

## Notice of the Final Oral Examination for the Degree of Doctor of Philosophy

of

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MSc (University of Victoria, 2021) BASc (Quest University Canada, 2018)

"Graph-theoretic and chemical properties of anionic fullerenes"

Department of Mathematics and Statistics

Tuesday, April 15, 2025 9:00 A.M. **Clearihue Building** Room B019

Supervisory Committee:

Dr. Gary MacGillivray, Department of Mathematics and Statistics, UVic (Co-Supervisor) Dr. Wendy Myrvold, Department of Mathematics and Statistics, UVic (Co-Supervisor) Dr. Jon Noel, Department of Mathematics and Statistics, UVic (Member) Dr. Peter Loock, Department of Chemistry, UVic (Outside Member)

External Examiner:

Dr. Nino Bašić, Department of Information Sciences and Technologies, University of Primorska

Chair of Oral Examination: Dr. Marco Cozzi, Department of Economics, UVic

Dr. Robin G. Hicks, Dean, Faculty of Graduate Studies

## Abstract

A *fullerene* is an all-carbon molecule with a polyhedral structure where each atom is bonded to three others and each face is either a pentagon or a hexagon. Fullerenes correspond to cubic planar graphs whose faces have sizes 5 or 6. The *p*-anionic Clar number  $C_p(G)$  of a fullerene *G* is equal to p + h, where *h* is maximized over all choices of p + h independent faces (*p* pentagons and *h* hexagons) the deletion of whose vertices results in a graph that admits a perfect matching. This definition is motivated by the chemical observation that pentagonal rings can accommodate an extra electron, so that the pentagons of a fullerene *p*-anion compete with the hexagons to host 'Clar sextets' of six electrons, and pentagons preferentially acquire the excess electrons of the anion.

Tight upper bounds are established for the *p*-anionic Clar number of fullerenes for p > 0. The upper bounds are derived via graph theoretic arguments and new results on minimal cyclic-*k*-edge cuts in *IPR fullerenes* (fullerenes that have all pentagons pairwise disjoint). These bounds are shown to be tight by infinite families of fullerenes that achieve them.

A fullerene G is said to be *k*-anionic-resonant if the deletion of the vertices of any k independent pentagons in G results in a graph that admits a perfect matching. We prove necessary and sufficient conditions for a fullerene to be 2-anionic-resonant. This result is used to prove that all fullerenes have a non-zero 2-anionic Clar number.

Chemical aspects of the anionic Clar model and its utility are also explored in this work. These include the central question of the general comparison between predictions of the anionic Clar model and qualitative molecular-orbital theory for relative stability of charged fullerenes. Hückel accounts of stability, including the chemical concepts of total  $\pi$  energy, resonance energy, HOMO-LUMO gap and Coulson bond order, and the unified perspective offered by CSI (the recently defined *charge stabilization index*) are used in this analysis.