

PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

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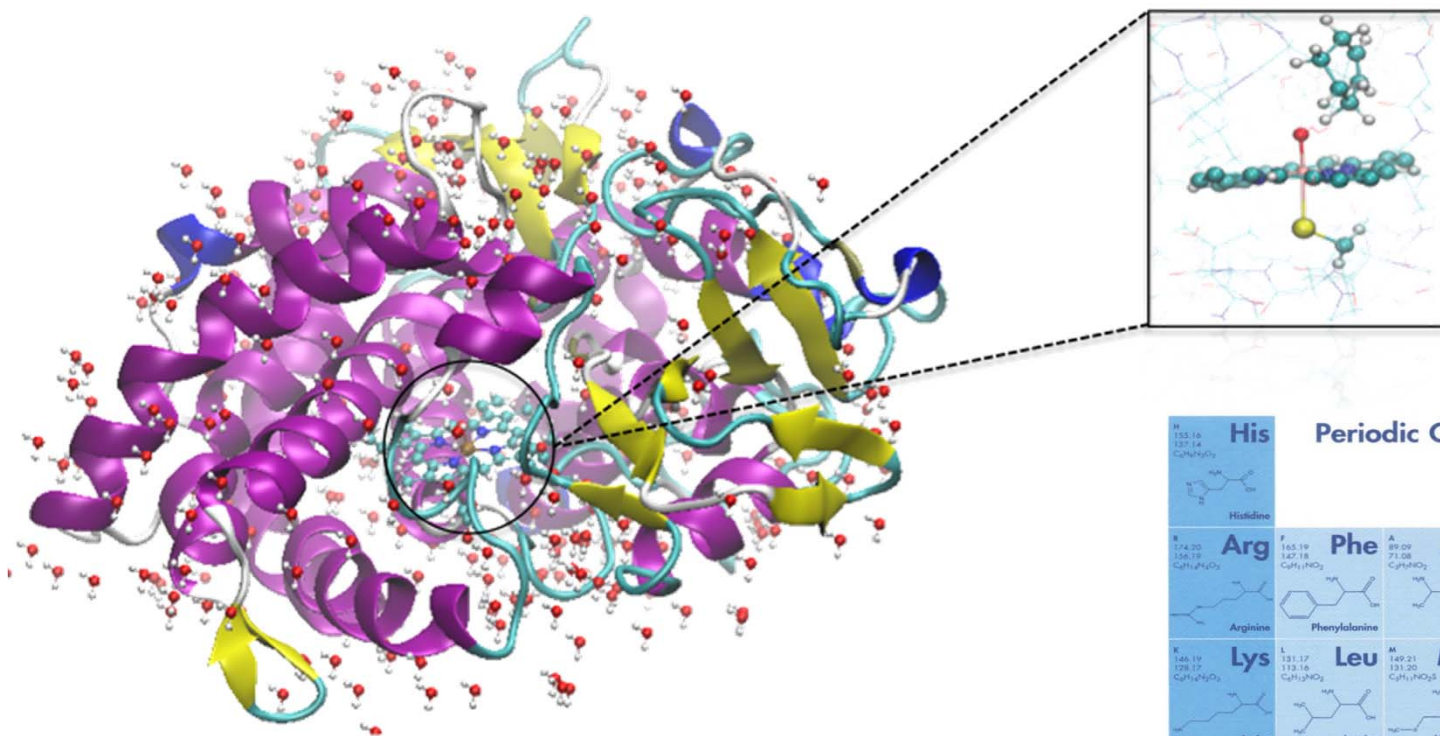
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



















ANTHONY C. LEGON

School of Chemistry

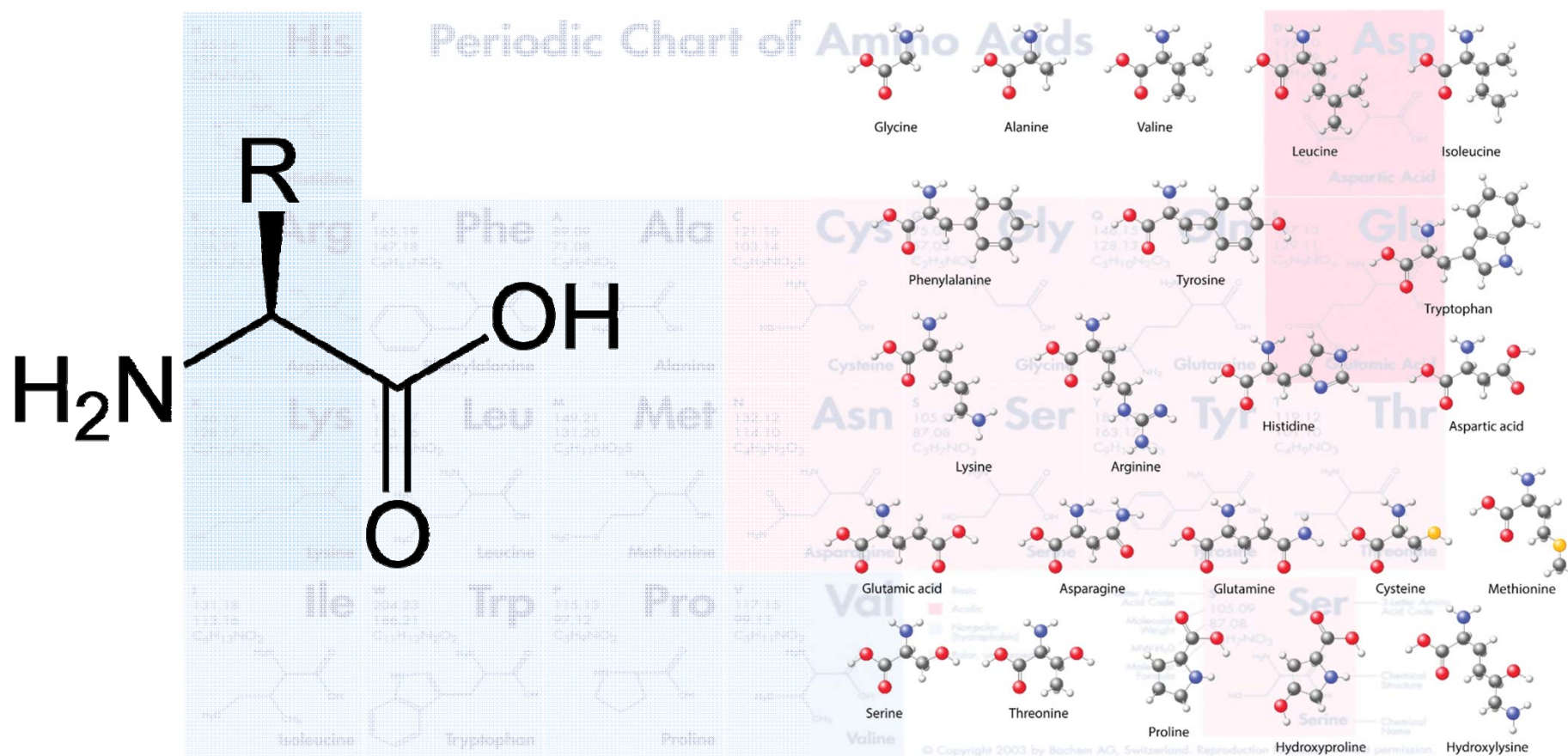
University of Bristol, Bristol, United Kingdom

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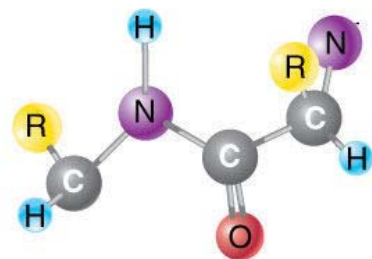


