

ERRATA

The Walk ID Number Revisited [*J. Chem. Inf. Comput. Sci.* 33, 231–233 (1993)] By Wolfgang R. Müller, Klaus Szymanski, Jan V. Knop, Zlatko Mihalić, and Nenad Trinajstić*. The Computer Centre, The Heinrich Heine University, D-40225 Düsseldorf, The Federal Republic of Germany, Faculty of Science and Mathematics, The University of Zagreb, HR-41001 Zagreb, The Republic of Croatia, and The Rugjer Bošković Institute, HR-41001 Zagreb, The Republic of Croatia

Pages 231 and 233. In his recent letter Professor Lu Xu from the Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China, informed us that he could not repeat our results reported as Figures 1 and 2 in our paper. The consequent analysis performed by us has shown that we did not report the self-returning walk ID (SID) numbers in these figures. The error was introduced during the preparation of Figures 1 and 2 when we printed by accident the walk ID (WID) numbers instead of the SID numbers underneath each structure in both figures. Below the corrected Figures 1 and 2 are given that now contain the SID numbers.

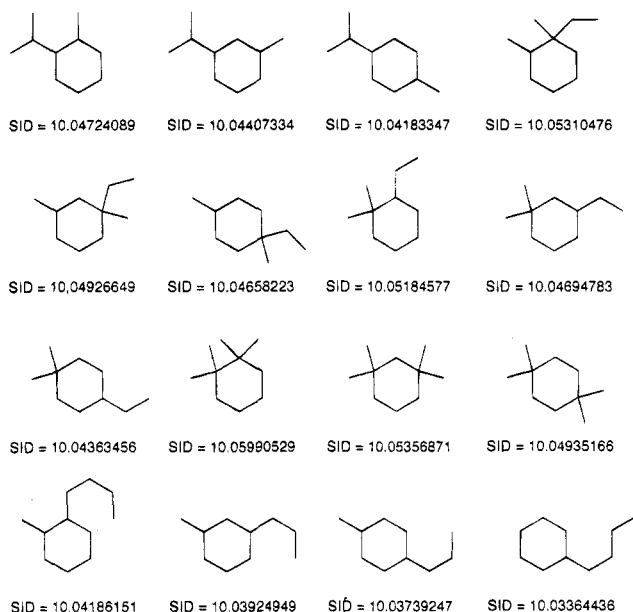


Figure 1. SID numbers for a class of cyclic graphs with 10 vertices and 10 edges.

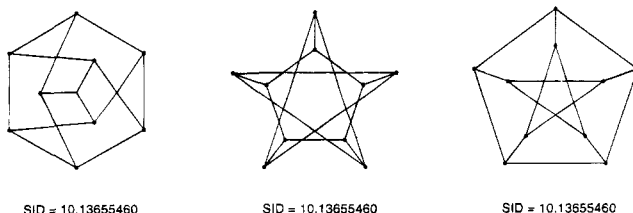


Figure 2. Three representations of the Petersen graph and the corresponding SID numbers.

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A Simplified Algorithm Using Base 5 Numbers To Assign Canonical Names to Cata-Condensed Benzenoid Polybenzenes [*J. Chem. Inf. Comput. Sci.* 34, 637–640 (1994)] By Seymour B. Elk. Elk Technical Associates, New Milford, NJ.

Pages 637–640: As pointed out by Nenad Trinajstić in his paper¹ in this issue (p 759), my earlier paper,² contains the error he detected. Although the mistake noted is in obvious need of correction, it is easily rectified by rotating the molecule (if necessary) so that the incoming vector is progressing horizontally from left to right thus “anchoring” the molecule. We now include in the coding algorithm the proviso that whenever encountering the first polyfilar hexagon in a chosen path one follows the “upper” path before following the “lower”. In other words, this is the same scenario that I noted in an article³ that appeared in 1980 in *MATCH*. In that article, I described the “more than semantical” difference between what I termed a “synthetic” (locally generated and moving) vs an “analytic” (fixed initially and remaining invariant) nomenclature algorithm and noted how a synthetic code would eventually always lead to inconsistency in a large and sufficiently complex system. Using my code with this correction, the upper half of their Figure 7 would be named 114302 and the lower one 114203—which is precisely compatible with the results obtained by their DAST code.

REFERENCES AND NOTES

- (1) Müller, W. R.; Szymanski, K.; Knop, J. V.; Trinajstić, N. A Remark on the Naming of Cata-Condensed Benzenoids with Base 5 Numbers. *J. Chem. Inf. Comput. Sci.* **1995**, 35, 759–760.
- (2) Elk, S. B. A Simplified Algorithm Using Base 5 Numbers To Assign Canonical Names to Cata-Condensed Benzenoid Polybenzenes. *J. Chem. Inf. Comput. Sci.* **1994**, 34, 637–640.
- (3) Elk, S. B. A Nomenclature for Regular Tessellations and its Applications to Polycyclic Aromatic Hydrocarbons. *MATCH* **1980**, 8, 121–158.

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