

Hydrogen Bonding

Spoken Tutorial Project

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



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We will learn to:



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We will learn to:

- ▶ **Configure Avogadro**



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- ▶ **Show hydrogen bonding in molecules**



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- ▶ **Show hydrogen bonding in molecules**
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- ▶ **Show dipole moments in molecules**



System Requirement



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- ▶ **Ubuntu Linux OS v 14.04**



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- ▶ **Avogadro version 1.1.1**



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- ▶ **Avogadro version 1.1.1**
- ▶ **Working Internet connection**



Pre-requisites



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► Avogadro interface



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- ▶ Structures used in this tutorial are provided as code files for your reference



Quality



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High quality rendering:



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- ▶ is set for printing and publishing images



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- ▶ is set for printing and publishing images
- ▶ uses more CPU power



Significance of Hydrogen Bonding



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- ▶ *determine unique solvent capabilities of water & stabilize crystal structure of ice*



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Hydrogen bonds:

- ▶ *determine unique solvent capabilities of water & stabilize crystal structure of ice*
- ▶ *hold complementary strands of DNA together*
- ▶ *determine & stabilize structures of proteins & nucleic acids*
- ▶ *involve in the mechanism of enzyme catalysis*



Assignment

1. Show inter molecular Hydrogen bond in Para-hydroxybenzoic acid
2. Nucleobases, adenine and uracil



Dipole Moment



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- ▶ Dipole moment(μ) = charge(Q) * distance of separation(r)
- ▶ Dipole moment is expressed in Debye units



Summary

- ▶ *Configure Avogadro*
- ▶ *Show intermolecular hydrogen bonding in Methanol*
- ▶ *Show intramolecular hydrogen bonding in o-nitrophenol*
- ▶ *Measure length of hydrogen bonds*
- ▶ *Show Force display type in water*
- ▶ *Show dipole moment in HCN and H₂O molecules*



Assignment

1. Show dipole moments for carbondioxide and methyl chloride molecules
2. Show Force Display Type for ammonia molecules



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
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Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Acknowledgements

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- ▶ **It is supported by the National Mission on Education through ICT, MHRD, Government of India**
- ▶ **More information on this Mission is available at <http://spoken-tutorial.org/NMEICT-Intro>**

