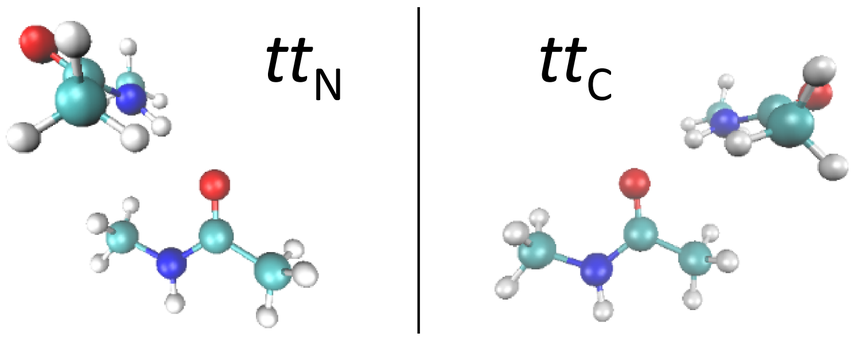




Raman spectroscopy of NMA clusters[2]

2 Method

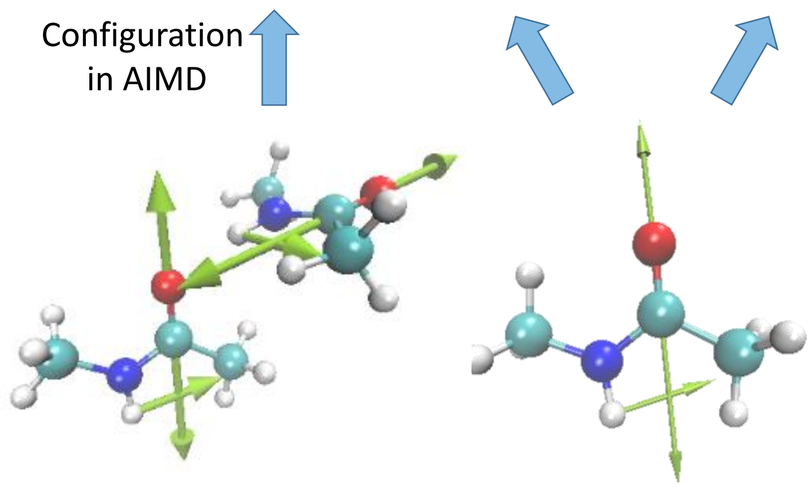
- Two AIMD trajectory



- Time-dependent frequencies

$$\boldsymbol{V}'(t, q_1, q_2) = H(t) - H_1(q_1) - H_2(q_2)$$

Configuration in AIMD



$$H_{ij,kl} = \langle l|\langle j|H_{(t)}|i\rangle|k\rangle = H_{ij}^{(1)}\delta_{ij} + H_{kl}^{(2)}\delta_{kl} + \sum\sum c_i^{(1)} c_j^{(2)} V'(q_1, q_2)$$

diagonalization

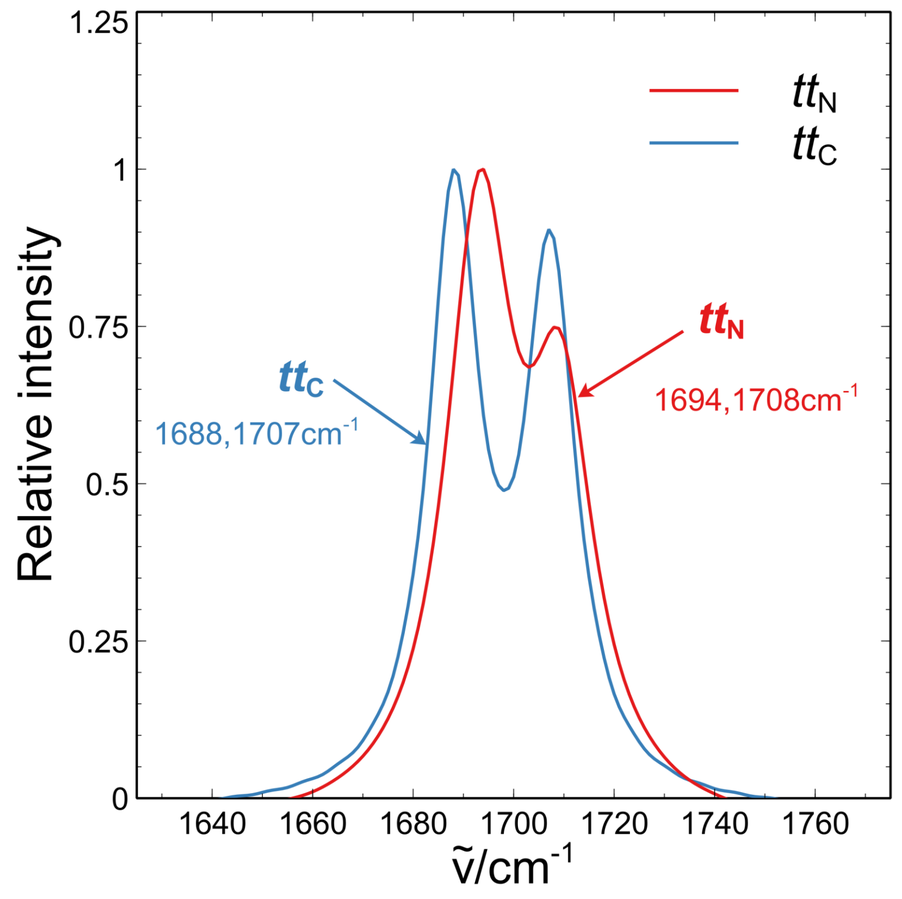
$$\begin{cases} E_1 - E_0 = \omega_1(t) \\ E_2 - E_0 = \omega_2(t) \end{cases}$$

3 Result and discussion

- PODVR convergence test

N_{PODVR}	ω_1/cm^{-1}	ω_2/cm^{-1}	$\langle 1\|q_1\|1\rangle$	$\langle 1\|q_2\|1\rangle$	$\langle 2\|q_1\|2\rangle$	$\langle 2\|q_2\|2\rangle$
3	1708.71	1721.14	-0.03814	-0.09118	-0.06258	-0.06699
5	1708.70	1721.02	-0.03825	-0.09115	-0.06216	-0.06717
9	1708.68	1721.014	-0.03821	-0.09121	-0.06218	-0.06714

- IR simulation result



4 Conclusion

- Extending QVP method to multi-chromophore resonance system. This method can provide a more accurate way to calculate protein IR in the future.
- Simulating Infrared spectrum of two NMA-dimer isomers. The frequencies gaps of them are 14cm^{-1} and 19cm^{-1}.

Acknowledgment

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Reference

1. Bridelli, M. G. (2017). In Fourier transforms-high-tech application and current trends. InTech.
2. Thomas Forsting et al., Phys.Chem.Chem.Phys.,2017, 19, 10727