

Shape of Model Potentials for a C₆₀ Shell

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Synopsis The spatial distribution of electric charges forming a square well potential has been analyzed. It has been shown that two concentric spheres each with a double layer of charges create the potentials of this type. It has been demonstrated that the phenomenological potentials simulating the potential of C₆₀ shell belong to a family of potentials with non-flat bottoms. A C₆₀ shell potential has been calculated under the assumption that it is formed by the averaged charge density of a neutral atom. It has been shown that this potential has a cusp-shaped form. Two model potentials of that type are proposed and their parameters have been calculated.

Phenomenological approaches on the basis of a rectangular (in the radial coordinate r) potential $U(r)$ for a C₆₀ shell are widely used to describe fullerene-like molecular systems [1]. The C₆₀ shell is formed by a superposition of the positive charge of carbon atomic nuclei and the negative charge of the tightly bound $1s^2$ -electrons and the collectivized $2s^22p^2$ -electrons. The spatial distribution of these charges is defined by the Poisson equation.

$$\frac{d^2}{dr^2}[rU(r)] = 4\pi\rho(r).$$

The solutions of this equation were analyzed for a family of spherically symmetric stepwise potentials (with a flat bottom and parallel potential walls). It was shown that the density of electric charges $\rho(r)$ for these potentials is equal to zero in all space except the epsilon neighborhoods of the inner r_o and outer r_i radii, i.e. at the points where the function $U(r)$ changes discontinuously from zero to $-U_0$ and *vice versa*. Thus, the positive and negative charges of C₆₀ shell can form the rectangular potential well only if one assumes that they are smeared over the surfaces of two concentric spheres and create a two-layer charge sandwich with a gap $\Delta = r_i - r_o$ between layers. This does not appear to correspond to the real structure of the C₆₀.

To obtain more detailed information on the behavior of the function $\rho(r)$ near the borders of potential walls, an exponential-power-law potential [2] was considered. This allows the potential shape to be changed continuously from a cusp-shaped type to a square-well type. It was shown that the potential well with the cusp-shaped bottom corresponds to real molecular

structure of C₆₀, namely the atomic nuclei of the carbon atoms are localized on the sphere with radius R , while the electronic clouds border on the positively charged sphere inside and beyond it, i.e., the C₆₀ shell charges form a three-layer charge sandwich. Here R is the distance between the center of the fullerene cage and nuclei of the carbon atoms.

The electrostatic potential created by the neutral atom charge density averaged over the sphere with radius R was calculated. It was shown that, calculated in such a way, the function $U(r)$ is very well approximated by the Lorentz-like curve, i.e., the potential $U(r)$ has a cusp-shape profile.

This analysis demonstrates that the phenomenological potentials simulating the C₆₀ shell potential should belong to a family of potentials with non-flat bottoms.

Two model potentials for the C₆₀ shell with a cusp-shaped bottom have been considered. The parameters of these potentials were chosen so that the bound state of the negative ion of C₆₀ with affinity energy $\varepsilon \approx 2.65$ eV (as it follows from the data of UV spectroscopy) could exist in these potential wells.

It should be noted that while the potentials with flat bottoms (particularly the square well potential) remain usable from a practical viewpoint as a fitting potential, it is necessary to keep in mind that the actual potential of C₆₀ has a cusp-shaped form.

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References

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