

Solvation and Vibrational Analysis of Propanamide

Connor J. Graça*, Dr. Jeffry D. Madura*

*Duquesne University, Bayer School of Natural and Environmental Science, The Cyril H. Wecht Institute of Forensic Science and Law

*Duquesne University, Bayer School of Natural and Environmental Science, Department of Chemistry and Biochemistry, Center for Computational Sciences



THE CYRIL H. WECHT

Institute of Forensic Science and Law

Background

- ▶ Propanamide: organic molecule
 - ▶ Amide of propanoic acid (see **Figure 1**)
- ▶ Used in ultraviolet resonance Raman (UVR) spectroscopy[1]
 - ▶ Model for hydrogen bonding
 - ▶ Model of a peptide backbone
- ▶ Raman spectral peaks correspond to specific amide vibrations
- ▶ Going from gas phase to aqueous solution
 - ▶ N–H stretch frequency increases
 - ▶ C=O stretch frequency decreases
- ▶ We hypothesize that the amide I (Am I) vibrational frequency of propanamide decreases upon hydrogen bonding with water, while the Am II and Am III vibrational frequencies will increase under the same conditions.

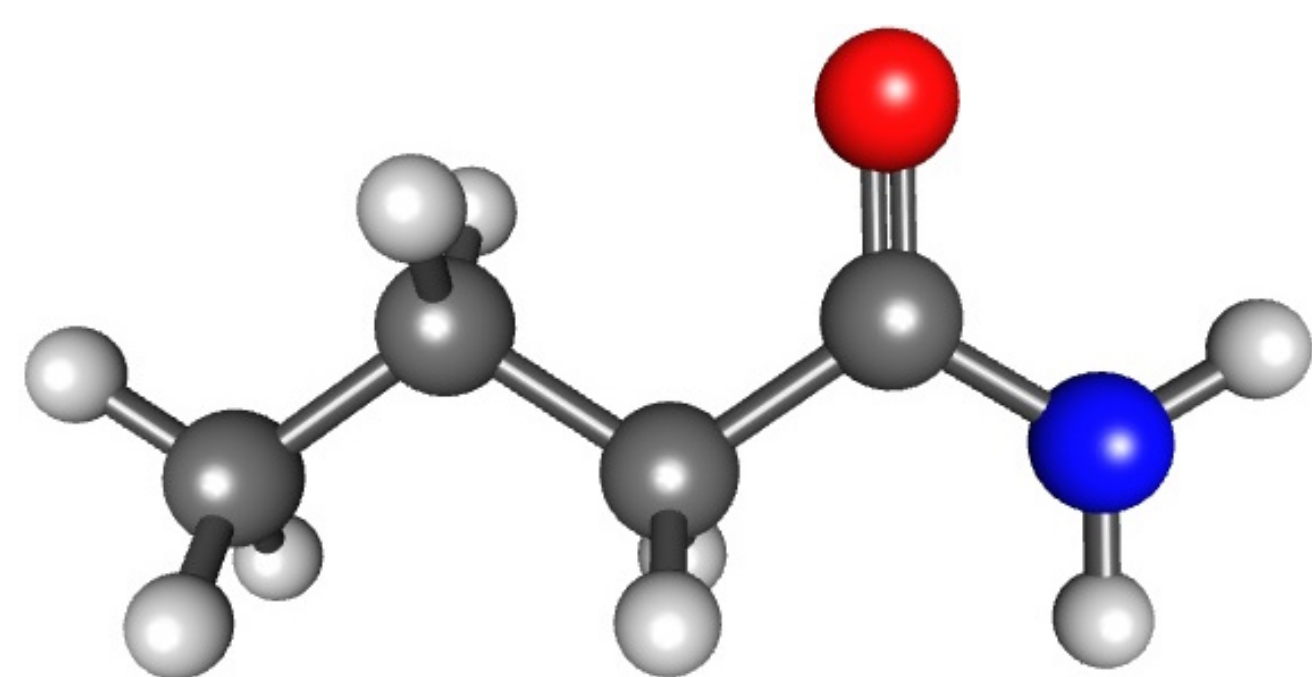


Figure 1: Ball and stick model of propanamide

Computational Methods

- ▶ Calculated the energy minimum of the system (propanamide and water)
- ▶ Calculated frequencies for minimum energy geometries

