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Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

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evolving topics like density functional theory, continuum solvation models, and computational thermochemistry brought firmly up-to-date

carefully guides the reader through key equations, providing background information and placing each in context.

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