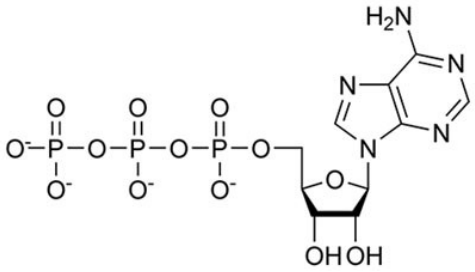
ATP

Adenosine triphosphate (ATP) is a small molecule consisting of an adenine base, a ribose sugar and three phosphate groups.

It is the direct energy source for the majority of cellular functions, such as synthesis of macromolecules, including DNA, RNA and proteins. It also plays an important role in the transport of macromolecules across cell membranes and it is involved in cellular motion and maintenance of the cell structure by facilitating assembly and disassembly of elements of the cytoskeleton. It is present in cytoplasm and nucleus of cells and almost all physiological mechanisms that require energy for their activity obtain it directly from ATP. It works as a chemical battery, storing energy and releasing it instantly when the organism requires it.

Chemical energy is stored in the ester bonds between phosphates, with the great amount of energy (7kcal/mole) in the bond between the middle and the outermost phosphate groups. The terminal phosphate group in particular is frequently split off by hydrolysis, being transferred to other molecules and releasing energy required for synthetic reactions. These covalent bonds are known as “high-energy” bonds.

The chemical structure of ATP is shown here:



For our rendering study, the coordinates for ATP were retrieved from PDB file 1XSC which contains 25 NMR conformations of an enzyme in complex with ATP. We used 20 ATP conformations forming a cluster. The atoms identity and positions were imported into virtual space of Maya as two different groups of particles superposed: the entire ATP is modelled as blobby particles (spheres that are blended together giving the impression of a surface that includes them) and the three phosphate groups are also modelled as overlapping clouds. The movement was realized by setting and key-framing at different moments of time all conformations coordinates as goals for the visible set of particles.

To render visible the surface properties of this hydrophilic molecule with “high-energy” bonds between phosphates we created two different shaders. The first surface shader applied to the entire ATP is a coarse-grained surface (created with displacement) and gives the impression of a molecule that can easily interact with water. The second surface shader created with displacement and high value of incandescence (like an emitting light source) was applied to the three phosphates in order to deliver in a visible way the chemical energy stored in these covalent bonds. RenderMan for Maya was used for rendering these images. For this rendering few ATP molecules are shown in the movie: each one is moving independently both as internal movement and in space (rotation and translation).