A STUDY OF THE FORMAMIDE-(H$_2$O)$_3$ COMPLEX BY MICROWAVE SPECTROSCOPY

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BY MICROWAVE SPECTROSCOPY

**Interactions between peptide groups and water** may be modelled from the study of gas phase microsolvated clusters of simple molecules.
A STUDY OF THE FORMAMIDE-(H₂O)₃ COMPLEX
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Interactions between peptide groups and water may be modelled from the study of gas phase microsolvated clusters of simple molecules.
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Interactions between peptide groups and water may be modelled from the study of gas phase microsolvated clusters of simple molecules such as formamide.

trans-peptide
~99%

FW-1:1c

14% in proteins

FW-1:1b

42% in proteins

cis-peptide
~1%

FW-1:1a

In proteins
We have analyzed the rotational spectra of formamide$_m$-(H$_2$O)$_n$ (m,n=1,2) clusters:

1) To characterize the different 1:1, 1:2, 2:1 conformers.

S. Blanco et al., *JACS* 128(37) 12111 (2006)
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We have analyzed the rotational spectra of formamideₘ-(H₂O)ₙ (m,n=1,2) clusters:
1) To characterize the different 1:1, 1:2, 2:1 conformers.
2) To search for evidences of cooperative effects such as polarization enhanced or resonance assisted hydrogen bonding.

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In these contest we have analyzed the rotational spectra of formamide-(H$_2$O)$_3$ cluster

1) To characterize the different 1:1, 1:2, 2:1 conformers.

2) To search for evidences of cooperative effects such as polarization enhanced or resonance assisted hydrogen bonding.

$\text{r}(C-N) \text{ decrease}$

$\text{shortening of HB lengths}$

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Formamide-(H$_2$O)$_3$ conformers

<table>
<thead>
<tr>
<th>Parameter$^{(a)}$</th>
<th>FW1-b b c</th>
<th>FW2a-FW1b</th>
<th>FW2a-FW1c</th>
<th>FW2b-FW1a</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta E/$ cm$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$\Delta E/$ kJmol$^{-1}$</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$A/$MHz</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$B/$MHz</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C/$MHz</td>
<td></td>
<td></td>
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</tbody>
</table>
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Formamide-(H₂O)₃ conformers

<table>
<thead>
<tr>
<th>Cloud</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Image of formamide-(H₂O)₃ conformers" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter(s)</th>
<th>C-top-u</th>
<th>C-top-d</th>
<th>C-back</th>
<th>C-front</th>
</tr>
</thead>
<tbody>
<tr>
<td>ΔE/ cm⁻¹</td>
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<td>B/MHz</td>
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<td></td>
</tr>
<tr>
<td>C/MHz</td>
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Spectrum

FTMW spectrometer  Fabry-Pérot cavity  supersonic jet - sample

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BY MICROWAVE SPECTROSCOPY

Spectrum

Heated Nozzle

Carrier gas
Ne
12 bar

H₂O

Ne + H₂O

Heater
50ºC

Liquid sample of formamide
b.p. 210ºC

(F)ₘ ∙∙∙ (H₂O)ₙ
A STUDY OF THE FORMAMIDE-(H₂O)₃ COMPLEX BY MICROWAVE SPECTROSCOPY
A STUDY OF THE FORMAMIDINE-(H₂O)₃ COMPLEX
BY MICROWAVE SPECTROSCOPY

Spectrum
A STUDY OF THE FORMAMIDE-(H\textsubscript{2}O\textsubscript{3}) COMPLEX
BY MICROWAVE SPECTROSCOPY

Evidences of cooperative effects such as \textit{polarization enhanced} or \textit{resonance assisted} hydrogen bonding.

\begin{align*}
  r_{Hf\cdots Ow} &= 2.062 \text{ Å} \\
  r_{Hw\cdots Of} &= 1.957 \text{ Å} \\
  r_{Ow\cdots Of} &= 2.813 \text{ Å} \\
  r_{Hf\cdots Ow} &= 1.791 \text{ Å} \\
  r_{Hw\cdots Of} &= 1.886 \text{ Å} / r_{Hw\cdots Of} = 1.810 \text{ Å} \\
  r_{Ow\cdots Ow} &= 2.774 \text{ Å} \\
  r_{Ow\cdots Of} &= 2.728 \text{ Å}
\end{align*}

\textbf{shortening of HB lengths}

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Evidences of cooperative effects such as polarization enhanced or resonance assisted hydrogen bonding.

\[ r_{\text{C-N}} = 1.361 \text{ Å} \quad 1.350 \text{ Å} \quad 1.343 \text{ Å} \]

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