

The Development of Computational Chemistry

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In the broadest sense, theoretical and computational chemistry may be thought of as being any aspect of chemistry that does not involve direct experimentation or observation of chemical phenomena. Theoretical chemistry provides the framework for making predictions about experimental observations and for explaining chemical phenomena involving atoms, molecules, and materials. Computational chemistry uses computers to apply the methods of theoretical chemistry to a broad range of topics in chemistry. In this talk I will trace the development of computational chemistry as a natural consequence of the development of digital computers. The importance of theoretical chemistry was recognized long before the terms theoretical and computational chemistry entered the language of chemists. My account will begin with the awarding of the 1901 Nobel Prize in Chemistry to Jacobus Henricus van't Hoff and will trace some of the major advances that followed.