Periodic Chart of Amino Acids				Asp		
<div>H 157.15 137.14 C₆H₉NO₂</div> <div></div> <div>Histidine</div>				<div>I 133.10 115.09 C₄H₇NO₄</div> <div></div> <div>Aspartic Acid</div>		
<div>F 165.19 156.18 C₆H₁₂N₄O₂</div> <div></div> <div>Arginine</div>	<div>F 165.19 156.18 C₉H₉NO₂</div> <div></div> <div>Phenylalanine</div>	<div>A 89.09 75.08 C₃H₇NO₂</div> <div></div> <div>Alanine</div>	<div>C 121.16 103.14 C₃H₇NO₂S</div> <div></div> <div>Cysteine</div>	<div>G 75.07 75.07 C₂H₅NO₂</div> <div></div> <div>Glycine</div>	<div>G 146.15 128.13 C₅H₉NO₃</div> <div></div> <div>Glutamine</div>	<div>F 147.15 129.11 C₅H₉NO₄</div> <div></div> <div>Glutamic Acid</div>
<div>K 146.19 129.17 C₆H₁₂N₂O₂</div> <div></div> <div>Lysine</div>	<div>L 131.17 113.16 C₆H₁₃NO₂</div> <div></div> <div>Leucine</div>	<div>A 149.21 131.20 C₅H₉NO₂S</div> <div></div> <div>Methionine</div>	<div>N 132.12 114.10 C₄H₈NO₂</div> <div></div> <div>Asparagine</div>	<div>S 105.09 87.08 C₃H₇NO₃</div> <div></div> <div>Serine</div>	<div>T 181.19 163.17 C₉H₉NO₃</div> <div></div> <div>Tyrosine</div>	<div>T 119.12 101.10 C₄H₉NO₃</div> <div></div> <div>Threonine</div>
<div>I 131.17 113.16 C₆H₁₃NO₂</div> <div></div> <div>Isoleucine</div>	<div>W 204.23 186.21 C₁₁H₁₁N₂O₂</div> <div></div> <div>Tryptophan</div>	<div>P 115.13 87.12 C₅H₉NO₂</div> <div></div> <div>Proline</div>	<div>V 117.15 99.13 C₆H₁₃NO₂</div> <div></div> <div>Valine</div>	<div><div><div>Basic</div><div>Acidic</div><div>Neutral</div><div>Nonpolar</div><div>Other: unchanged</div></div><div><div>1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100</div><div><div>1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 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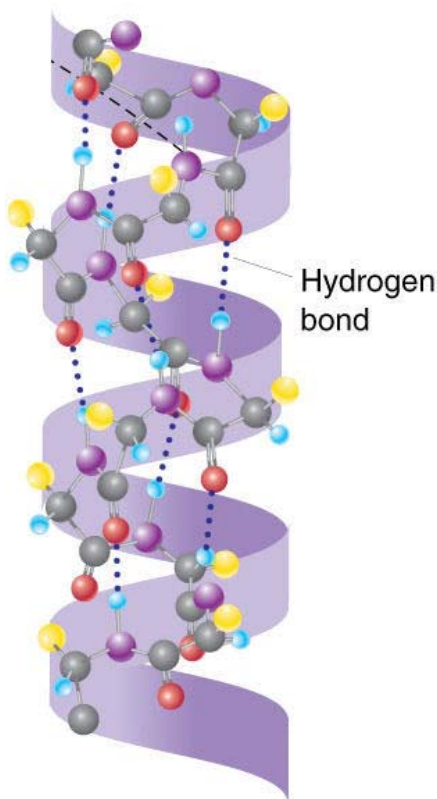
PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA



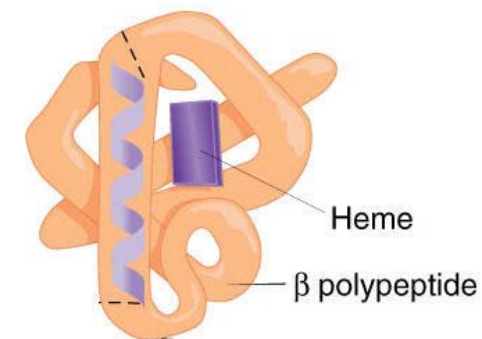
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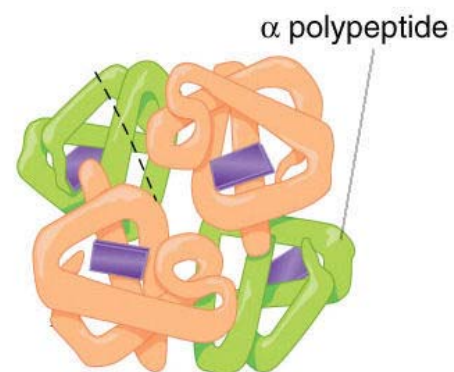
(a) Primary structure



(b) Secondary structure



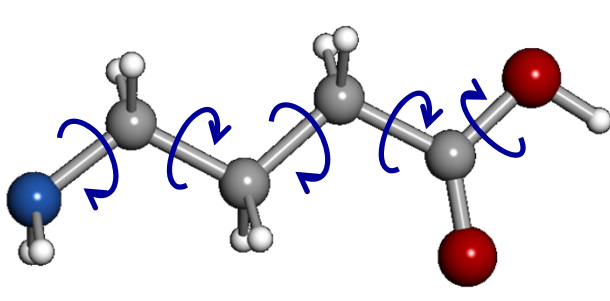
(c) Tertiary structure



(d) Quaternary structure

PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Single biomolecules: great torsional flexibility



Ang. Chem. Int. Ed.
49, 9187 (2010)

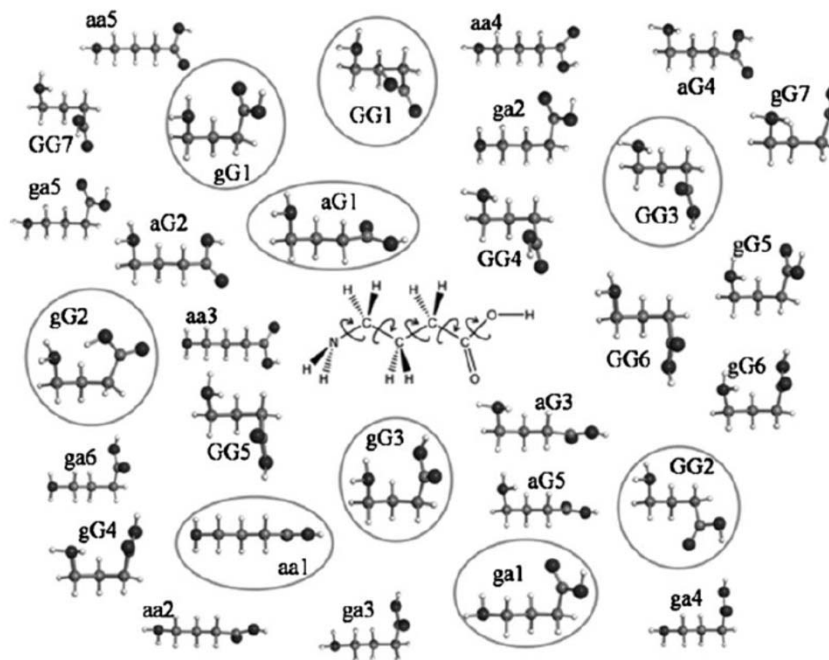
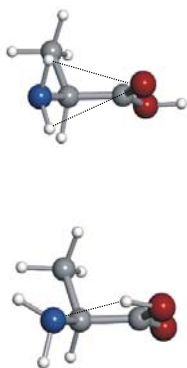


Figure 1. Predicted low-energy conformers of GABA. The nine observed conformers are circled.

PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

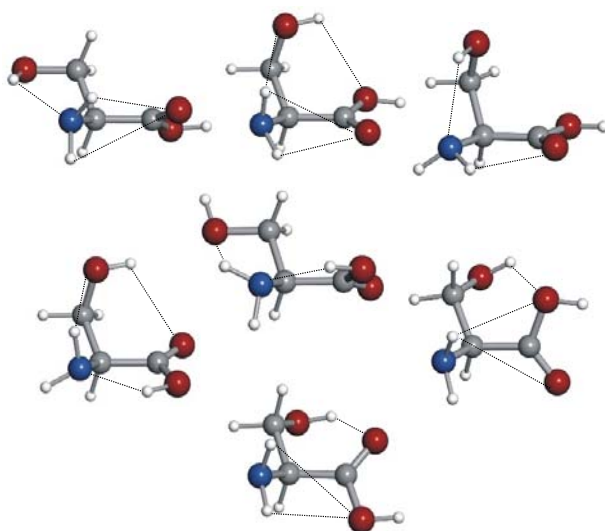
Single biomolecules: conformational panorama

Alanine



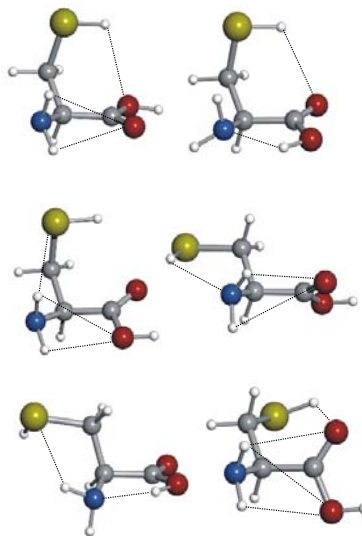
JACS, 126, 11675 (2004)

Serine



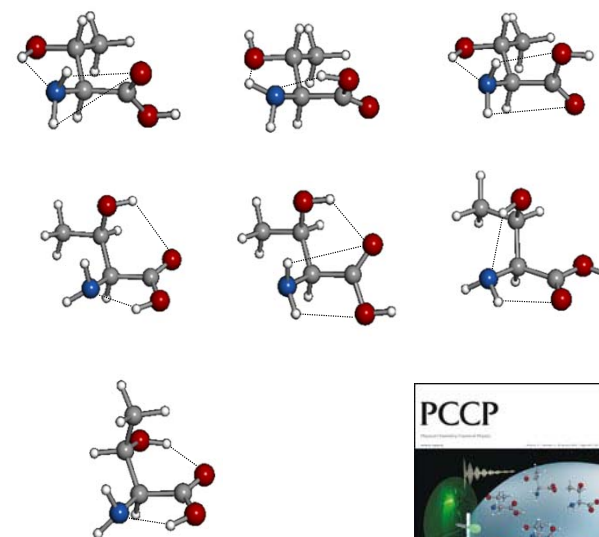
PNAS, 104, 20183 (2007)

Cysteine



Ang.Chem.Int. Ed.
47, 6216 (2008)

Threonine



PCCP 11, 617 (2009)

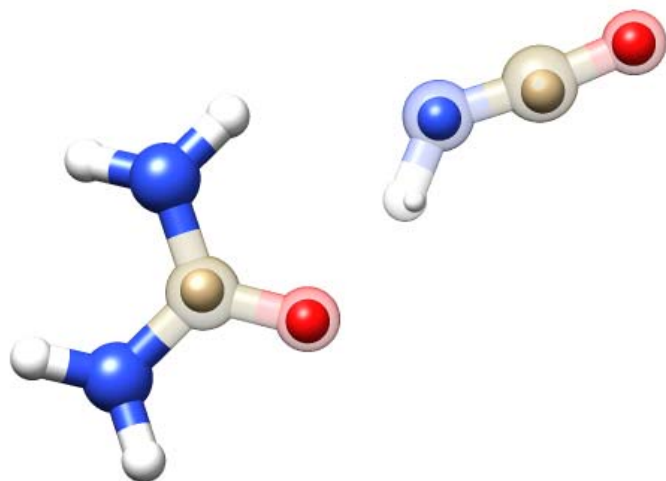
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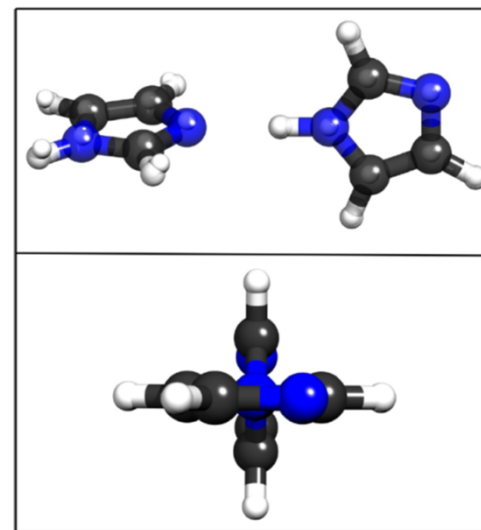
Biomolecules: complex

Urea - Isocyanic acid complex (ISMS: WC07)



N. Walker: to be published (2016)

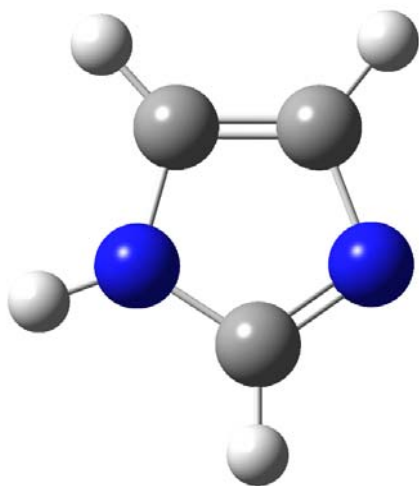
Imidazole dimer (ISMS:WC08)



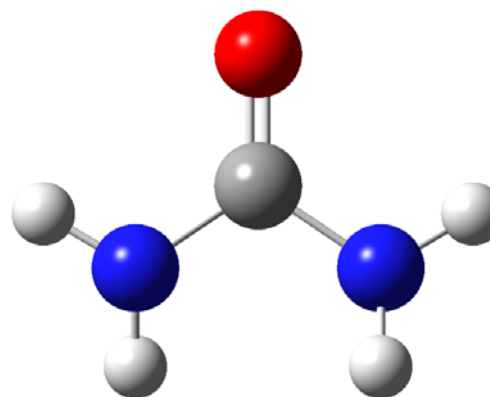
ChemPhysChem, 17, 1154 (2016)

PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Imidazole ... urea complex



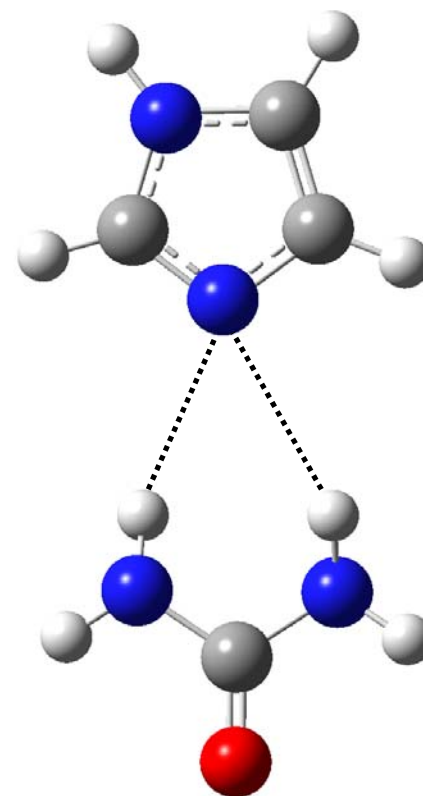
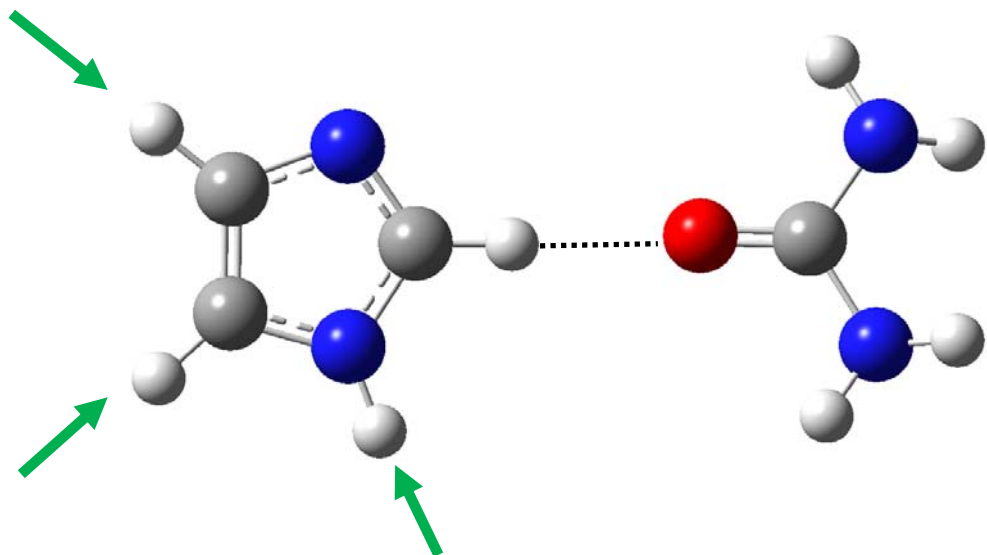
Imidazole ($\text{C}_3\text{N}_2\text{H}_4$: 68.08 g/mol)
mp. $\sim 90^\circ\text{C}$ (white solid)



Urea ($\text{C}_1\text{O}_2\text{N}_2\text{H}_4$: 60.06 g/mol)
mp. $\sim 133^\circ\text{C}$ (white solid)

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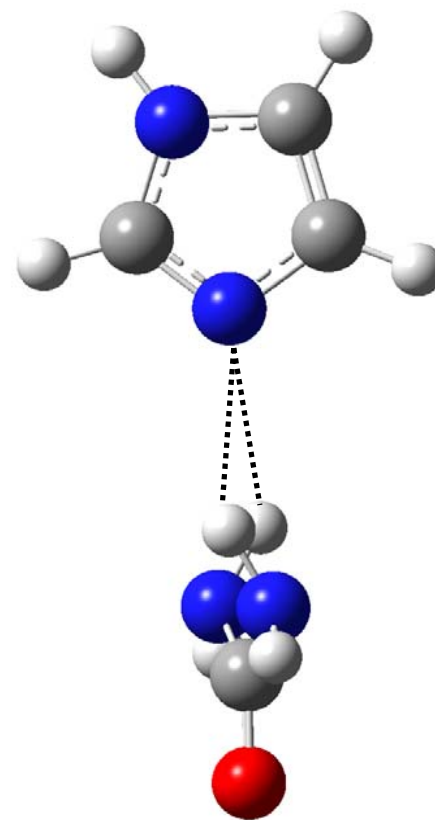
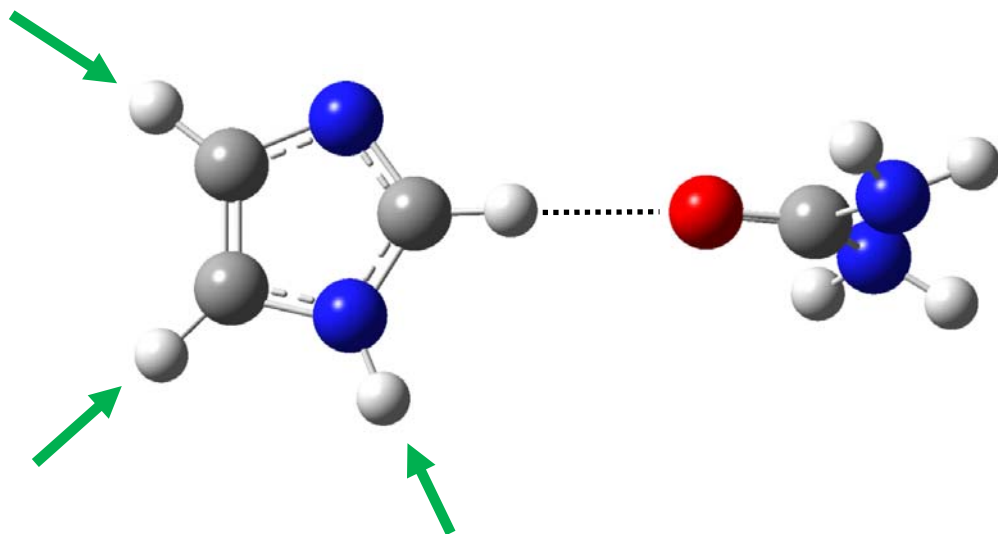
Conformational search - in plane



PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

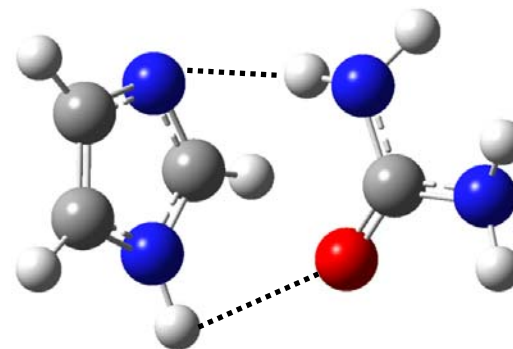
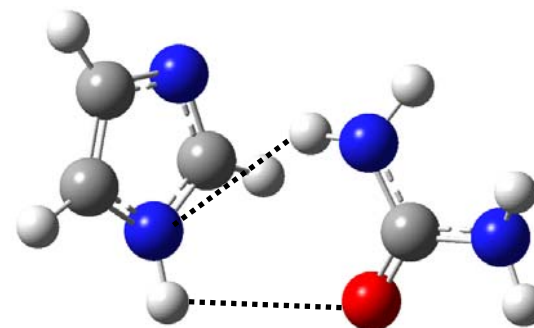
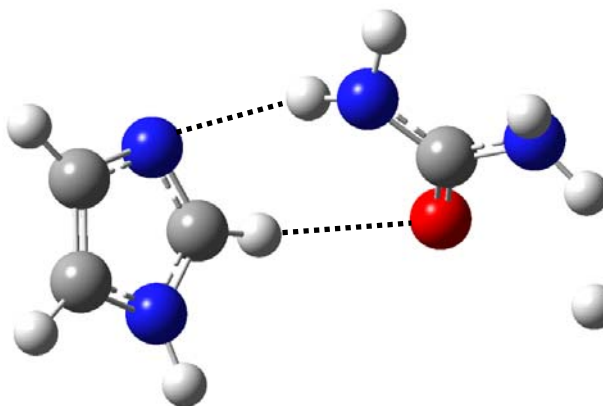
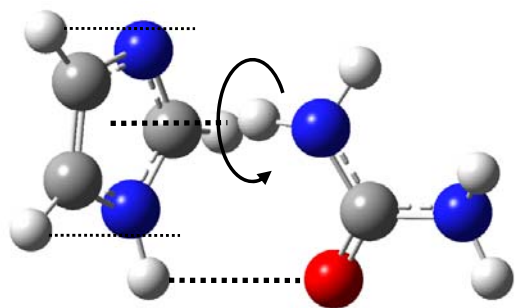
Conformational search

