

**Bartell L S.** Molecular geometry: bonded versus nonbonded interactions.  
*J. Chem. Educ.* 45:754-67, 1968.  
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Forces acting within a molecule are analyzed in the light of empirical and theoretical evidence. Procedures are outlined for incorporating elements of two contrasting approaches into a practical treatment of molecular properties, and the route to future progress is forecast. [The SCI® indicates that this paper has been cited in over 155 publications since 1968.]

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When I began my academic career in the mid-1950s, chemists paid only superficial attention to the structural consequences of the space-filling characteristics of atoms. Chemists assumed that molecular shapes are governed by certain quantum principles loftier than mere steric interactions. It took the stubbornness of my first graduate student at Iowa State University to provide evidence against accepted dogma.

Russell Bonham was brilliant and eager to grapple more intimately with molecules than would have been possible in the projects I first proposed. In desperation, I suggested determining some molecular structures with borrowed apparatus. As luck would have it, the bond angles in the first molecule we examined deviated from the values expected according to the quantum notions of the day. After a great deal of confusion, we suddenly realized that the discrepancy could be easily understood in terms of repulsions between nonbonded atoms.

Over the next few years, more and more evidence came to light suggesting the importance of nonbonded interactions. New ef-

fects were predicted, then measured. For several years, my papers invoking the nonbonded concept met with unrelenting referee hostility. Publication of several key papers was delayed by well over a year, and two or three papers were rejected outright by the first editors they were submitted to. Leading chemists ridiculed my ideas in public forums and in private correspondence, and I developed a certain notoriety that actually made me more attractive to organizers of some symposia. Gradually, however, my ideas began to be tolerated.

In the mid-1960s when I moved to the University of Michigan, another gifted student made a major advance. Jean Jacob applied powerful new computer techniques to develop a quantitative expression of these ideas. Her first paper was one of the founding formulations of a new field now popularly known as "molecular mechanics," a field that has become enormously important in industrial as well as academic research on organic substances.<sup>1</sup>

In the meanwhile, our investigations of some unusual inorganic molecules helped shed light on Gillespie's popular "Valence-Shell-Electron-Pair Repulsion Theory"<sup>2</sup> in which "bond interactions" formally resemble "nonbonded interactions." Just as I was diagnosing the distinctions, Brad Thompson organized a symposium for the American Chemical Society Division of Chemical Education to thrash out molecular theory. My contribution, this week's cited paper, was soon published in the division's journal. For pedagogical reasons, I introduced, in language accessible to nonspecialists, a quantum perturbation approach for polyatomic molecules known as second-order Jahn-Teller theory. This approach later became popular.<sup>3</sup> Because my review touched on a number of ideas that ultimately were developed independently by others into important research areas, my paper became a convenient one to cite. Although my original ideas may not be universally shared, at least they no longer spark controversy.

1. Burkert U & Allinger N L. *Molecular mechanics*. Washington, DC: American Chemical Society, 1982. 339 p. ACS Monograph 177.
2. Gillespie R J. *Molecular geometry*. London: Van Nostrand, 1972. 228 p.
3. Burdett J K. *Molecular shapes: theoretical models of inorganic stereochemistry*. New York: Wiley-Interscience, 1980. p. 64-88.