GRAPHS MAXIMIZING THE GENERALIZED COMPLEMENTARY SECOND ZAGREB INDEX

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The complementary second Zagreb index exhibits strong correlations with physicochemical properties and effectively models the heat of vaporization, particularly its normalized form, in compounds such as octanes and benzenoid hydrocarbons. We confirm a conjecture by Furtula and Oz [1] concerning graphs that maximize the second complementary Zagreb index.[2] We further extend this result to a broader class of parameter-dependent indices, which we term the *generalized complementary second Zagreb index*. We prove that all indices within this class attain their maximum on complete split graphs. Additionally, we analyze the behavior of the clique order in extremal graphs [2,3]. For the classical second complementary Zagreb index, we derive an explicit formula for the maximum value, thereby confirming the conjectured result of Furtula and Oz [1].

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2024-05-2130.

[1] B. Furtula, M. S. Oz, *MATCH Commun. Math. Comput. Chem* **2025**, 93, 247–263.

[2] S. Majstorović Ergotić, T. Došlić, *MATCH Commun. Math. Comput. Chem* **2026**, 95, 265–283.

[3] S. Stevanović, D. Stevanović, *MATCH Commun. Math. Comput. Chem* **2026**, 96, 43–52.