Software IQmol and QChem
Functional M06-2X[2, 3]
Basis Set 6-31G**[4]

Results

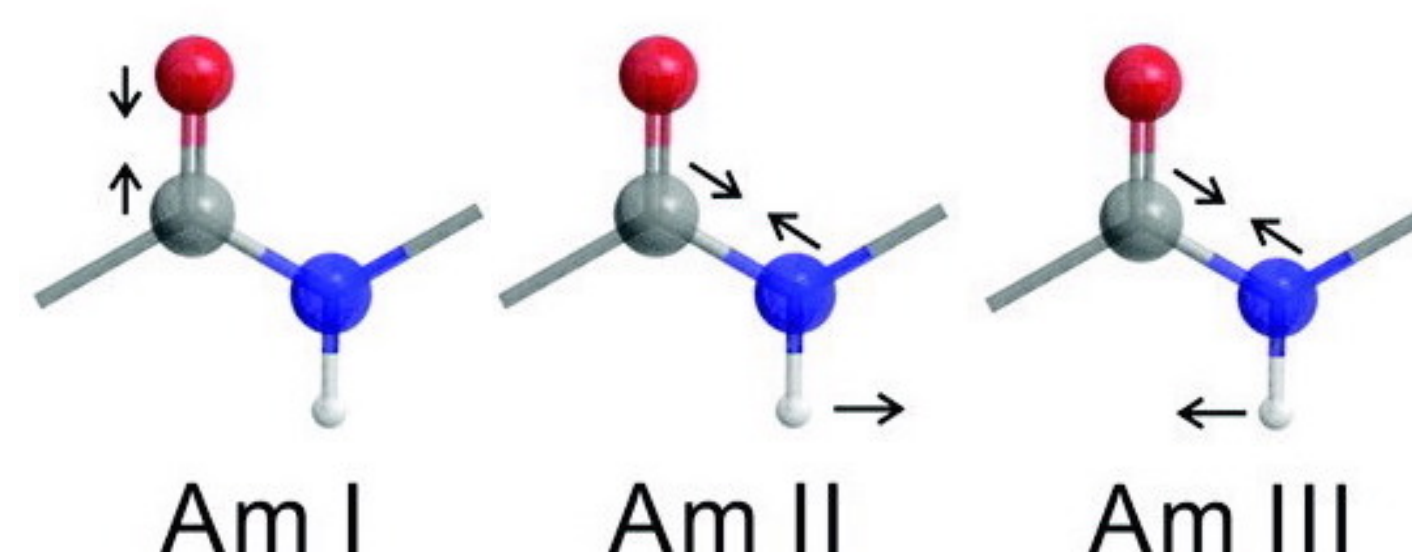


Figure 2: Primary amide modes of peptide backbone[5]

