ON THE THREE-DIMENSIONAL WIENER NUMBER. A COMMENT

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"... What happened before that beginning? Another beginning and another beginning? And before that?..."

(E.F. Benson, In the Tube, in Roald Dahl's Book of Ghost Stories, Penguin, Harmondsworth, Middlesex, 1985, p. 65.)

Abstract

The origin of the concept of the three-dimensional Wiener number is discussed.

Recently, we reported in this journal a novel approach to the Wiener number [1]. It is based on the distance matrix [2] in which topographic (geometric) distances rather than topological (graph-theoretical) distances are the input entries. The Wiener number defined in this way is thus a representative of three-dimensional (topographic) molecular descriptors [3]. It has been named the three-dimensional (3D) Wiener number and is denoted by ^{3D}W.

Shortly after the report appeared, we received several letters (e.g. [4]) in which authors pointed out that we were not the first to introduce this concept. A close scrutiny of the literature revealed that there are indeed several papers in which a metric analogue of the traditional (two-dimensional) Wiener number [5] has been mentioned without a detailed analysis. All these contributions [6–10] came from the Burgas Group. However, it appears that Dr. Ovanes Mekenyan from Burgas was the first person to suggest this concept, and a very complete discussion of the 3D Wiener number will be given in his D.Sc. Thesis [11]. On the other hand, our report [1] is the first published work with a detailed mathematical and computational analysis of the 3D Wiener number.

A final point we wish to mention is the following. Since one of us contributed to the work which appeared as refs. [6] and [7], we perhaps confirmed with ref. [1] the Whole Picture Principle of Murphy [12] which states that (some) research scientists are often so wrapped up in their current endeavours that they cannot possibly see the whole picture of anything, including their own research.

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