

In Memory of Professor Ali Reza Ashrafi (1964-2023):  
A Matchless Role Model in Mathematical Chemistry  
in Iran

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With great sorrow, Professor Seyed Ali Reza Ashrafi (1964-2023), the distinguished professor of mathematics at the University of Kashan, and an excellent teacher with brilliant ideas passed away in a car accident on the way home in Kashan on 9 January 2023, when a drunk driver was driving in the wrong direction. As must have been many of his friends and colleagues, we were utterly shocked and unprepared for the news of his sudden death. Two days after the

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accident he was buried in Tehran, the capital of Iran. His passing was not only a great loss for his family and friends but also for the Iranian mathematical community. Let us write about a scientist who was well known not only for his knowledge, but also for his humanity. Professor Ashrafi was born on 10 May 1964 in Tehran. He received his bachelor's degree from the Teacher Training University of Tehran in 1989 and his master's degree from Shahid Beheshti University in 1991. He obtained his Ph.D. degree in computational group theory, under the supervision of Professor Mohammad Reza Darafsheh, from the University of Tehran in 1996. The title of his Ph.D. thesis was "The Irreducible Character Table of the Group  $\text{Aut}(\text{PSL}(5,3))$ ".



Figure 1: Some members of the world academy of Mathematical Chemistry, Slovenia

Professor Ashrafi became a member of the faculty of mathematical sciences at the University of Kashan in 1996. He continued his research work alongside teaching with perseverance and dedication. He was a hardworking scientist and often worked until late at night in his office at the university. In 2005 he became a full professor at the University of Kashan. His interests were in mathematical chemistry, computational group theory, chemical graph theory, finite groups, mathematical physics, mathematical education and history of mathematic.

Professor Ashrafi used the computer algebra system Gap, which was probably unknown to chemists in 2002. In 2008, at his suggestion, the first mathematical chemistry conference was held at Tarbiat Modares University, in Tehran. In 2009, the second mathematical chemistry conference was held at the University of Kashan and it was decided to continue holding these conferences. As many students participated in these conferences, interest in mathematical chemistry in Iran increased significantly. We refer the interested reader to [1] to see how the mathematical chemistry topic started in Iran and the role of Professor Ashrafi in it. It is not really an exaggeration to say that Dr. Ashrafi was the father of Iranian mathematical chemistry.

One of his most important achievements was being a member of international academy of mathematical chemistry. In 2010, Professor Ashrafi was elected as a member of the academy. Also, in 2017, he was selected as the first deputy of the international academy of mathematical chemistry. In addition, Professor Ashrafi was the representative of Iran in two sessions of the

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Figure 2: Page of A.R. Ashrafi in zbMATH (May 2023)

International Congress of Mathematicians in 2010 and 2014. Moreover, he is being included in the list of highly cited researchers of the world in the mathematics field for several years.

During about three decades of professional activity, Professor Ashrafi achieved valuable research and educational achievements, including publishing hundreds of scientific articles in international and national journals, writing more than twenty international books and six Persian books, serving as editor-in-chief of two scientific research journals, i.e., "Iranian Journal of Mathematical Chemistry" (IJMC), and "Mathematics Interdisciplinary Research" (MIR). He was the editor-in-chief of the "Bulletin of Iranian Mathematical Society" (BIMS) for a period of three years. He also being a member of the editorial board of more than ten international journals, reviewing numerous domestic and international journals, being a member of the Iranian Mathematical Society, American Mathematical Society, European Mathematical Society and International Mathematical Chemistry Society, being a keynote speaker at many conferences, serving as scientific secretary and committee member at many domestic and international conferences, and receiving numerous awards during his years of activity. He was the organizer of many conferences in Iran and was a member of the scientific committee of most domestic and foreign conferences.

About the end of 1994, he became interested in the subject of mathematical chemistry and turned to topics such as symmetry and topological indices of molecules. The first article in the field of chemical graph theory, was co-authored by a student from Kashan (Amir Loghman), entitled "PI Index of Zig-Zag Polyhex Nanotubes", see [2]. Although this article was published after Dr. Ahmadi's subsequent articles, Dr. Ashrafi's first article in the field of mathematics and chemistry, co-authored with Dr. Hamedanian, was published in the journal "Croat. Chem. Acta" in 2003. The title of this article was "The Full Non-Rigid Group Theory for Tetraamino Platinum (II)", see [3].

