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0521839068 - Van der Waals Forces: A Handbook for Biologists, Chemists, Engineers, and Physicists

V. Adrian Parsegian

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VAN DER WAALS FORCES

This should prove to be the definitive work explaining van der Waals forces, how to calculate them and to take account of their impact under any circumstances and conditions. These weak intermolecular forces are of truly pervasive impact, and biologists, chemists, physicists, and engineers will profit greatly from the thorough grounding in these fundamental forces that this book offers. Parsegian has organized his book at three successive levels of sophistication to satisfy the needs and interests of readers at all levels of preparation. The Prelude and Level 1 are intended to give everyone an overview in words and pictures of the modern theory of van der Waals forces. Level 2 gives the formulae and a wide range of algorithms to let readers compute the van der Waals forces under virtually any physical or physiological conditions. Level 3 offers a rigorous basic formulation of the theory.

V. Adrian Parsegian is chief of the Laboratory of Physical and Structural Biology in the National Institute of Child Health and Human Development. He has served as Editor of the *Biophysical Journal* and President of the Biophysical Society. He is happiest when graduate students come up to him after a lecture and ask hard questions.

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ENGINEERS, AND PHYSICISTS**

V. Adrian Parsegian

National Institutes of Health



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PREFACE

“What is this about entropy really decreasing?” I didn’t know how to answer my family, worried by some preposterous news report. My best try was, “I don’t know the words that you and I can use in the same way. I tell you what. Let me give you examples of where you see entropy changing, as when you put cream and sugar in coffee. You think a while about these examples. Then we can answer your question together.”

That was part of the dream to which I woke the morning I was to write this welcome to readers. I connected the dream with the way my friend David Gingell came to learn about van der Waals forces 30 years ago. He began immediately by computing with previously written programs, then improved these programs to ask better questions, and finally worked back to foundations otherwise inaccessible to a zoologist.

Written using the “Gingell method,” this book is an experiment in what another friend called “quantum electrodynamics for the people.” First the main ideas and the general picture (Level 1); after that, practice (Level 2); then, finally, the bedrock science (Level 3), culled and rephrased from abstruse sources. This is a strategy intended to defeat the fear that stops many who need to use the theory of van der Waals forces from taking advantage of progress over the past 50 or 60 years.

Many excellent physically sophisticated texts already exist, but they remain inaccessible to too many potential users. Many popular texts simplify beyond all justification and thus deprive their readers of an exciting peek into the universe.

Although intended to be popular, the present text is not sound-bite science. There are no skimmable captions, side boxes, or section headings intended to spare the reader careful thinking. See this text as a set of conversations-at-the-blackboard to support the tables of collected or derived formulae suitable for knowing application. Peter Rand, with whom I have done more science than with any other person, says I rely heavily on the intelligence of my readers. Yes, I accept that. I hope that I can also rely on readers’ motivation and pleasure in learning about a subject that reaches into all the basic sciences and into several branches of engineering.

As the book grew, I wondered if there could be more examples of applications, more details on the mechanics of computation, more exhaustive review of works in progress.

Regarding applications: I have found that many people are already eager to learn about van der Waals forces because of prior need or interest. I prefer to devote space to satisfy those needs.

Regarding computation: Spectroscopy and data processing are finally catching up with possibilities revealed by basic physical theory; any detailed How-To given here would soon be obsolete.

Regarding works in progress: “*Perfection can be achieved if a limit is accepted; without such a boundary, the end is never in sight.*” These painful phrases from Mary McCarthy’s *The Stones of Florence* can burden any author who is worrying about what not to include, where to stop. The “maybe-include” list—excited states, ions in solution, atomic beams, weird geometries, etc.—grew faster than I could rationally consider. The only option was to reassure myself that, after absorbing what has been written, readers would be newly able to learn on their own. In that spirit of learning to learn, this book is designed. Through this design, I hope now to learn from my readers.

The *Prelude* gives the kind of too-brief summary and overview students might get from their pressured professors—history, principles, forms, magnitudes, examples, and measurements.

Level 1, a word-and-picture essay, tells the more motivated readers what there is for them in the modern theory. After the *Prelude*, it is the only part of the book best read through consecutively.

Level 2 is the doing.

Its first part, *Formulae*, examines the basic forms in a set of tables and essays that explain their versions, approximations, and elaborations. The formulae themselves are tabulated by geometry and physical properties of the interacting materials. (Take a look now. Pictures on the left; formulae on the right; occasional comments at the bottom.)

The second part, *Computation*, advises the user on algorithms as well as ways to convert experimental data into grist for the computational mill. It includes an essay on the physics of dielectric response, the aspect of van der Waals force theory that needlessly daunts potential users.

Level 3, the basic formulation, was the easiest part to write but is probably the most difficult to read. I put it last because people have a right to know what they are doing, though they need not be pushed through derivations before learning to use the theory. It is, as I imagined in the dream with my family, better to stir the coffee and have a few sips before getting into the principles of coffee making.

This brings me to think of a far more learned group of friends and fellow coffee drinkers with whom I have been lucky to study this subject (none of whom is responsible for inevitable errors or shortcomings in this text). Among them:

Barry Ninham, my original collaborator; our high moment together set our paths of learning over the next decades and founded lifelong friendship; Aharon Katzir-Katchalsky and Shneior Lifson, wise, shrewd, inspiring teachers who introduced me to this subject and who guided my early scientific life; George Weiss, my one-time “boss” who made sure that I always had complete freedom, whose corny jokes and mathematical wit have nourished me for decades; Ralph Nossal, steady friend of forty years, who has reliably provided wise advice on book writing, bike riding, and much else; Rudi Podgornik, whose “you’re the one to do it” kept me doing it, and whose fertile

PREFACE

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And David Gingell (1941–1995). I wish I could will myself another dream, talking with David:

Here is the book you asked me to write 30 years ago. It is not as good as it would have been after your unpredictable comments. There were not the laughs we would have had while I was writing. The book misses you. So do I. Still, it is from working with you that I wrote as I did.

From me.

For you.