- out of plane / perpendicular molecular planes



PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

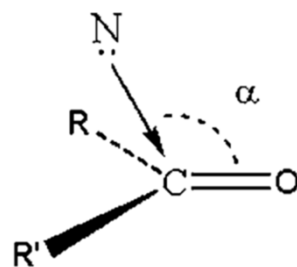
Conformational search - out of plane



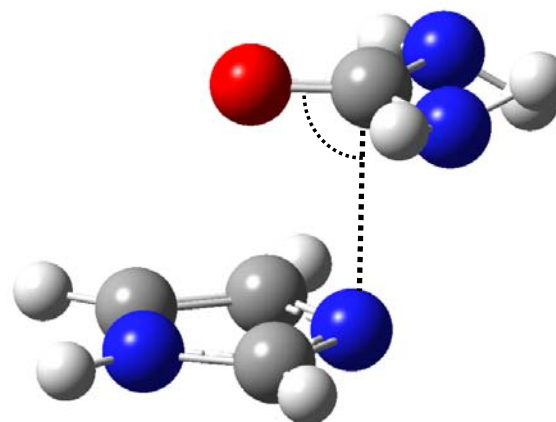
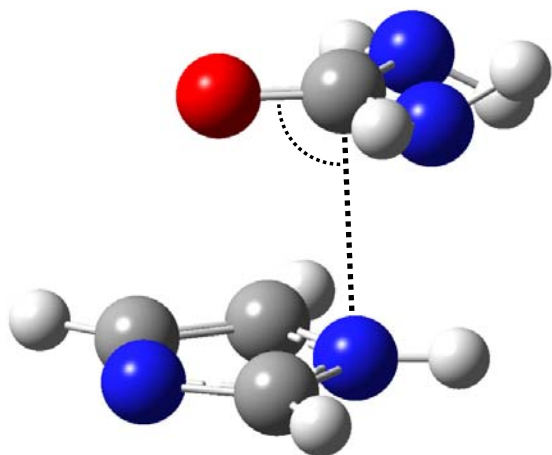
PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Conformational search

- parallel / $n \cdots \pi^*$



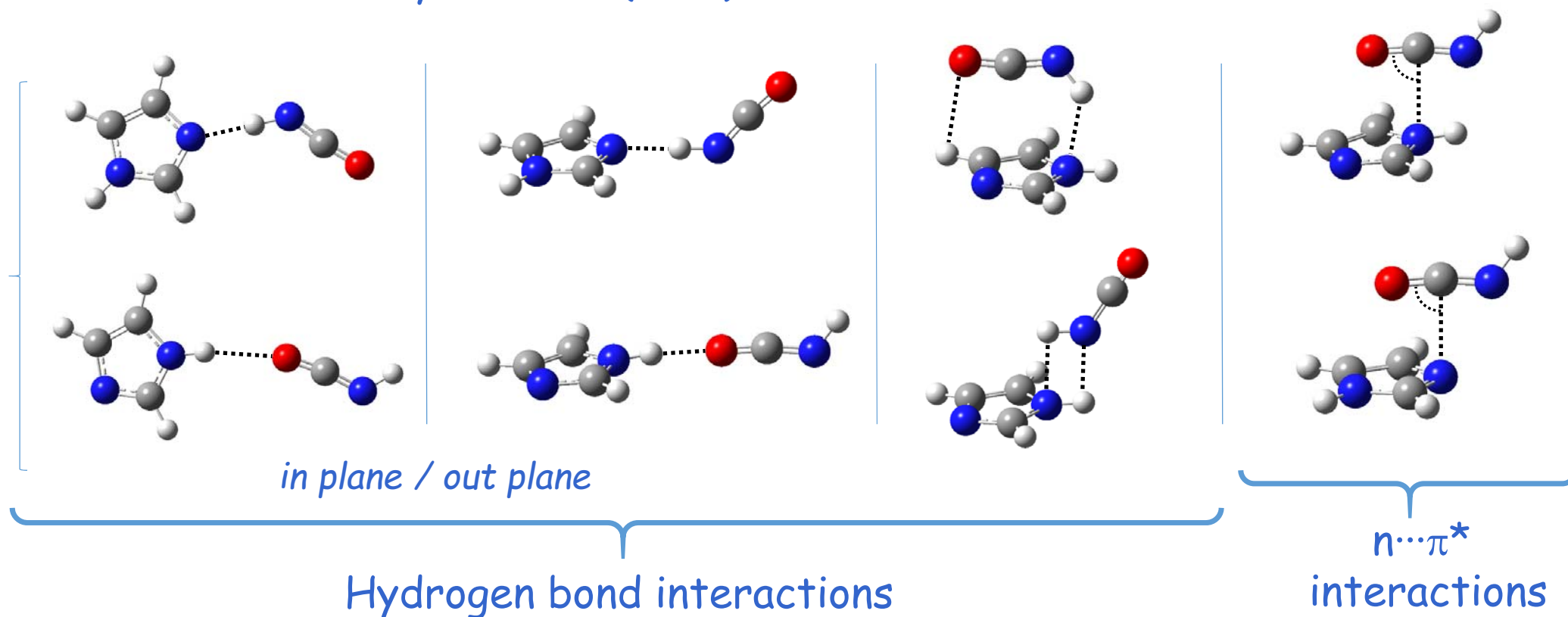
Bürgi – Dunitz trajectory



PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Conformational search

- Imidazole - isocyanic acid (urea)



PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Spectrometer: CP-FTMW

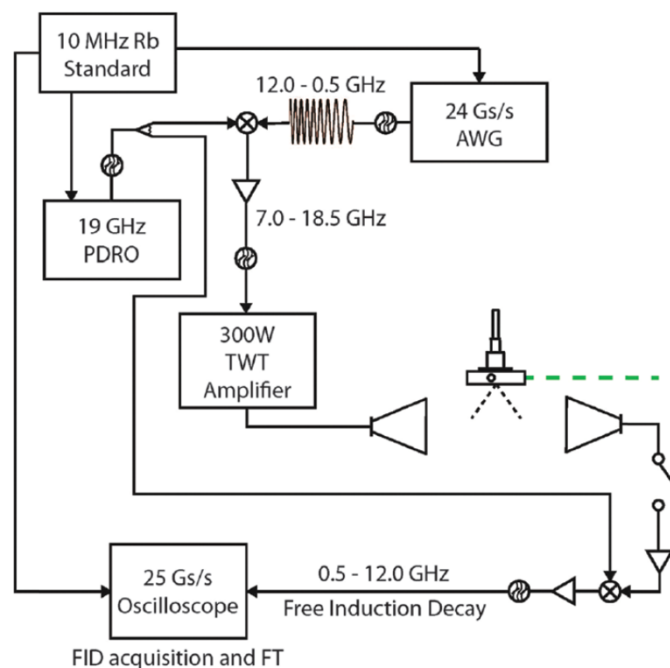
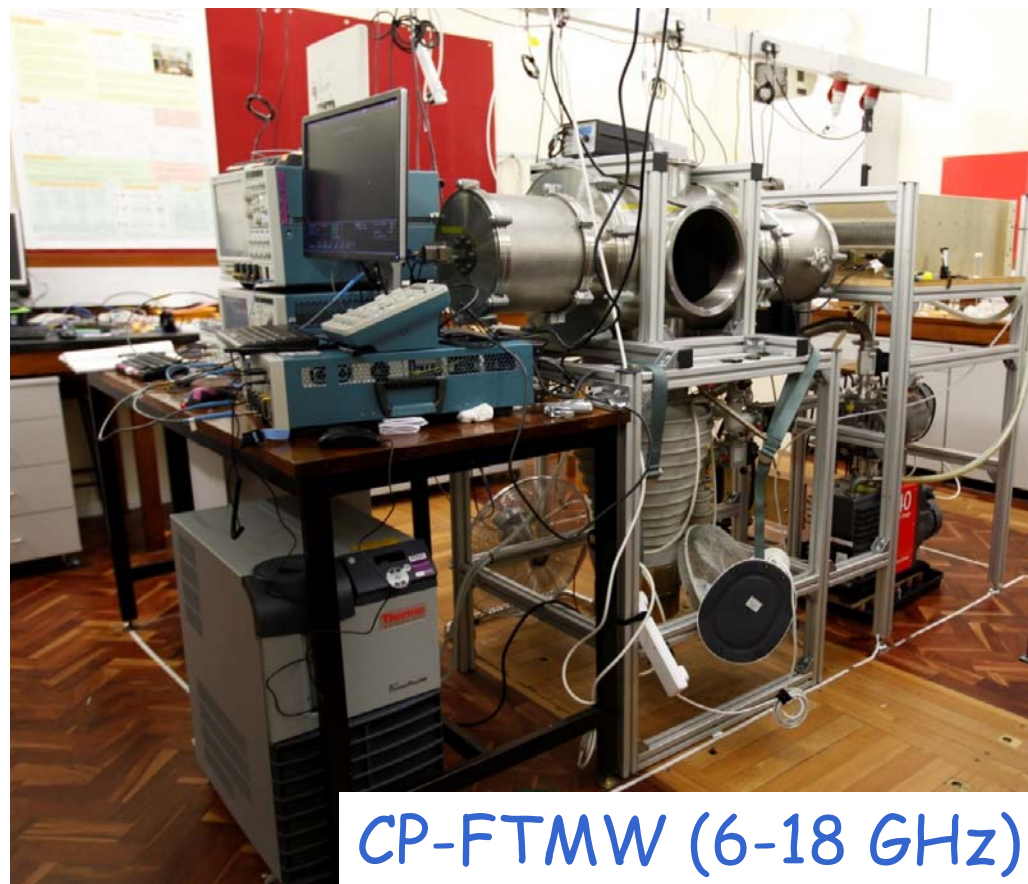