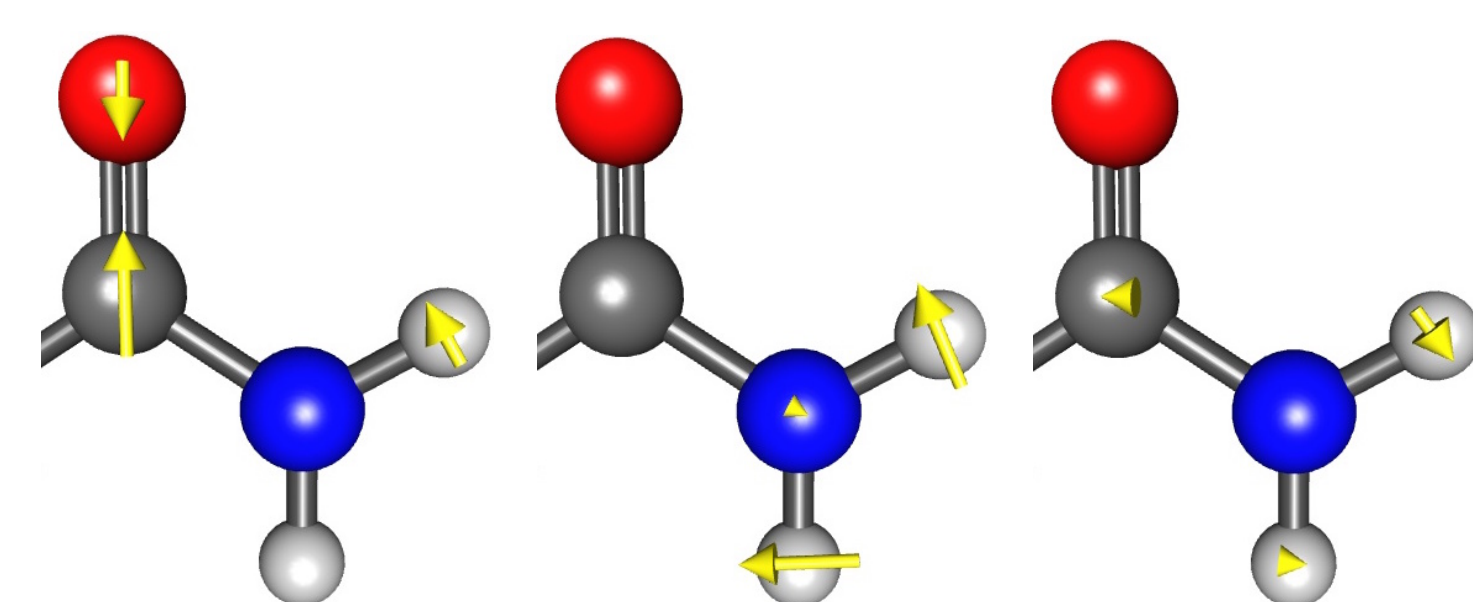


Figure 3: Primary amide vibrational modes of propanamide in the gas phase

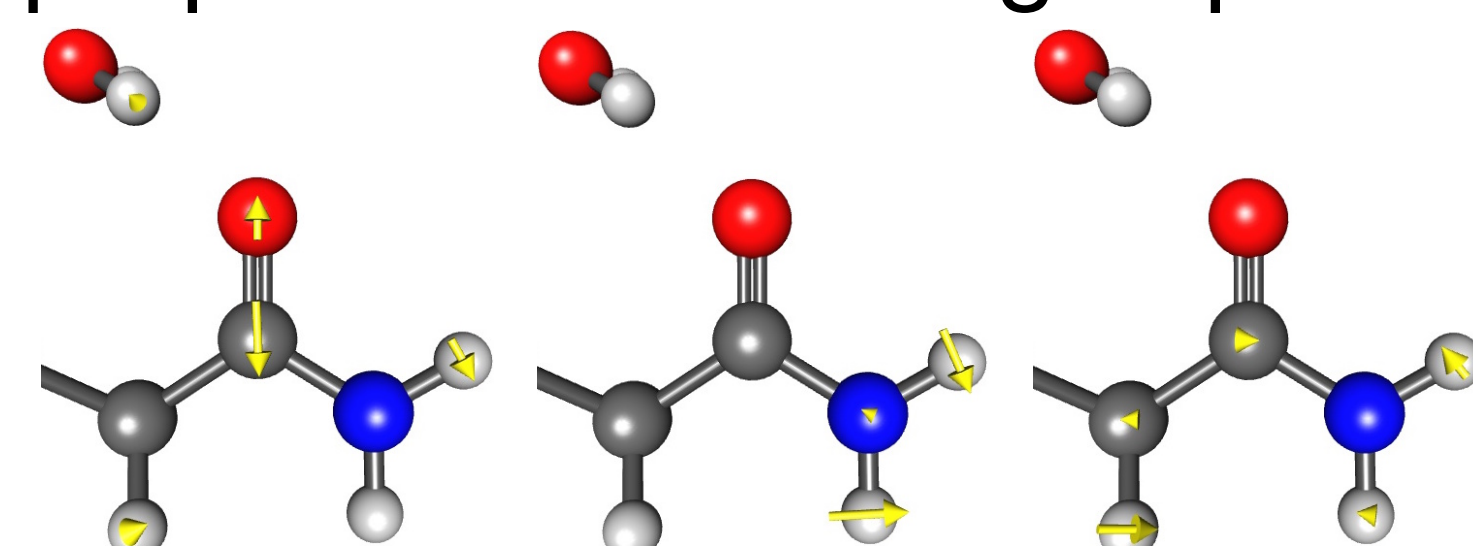


Figure 4: Primary amide vibrational modes of propanamide and one water molecule

$\Delta\nu$ is the change in the frequency from propanamide to propanamide with one water molecule

