Answer on Question #53289 – Chemistry – Inorganic Chemistry

Question:

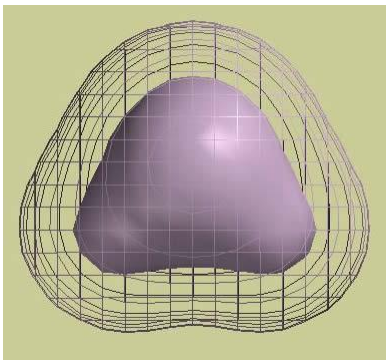
What is the meaning of electron density? Explain with an example.

Answer:

If $P(x,\ y,\ z)\ \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z$ is the probability of finding an electron in the volume element $\mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z$ at the point of a molecular entity with coordinates $x,\ y,\ z$, then $P(x,\ y,\ z)$ is the **electron density** (**ρ**)at this point.

An example

The following picture is a graph of the electron density in a water molecule. The graph consists of two surfaces, a "solid" inner surface and a "mesh" outer surface. Each surface is constructed so that **ρ** (rho) has the *same value* at every point on the surface.



This particular graph is constructed so that **ρ** is 10 times larger on the solid surface than on the mesh surface. In other words, if we randomly select one point (**r**solid) on the solid surface and one point (**r**mesh) on the mesh surface, the value of **ρ** at **r**solid is 10 times larger than the value at **r**mesh. Of course, this also means that it is 10 times more likely that an electron will be at **r**solid than at **r**mesh.

We can also compare the probabilities of finding electrons anywhere on each surface. The probability of finding an electron anywhere on a surface is proportional to **ρ** x A, the electron density multiplied by the area of the surface. It so happens that the area of the solid surface is about 2.5 times *smaller* than the area of the mesh surface. Therefore, it is only about 4 times more likely that an electron will be *somewhere* on the solid surface (4 = 10/2.5).