

Dewar M J S & Thiel W. Ground states of molecules. 38. The MNDO method. Approximations and parameters. *J. Amer. Chem. Soc.* 99:4899-907, 1977.
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This paper reported the first quantum mechanical treatment of organic molecules that could be used as a practical tool by organic chemists in their own research. Many organic chemists are now using it, which is why the paper has been cited so often. [The SCI® indicates that this paper has been cited in over 695 publications since 1977.]

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How do chemical reactions take place? This is the question that has been my main concern throughout my chemical research career. It cannot be answered directly because reactions take place too quickly to be observed by any possible experimental technique. The mechanisms stated so confidently in textbooks are in fact based on devious inferences from experiments and qualitative theories of molecular behavior.

Twenty-five years ago, I was becoming increasingly skeptical about this approach. What was clearly needed was a better theory, a quantitative theory that could predict the course of reactions unambiguously, in other words, one based on quantum mechanics. At that time, however, this seemed far beyond the bounds of possibility, certainly not achievable in my own scientific lifetime. Indeed, in spite of prodigious efforts, attempts based on approximate solutions of the Schrödinger equation, i.e., *ab initio* treatment, are still far from this goal.¹

At this point, a serendipitous discovery convinced me that the problem could be solved by an artifice that has

often been used in other analogous connections, i.e., upgrading the accuracy of a crude and correspondingly cheap procedure by introducing adjustable parameters. This "semiempirical" approach had been tried by others but abandoned as hopelessly unpromising. My group was able to show that their failure was due simply to lack of effort. Many man-years and many millions of (computer time) dollars later, we finally developed a procedure (MINDO/3—modified intermediate neglect of differential overlap/3)² good enough to be chemically useful. (For a detailed but informal account, see reference 2.) This was followed by the better procedure (MNDO—modified neglect of diatomic overlap) referenced above. Very recently we have developed one that is better again (AM1—Austin model 1).¹

Why did we succeed when others had, and have, failed? Simply because I, and the members of my group, were organic chemists, not theoreticians. No organic chemist ever expects anything to work the first time he or she tries it. One just goes on trying until it does. However, I must confess that if I had known what I was letting myself in for 20 years ago in Chicago, I might not have been quite so enthusiastic!

While MNDO is not as accurate as one would like, it is good enough to be useful. It can also be applied to quite large molecules, using readily available computers. Tests indicate that it is comparable with *ab initio* methods that need at least 1,000 times more computing time. MNDO can therefore serve as a practical chemical tool for studying molecular properties and reactions, as a large and increasing number of organic chemists have discovered. This is why the source paper has been cited so often. I might add that the Royal Society awarded me the Davy Medal (1982) in recognition of my work in this area.

1. Dewar M J S. Quantum mechanical molecular models. *J. Phys. Chem.* In press, 1985.
2. -----, Development and status of MINDO/3 and MNDO. *J. Mol. Struct.* 100:41-50, 1983.