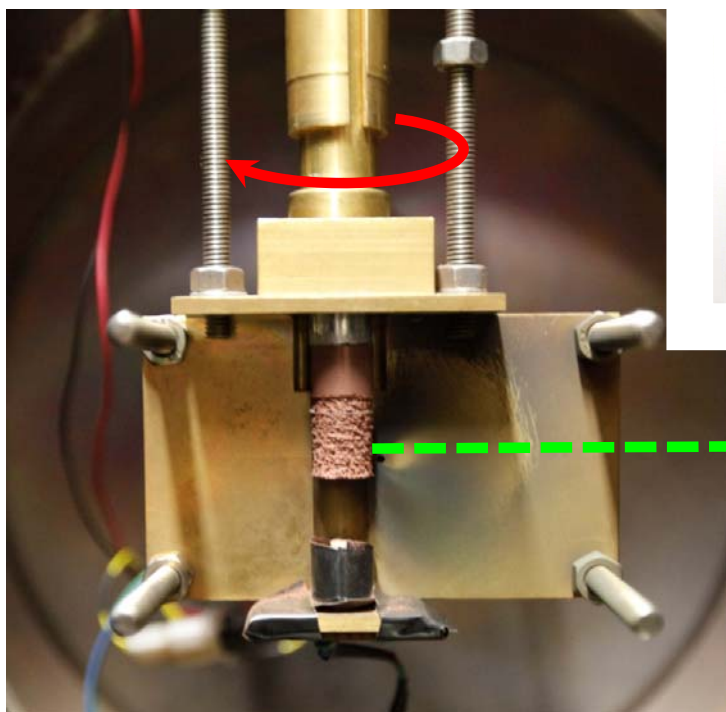
Fig. 1 Schematic of the Newcastle CP-FTMW spectrometer. The green dashed line represents the laser beam path.

PCCP, 16, 25221 (2011)

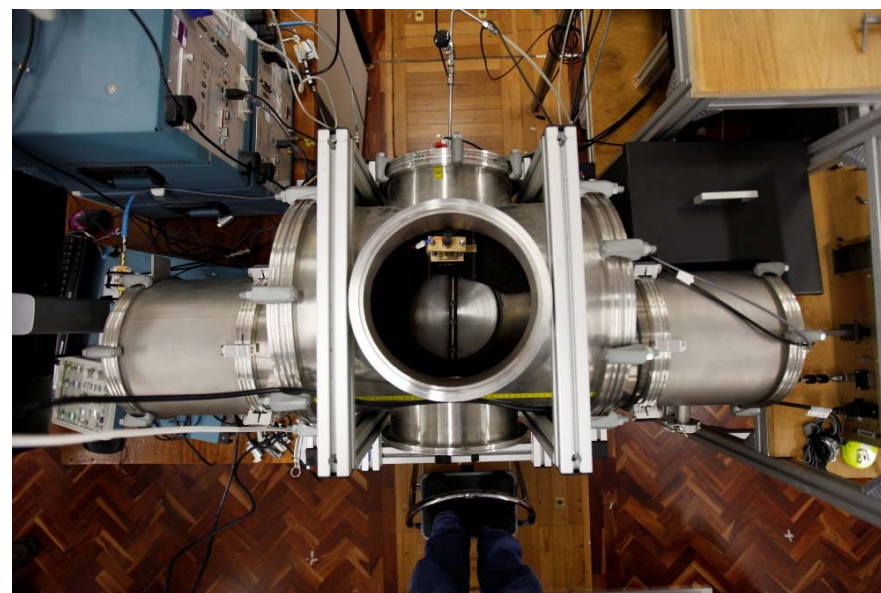
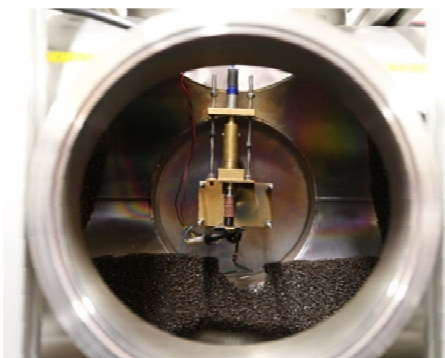


PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Spectrometer: CP-FTMW



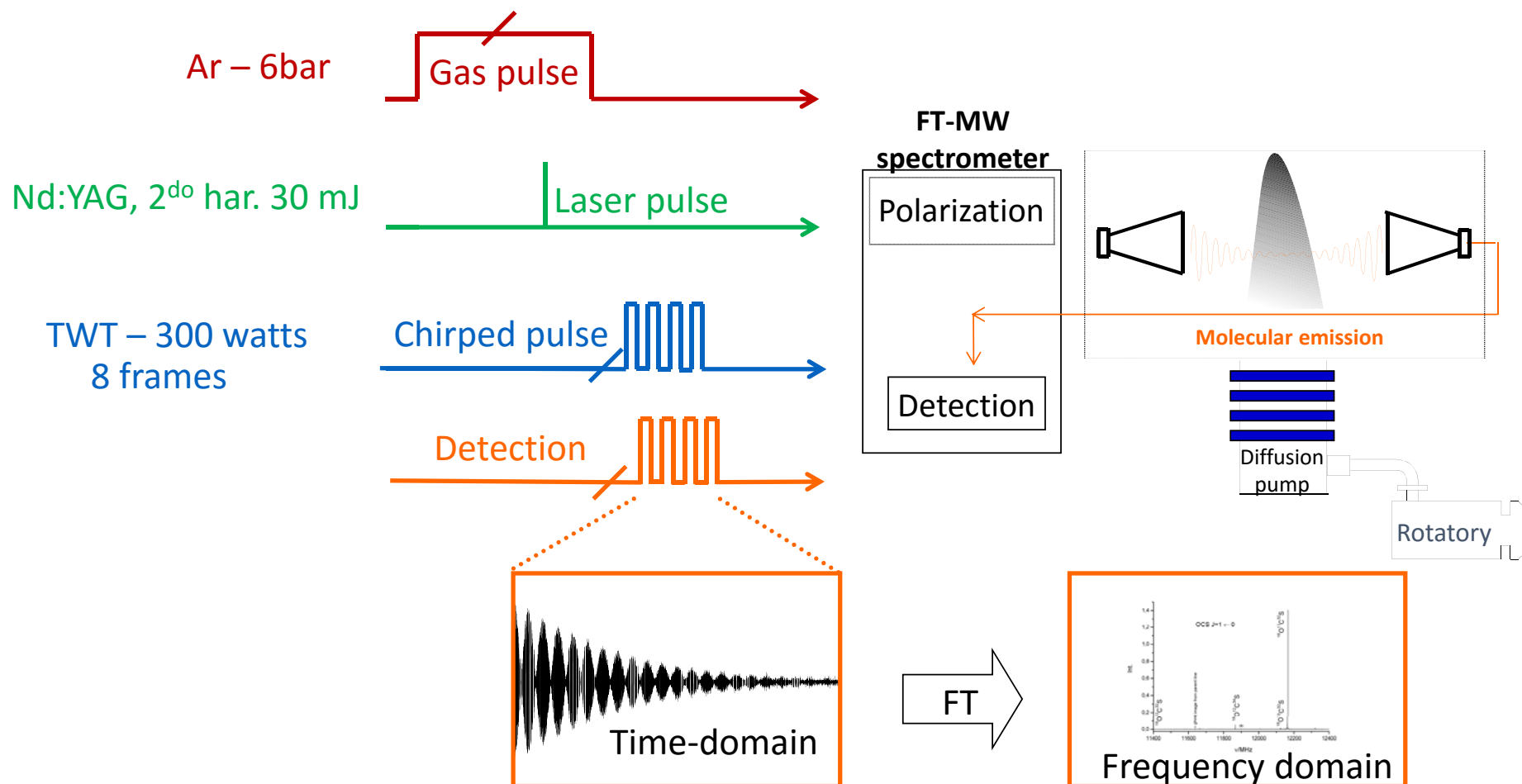
Nd:YAG
2^{do} har. 30 mJ



Laser Vaporization
CP-FTMW (6-18 GHz)

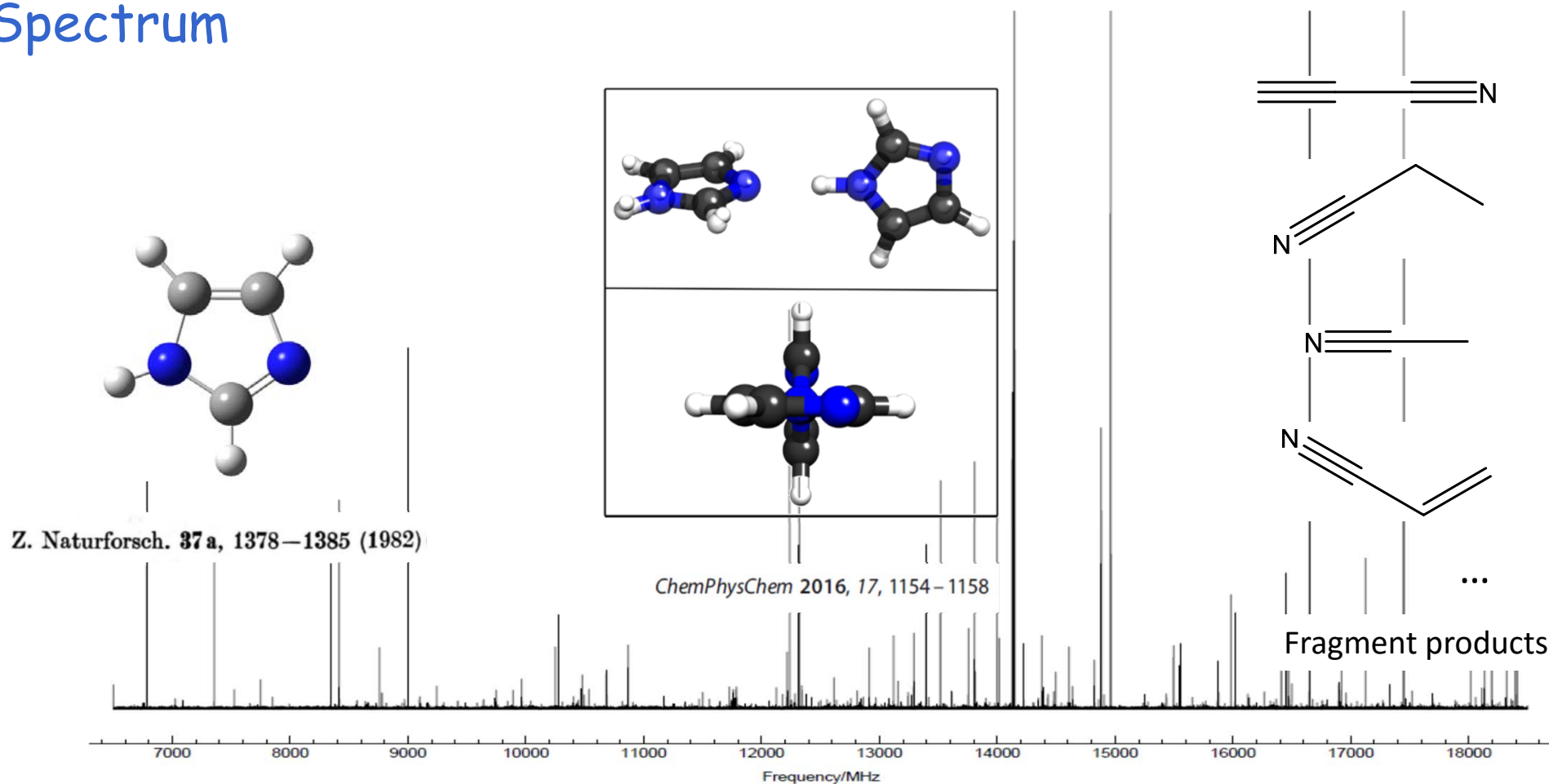
PCCP, 16, 25221 (2011)

