

TPA 2: Chemical formula visualizer

Biomolecules, such as proteins and nucleic acids (DNA and RNA), are involved in every aspect of cellular function. Often times, understanding their structure is key to understanding their function. In the past, crystallographers and biologists created detailed real-world models, called Corey- Pauling-Koltun models, using wooden or synthetic spheres to represent atoms and sticks to represent bonds. Today, these models of protein structures, referred to as space-filling and ball-stick models, have been adopted in computer graphics systems to create visual representations.

Your job is as follows:

Input:

A Chemical Formula eg. C₆ H₁₂ (Cyclohexane).

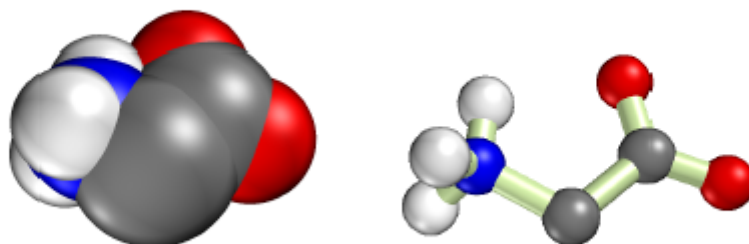
Output:

Visualize it using ball-stick models and Space filled models.

Your demo should produce smooth edges around the intersection of spheres and cylinders, and control view angle at different zoom level.

Figure

1:



Example of Glycine molecule: Left - space-fill model; Right - Ball Stick model

References :

1. Pranav D Bagur, Nithin Shivashankar and Vijay Natarajan, Improved Quadric Surface Impostors for Large Bio-Molecular Visualization, Proceedings of the 8th Indian Conference on Vision, Graphics and Image Processing, 16-19 Dec. 2012, Bombay, India.

2. Molecular Visualization Freeware www.umass.edu/microbio/rasmol/