

electron density function

The electron probability distribution function, ρ , defined as

$$\rho(\mathbf{r}) = n \int \Psi^*[\mathbf{r}(1), \mathbf{r}(2) \dots \mathbf{r}(n)] \Psi[\mathbf{r}(1), \mathbf{r}(2) \dots \mathbf{r}(n)] d\mathbf{r}(2) \dots d\mathbf{r}(n)$$

where Ψ is an electronic wave-function and integration is made over the coordinates of all but the first electron of n . The physical interpretation of the electron density function is that $\rho d\mathbf{r}$ gives the probability of finding an electron in a volume element $d\mathbf{r}$, *i.e.*, electron density in this volume.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1937