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Model Potentials for a C_{60} Shell A.S. BALTENKOV, Inst. of Ion-Plasma and Laser Tech., S.T. MANSON, Georgia State University, A.Z. MSEZANE, Clark-Atlanta University — Radial square wells are commonly used to model the potential effects of the C_{60} fullerene molecule [1]. The spatial distribution of electric charges forming such a square well potential has been analyzed. It is shown that this potential is created by two concentric spheres with a double layer of charges. This does not seem to be representative of the actual placement of the carbon nuclei in the molecule. A C_{60} shell potential has been calculated under the more realistic assumption that it is formed by the averaged charge density of neutral carbon atoms. It is further demonstrated that the phenomenological potentials simulating the C_{60} shell potential belong to a family of potentials with a non-flat bottom and non-parallel inner and outer potential walls. Two possible types of C_{60} model potentials are proposed and their parameters have been calculated. However, experiment indicated that the potential does have identifiable (parallel) walls [2]. Thus, we are left with something of a conundrum.

[1] V. K. Dolmatov, Adv. Quantum Chem. 58 13 (2009).

[2] A. Rüdel, R. Hentges, U. Becker, H. S. Chakraborty, M. E. Madjet and J. M. Rost, Phys. Rev. Lett. 89 125503 (2002).

> Steven T. Manson Georgia State University

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