

# Create Surfaces

**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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- ▶ **View properties of the molecule**



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- ▶ **Create Van der waals surface**



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**We will learn to:**

- ▶ **View properties of the molecule**
- ▶ **Label the atoms with partial charge**
- ▶ **Create Van der waals surface**
- ▶ **Color the surface according to the electrostatic potential energies**



# System Requirement





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- ## ► Ubuntu Linux OS v 14.04



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- ▶ **Ubuntu Linux OS v 14.04**
- ▶ **Avogadro version 1.1.1**



# Pre-requisites



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## ► Avogadro interface





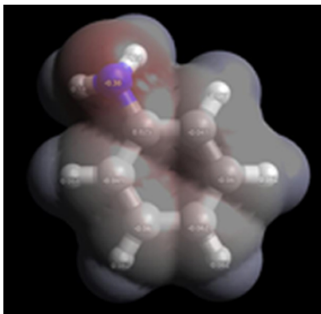
# Electrostatic potential surface

- ▶ **Electrostatic potential surface illustrates charge distributions of the molecule**
- ▶ **They are also used in predicting the behavior of molecules**
- ▶ **By default, areas of high electronegativity are colored in red and least in blue**

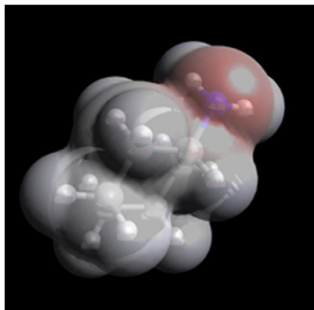


# Electrostatic potential surfaces

Aniline



Cyclohexylamine



Cyclohexylamine is more reactive than Aniline







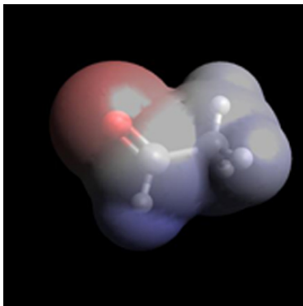
# Assignment

1. Compare the reactivity of acetaldehyde and formamide using electro-static potential surface
2. Label the atoms with partial charge

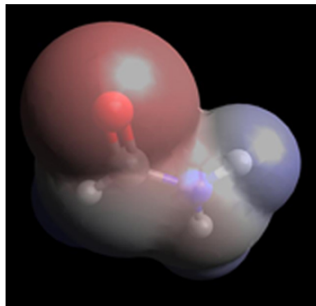


# Electrostatic potential surfaces

Acetaldehyde



Formamide



Acetaldehyde is more reactive than Formamide



# About the Spoken Tutorial Project

- ▶ Watch the video available at [http://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project




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- ▶ It summarises the Spoken Tutorial project
- ▶ If you do not have good bandwidth, you can download and watch it



# 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](mailto:contact@spoken-tutorial.org)
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- The logo of Spoken Tutorial, featuring a stylized orange and black circular design with a white swoosh.



# Acknowledgements

- ▶ **Spoken Tutorial Project is a part of the Talk to a Teacher project**
- ▶ **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>**

