

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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