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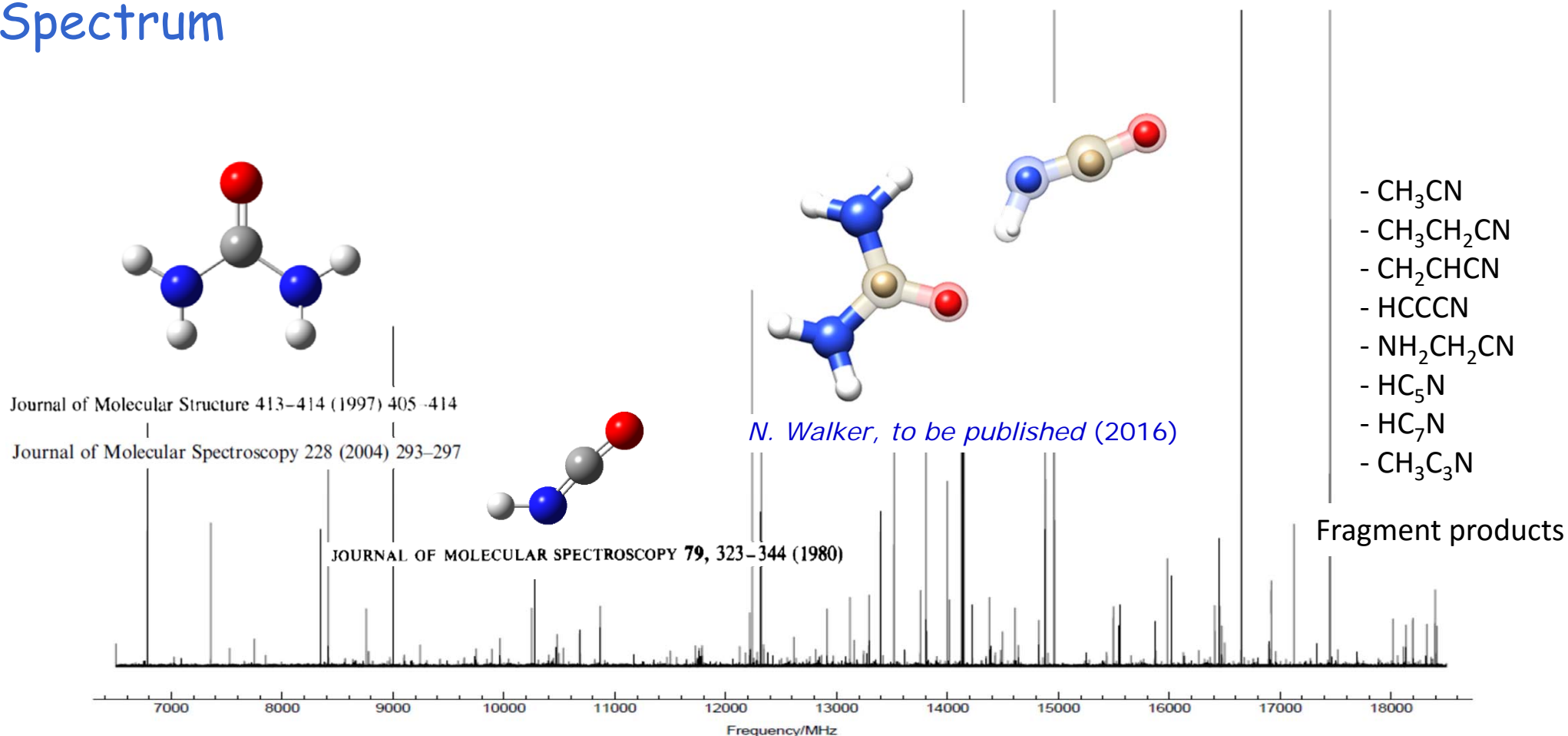
PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Spectrum



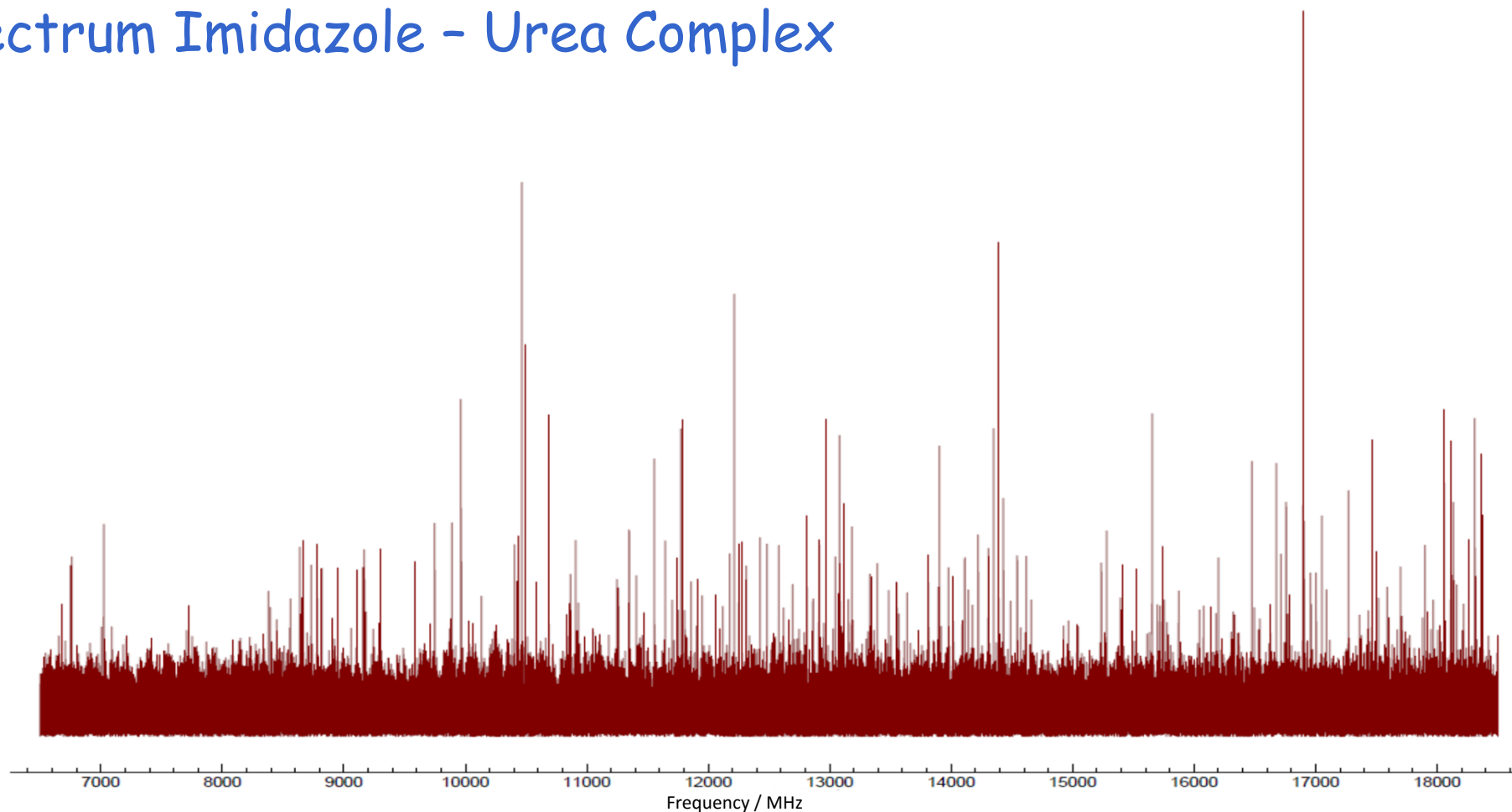
PURE ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF AN ISOLATED COMPLEX OF IMIDAZOLE AND UREA

Spectrum



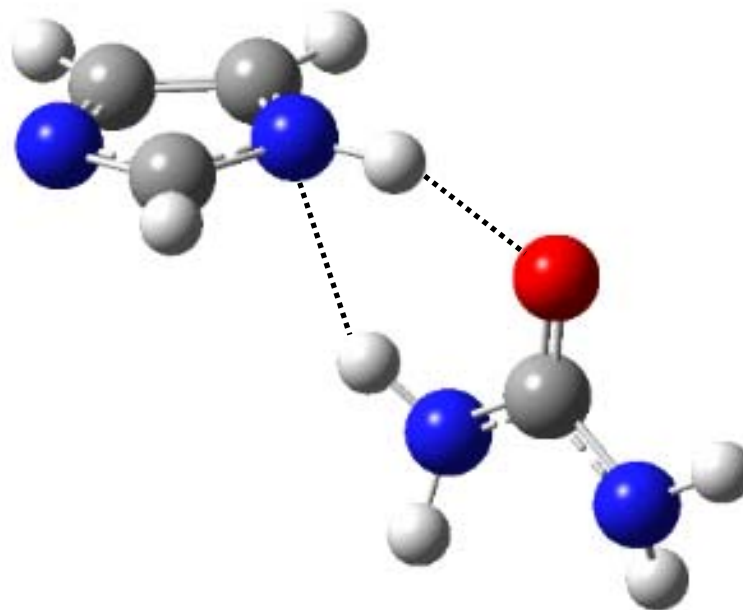
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Spectrum Imidazole - Urea Complex



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Results



MP2/6-311++G(d,p)

Spectroscopy Group

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