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Séminaire conjoint CIRRELT / CIMMUL

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DETERMINING OPTIMAL MOLECULES VIA A POLYHEDRAL DESCRIPTION OF CHEMICAL GRAPHS

Abstract: A chemical graph is a simple, connected graph of maximum degree 3 or 4 (depending on the context). Such graphs represent molecules, where vertices are associated to atoms and edges to chemical bonds. Degree-based topological indices play a fundamental role in mathematical chemistry by capturing the structural properties of molecules and predicting their physicochemical behavior. These indices are calculated as the sum of the edge weights of the chemical graph, each edge having a weight defined by a formula that depends only on the degrees of its endpoints.

Numerous scientific papers have been published with the primary objective of characterizing chemical graphs that optimize (maximize or minimize) one of these degree-based topological indices. Restricting our attention to chemical graphs with maximum degree at most 3, we show that whatever the degree-based topological index (more than fifty have already been defined, and new ones are proposed regularly), it is sufficient to evaluate at most 16 chemical graphs to determine an optimal one. This follows from a complete polyhedral description of all chemical graphs with n vertices, m edges and maximum degree at most 3. Our main results is that whatever n and m, the associated polytope has at most 16 extreme points, and at least one of them corresponds to the structure of an optimal molecule.

Short Biography: Alain Hertz graduated in mathematical engineering and obtained a Ph.D in operations research at the École Polytechnqiue Fédérale de Lausanne. Since 2001, he is professor at the department of mathematics and industrial engineering at Polytechnique Montréal, Canada. He is also member of the multi disciplinary GERAD research group that includes nearly sixty researchers and experts in operations research and discrete mathematics. He is the author of around 200 scientific publications and 4 detective novels. His main research domains are combinatorial optimization, graph theory, algorithmics, and the development of decision aid systems for scheduling and distribution problems.

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23 octobre / October 23rd, 2025
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Responsable / Organizer:
Pierre Miasnikof

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