Solvation and Vibrational Analysis of Propanamide

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Background

- Propanamide: organic molecule
  - Amide of propanoic acid (see **Figure 1**)
- Used in ultraviolet resonance Raman (UVRR) 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.

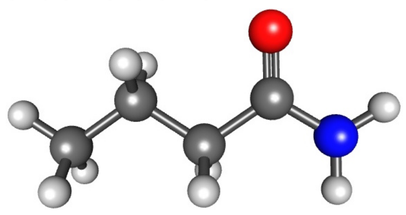

Figure 1: Ball and stick model of propanamide

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

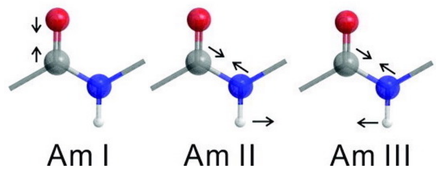

Figure 2: Primary amide modes of peptide backbone[5]

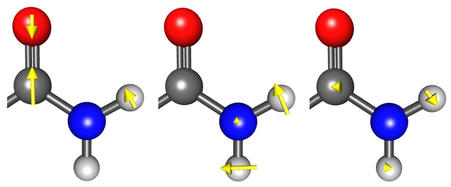

Figure 3: Primary amide vibrational modes of propanamide in the gas phase

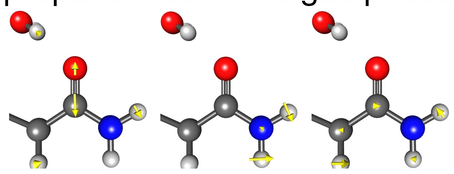

Figure 4: Primary amide vibrational modes of propanamide and one water molecule

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

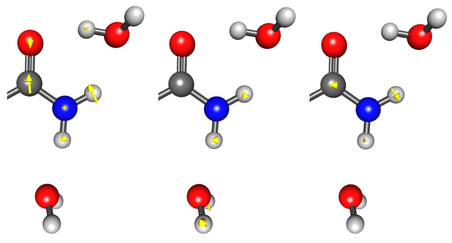

Figure 5: Primary amide vibrational modes of propanamide and two water molecules

Mode	ν (cm^{-1})
Am I	$\approx$ 1600
Am II	$\approx$ 1550
Am III	$\approx$ 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 shpere
- Hypothesis: Supported
  - Am I frequencies showed decreasing trend
  - Am II and Am III frequencies showed increasing trend

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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.