

# E D I T O R I A L

## 05C09 & 05C92

With great joy we inform the readers of MATCH COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY that in 2020, in the newest version of MATHEMATICS SUBJECT CLASSIFICATION, the following two new mathematical subjects have been included:

- **05C09 Graphical indices** (Wiener index, Zagreb index, Randić index, etc.), and
- **05C92 Chemical graph theory**

both in the section **05 Combinatorics** and subsection **05C Graph theory**.

By this, for the first time, i.e., since 2020, one of the main directions of applications of mathematics in chemistry has been officially recognized and classified as a regular part of modern-day mathematics. Bearing in mind that MATCH COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY is one of the main journals covering the applications of mathematics in chemistry, we may consider the present update of MSC as a great and significant confirmation of the scientific value of our endeavor. In the same time, this is a major success of all those colleagues who over several decades worked and/or are working in “*chemical topology*”, a field of research considered by many as worthless.

One should recall that, in an earlier version of the MSC, chemistry was classified under section 92 “*Biology and other natural sciences*”, where at its very end, in the subsection 92E, there were the subjects

- **92E10** Molecular structure (graph-theoretic methods, methods of differential topology, etc.)
- **92E20** Classical flows, reactions, etc.
- **92E99** None of the above, but in this section

This reflects the low opinion that mathematicians have/had with regard to what we call “*mathematical chemistry*” and what our journal is concerned with.

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Returning to MSC-2020, it should be pointed out that the name “*chemical graph theory*” seems to have been coined by NENAD TRINAJSTIĆ, and used as the title of his seminal book *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd revised ed. 1992.

Under subject 05C09, the following three topological indices are explicitly mentioned:

- **Wiener index** was put forward in 1947 by 23-year-old HARRY WIENER (1924–1998). Later, Wiener became a psychiatrist and completely abandoned scientific activities.
- **Zagreb index** was put forward in the 1970s. Originally, there were two such indices, whereas later their number further increased. These were initially referred to as the “*Zagreb group indices*”, where under “group” was understood a research team at the “Ruđer Bošković” Institute in Zagreb. The actual authors of the two Zagreb indices are NENAD TRINAJSTIĆ (1936– ) and IVAN GUTMAN (1947– ).
- **Randić index** was put forward in 1975 by MILAN RANDIĆ (1930– ). Note that this year Milan is 90, and he is still active and productive. Congratulations!
- **etc.** in 05C09 stands for the many hundreds of topological indices that are in the focus of interest of present-day mathematical chemists.

**Ivan Gutman**