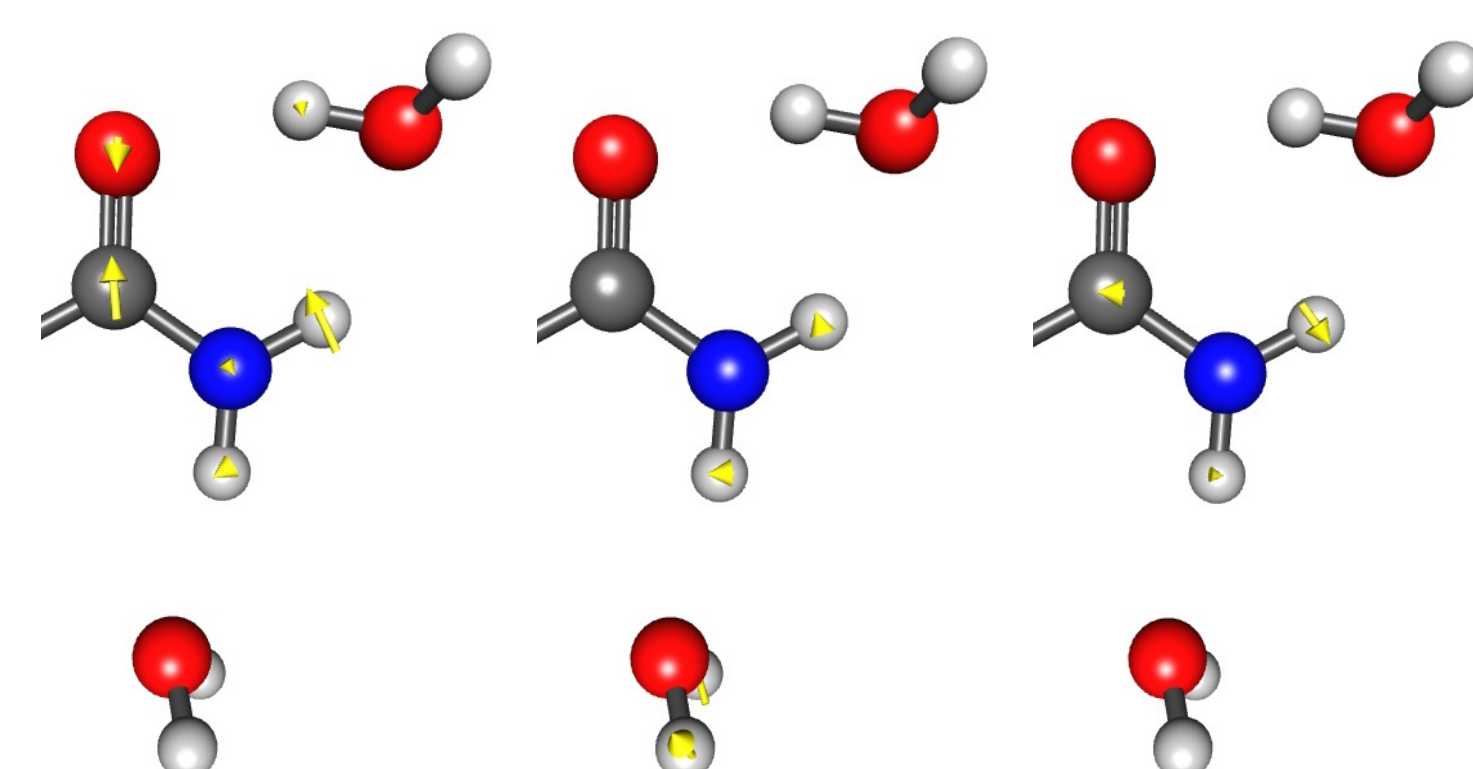


Figure 5: Primary amide vibrational modes of propanamide and two water molecules

Mode	ν (cm ⁻¹)
Am I	≈ 1600
Am II	≈ 1550
Am III	≈ 1200 to 1340

Table 1: Experimentally determined normal modes of peptide backbone[5]

Mode	ν (cm ⁻¹)
Am I	1852
Am II	1622
Am III	1441

Table 2: Frequency of propanamide vibrations in the gas phase

Mode	ν (cm ⁻¹)	$\Delta\nu$ (cm ⁻¹)
Am I	1852	-28
Am II	1622	8
Am III	1441	6

Table 3: Frequency of propanamide vibrations and one water molecule

Mode	$\Delta\nu_1$ (cm ⁻¹)	$\Delta\nu_t$ (cm ⁻¹)
Am I	-35	-63
Am II	2	10
Am III	26	32

Table 4: Frequency of propanamide vibrations and two water molecule

Results, Continued

$\Delta\nu_1$ is the change in frequency between propanamide with one water molecule and propanamide with two water molecules, and $\Delta\nu_t$ is the change in frequency between propanamide and propanamide with two water molecules

Conclusions and Future Work

- ▶ Continue adding water molecules to the system (three, four, five water molecules)
- ▶ Calculate primary amide vibrational modes of propanamide in a water sphere
