



The Algebra of Organic Synthesis: Green Metrics, Design Strategy, Route Selection, and Optimization

John Andraos

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The Algebra of Organic Synthesis combines the aims, philosophies, and efforts involved in organic synthesis, reaction optimization, and green chemistry with techniques for determining quantitatively just how "green" synthesis plans are. It provides the first complete quantitative description of synthesis strategy analysis in the context of green chemistry and reaction optimization.

Providing what is perhaps the first complete description of synthesis strategy analysis, this book:

- Explores quantitative material efficiency for synthesizing molecules, including 1,000+ worked out synthesis plans to important target molecules
- Explains, in simple language, the most useful ideas in graph theory that have direct application in organic synthesis
- Reinforces the value of simple mathematical analysis in organic synthesis to help any synthetics or process chemist understand presented ideas and apply them to their own work
- Illustrates concepts with example target plans to classical targets that are considered milestones in synthetic chemistry, from pharmaceuticals, industrial commodity chemicals, dyestuffs, agrichemicals, flavorings, natural products, and molecules of theoretical interest

The accompanying CD-ROM includes a reproduction of the tables in the book, with direct electronic links to files for all plans. Files contain a list of references for each plan, including secondary references for the synthesis of starting materials if applicable. Ancillary materials also include a complete synthesis scheme with fully balanced chemical equations, a synthesis tree, a summary of green metrics parameters, a target bond map and list of reagents that end up in the target molecule, and a series of graphs that offer a visual depiction of the plan performance.

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