Although this article primarily focused on the molecular symmetry group mentioned above, it can be considered the first article by an Iranian mathematician in the field of mathematics and chemistry. Prior to this, many chemists had published articles in this field. Following

the publication of this article, many other articles were co-authored by Dr. Ashrafi with Dr. Hamedanian and Dr. Darafsheh until 2005. Dr. Ashrafi also co-authored articles in this field with Dr. Vakili-Nezhaad and Dr. Moghani, see [4-8]. Also in 2006, Gholami, Safaei, Ashrafi, and Ghorbani published an article titled "Symmetry of Tetrahydroxycalix[4]Arenes" in the journal "Journal of Serbian Chem. Soc.", see [9]. Additionally, Dr. Ashrafi was also active in the field of group theory, publishing many articles about groups and Cayley graphs. Please note that our evaluation criterion is based on the documentation of the Google Scholar site. There were works that were initiated earlier and were even submitted to journals but were ultimately published after 2006. From zbMATH observed that Alireza has 301 publications since 1995 with 150 coauthors. These articles including 210 articles on the topics of graphs, combinations and chemical graphs, 102 articles on the topics of group theory and generalizations, 74 articles on biology and other natural sciences, 10 articles on statistical mechanics and the structure of matter and 7 articles in lattices and ordered algebraic structures (Figure 2). According to the website of MathSciNet, Dr. Ashrafi's most recent article in group theory was titled "Counting Centralizers of a Finite Group with an Application in Constructing the Commuting Conjugacy Class Graph", see [10]. Also most recent article in mathematical chemistry was titled "On Vertex-Edge and Edge-Vertex Connectivity Indices of graphs" ([11]). The highly cited paper of A.R. Ashrafi is [12]. In this paper, some exact expressions for the first and second Zagreb indices of graph operations containing the Cartesian product, composition, join, disjunction and symmetric difference of graphs presented. Also some of results of this paper applied to compute the Zagreb indices of arbitrary  $C_4$  tube,  $C_4$  torus and  $q$ -multi-walled polyhex nanotorus. His paper entitled "Some new results on distance-based graph invariants" which is one of the his highly cited paper ([13]) considered several distance-based graph invariants such as the Wiener index (half the sum of all inter-vertex distances), the Szeged index (half the sum over all edges  $uv$  of the number of vertices closer to  $u$  than to  $v$  multiplied by the number of vertices closer to  $v$  than to  $u$ ) and the related Schultz and Padmakar-Ivan indices, together with their extensions obtained by replacing one of both vertices by edges in the defining formulas. Also several relations between these indices proved for trees, for the edge graph of a graph and for products of graphs, leading to exact formulas for some indices for some new classes of graphs including Hamming graphs and  $C_4$ -nanotubes. Some extremal value bounds for Wiener and Szeged indices are obtained together with some asymptotic bounds, disproved a conjecture about the Szeged index.

Alireza Ashrafi guided more than 20 Ph.D. students and was literally a unique professor. He never being too busy to set regular time aside for getting together with his students. He was everything that one could hope for in a supervisor, and more. He was a role model in ethics and politeness and these qualities made him very popular and lovely among his colleagues and students.

He loved his homeland and his father's hometown such that he always used the affiliation of Kashan and Iran for his books and articles, and in response to some foreign publications, he answered politely and firmly that "My country is my first love". Because of his love, Kashan's post office unveiled a stamp in a ceremony for the seventh day of Ashrafi's death (Figure 3). Also, Iranian Mathematical Society (IMS) published a special issue of the IMS's Newsletter (Number 173-174) in memory of this mathematician (available at [https://nims.ims.ir/article\\_171930.html](https://nims.ims.ir/article_171930.html)). In this special issue, colleagues and students of the late Prof. Ashrafi have expressed their memories with Alireza.

In conclusion, Professor Ashrafi was a brilliant mathematician, a dedicated teacher, and a valued member of the academic community. His contributions to the field of mathematics have left a lasting impact, and his legacy will continue to inspire future generations of mathematicians. Until the day of his death, he worked continuously with great hope for the future, he had



Figure 3: Stamp of Ashrafi and a photo of International Conference on Math. Chemistry, China, 2016

high expectations for research projects and student dissertations in the future. His presence was attractive and his words were insightful and all these placed Professor Ashrafi one of the outstanding role models for students and teachers. He left behind two daughters named Ghazal and Maryam. His love for not only his family and children, but also his students, friends and colleagues is unforgettable. We are grateful for his contributions and will always remember him with fondness and respect. Alireza used to tell us “there is justice in mathematics! Thus try to be as good as you can in mathematics.” And with this quotation of his we will finish these notes. When we close our eyes, we will always remember him, walking in some deep thoughts, with almost white hair, with loud laughs, quiet and lovely voice, always ready to pour out formulas, ideas and problems. The our world of mathematics will be never the same without him.

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