- ▶ Hypothesis: Supported
 - ▶ Am I frequencies showed decreasing trend
 - ▶ Am II and Am III frequencies showed increasing trend

Acknowledgements

Thank you to:

- ▶ Dr. Jeffry D. Madura
- ▶ Madura Research Group
 - ▶ Matthew N. Srnc, Shiv Upadhyay and Riley Workman
- ▶ Duquesne University
- ▶ Bayer School of Natural and Environmental Science
- ▶ Scott Boesch
- ▶ Undergraduate Research Program
- ▶ National Institutes of Health R25, National Institute on Drug Abuse (NIDA) Grant
 - ▶ 1R25 DA032519 - 01
- ▶ National Science Foundation (NSF), Major Research Instrumentation (MRI)
 - ▶ CHE - 1126465

References

1. Punihaole, D.; Jakubek, R.; Dahlburg, E.; Hong, Z.; Myshakina, N.; Geib, S.; Asher, S. *J. Phys. Chem. B* **2015**, *119*, 3931–3939.
2. Zhao, Y.; Truhlar, D. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
3. Zhao, Y.; Truhlar, D. *Accounts Chem. Res.* **2008**, *xxx*, 1–11.
4. Janis, J.; Kaijser, P.; Sabin, J.; Smith, V. *Mol. Phys.* **1979**, *37*, 463–472.
5. Oladepo, S.; Xiong, K.; Hong, Z.; Asher, S. *J. Phys. Chem. Lett.* **2011**, *2*, 2604–2628.