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COMPUTER SOFTWARE REVIEWS

STR3DI32.EXE v3.000.3.A. P.O. Box 56, Colonia, NJ 07067. http://www.exorga.com. See Web site for pricing information.

When I was preparing to review the STR3DI32 software, I was rather excited. The size of the distribution was only 2.09 MB. It could fit on just two 3.5" diskettes (remember those?), and I was looking forward to working with software that is apparently so space-efficient. However, the rest of the story was a disappointment. The trouble started when I tried to install the program. After repeatedly following the directions to the letter, I still could not make it run. Apparently, STR3DI32 and my Windows Vista were not very happy together. The Exorga customer support offered some options, which did not help, and they actually got frustrated with me. After several days of downloading additional libraries and reinstalling the software, I was eventually successful in getting it to run.

Nevertheless, the performance of the program was not great, especially in view of the numerous commercial programs available for molecular modeling at this time. To name a few, one can use XChemedit, Maestro, or Spartan. The student edition of the latter is even available with some organic and physical chemistry textbooks, and it provides excellent molecule-building and molecular mechanical capabilities *in addition* to the quantum mechanical ones.

Overall, the STR3DI32 does what it promises to do. You can build a molecule, rotate, or move it, and you can run a geometry optimization. But there are reasons why I would not choose this software for my work. The program interface is not very user-friendly, despite the numerous claims to the contrary in the manual. Sometimes it is very old-fashioned: there is no click-and-drag option—you use the mouse to push buttons on the screen. This is not a fatal flaw, but it is certainly a disappointment. And sometimes going through a task is so difficult that it simply takes too much time and effort, such as, for example, in building a molecular structure. The manual does not provide sufficient help and explanations. The "versatile molecular drawing capabilities" mentioned in the manual are at the very least questionable. Moreover, the program dies from time to time, in spite of the claim made in the manual that it is "almost crash-proof". It is possible that it would work better with a non-Vista version of Windows. Geometry optimizations are performed with QVBMM, which is not exactly a widely used force field. The manual does not present a proof, or even sufficient references, that would convince one to use this force field in production calculations.

If one compares STR3DI32 with, for example, the student edition of Spartan, the latter is clearly superior. It permits both quantum mechanical and molecular mechanical (MMFF94 force field) calculations. Building molecular systems is a breeze, it is reasonably crash proof, and the interface is eye candy compared with STR3DI32. A free system named Avogadro by Geoff Hutchinson, available from http://avogadro.sf.net, is also worth mentioning. It offers a molecule building and viewing interface that is definitely easier than that of STR3DI32. It also includes a large library of molecular fragments and a choice of four force fields, including MMFF94, Ghemical, and UFF.

All of the above is not to say that the STR3DI32 software has no value. It is small in size, it does what it promises, and I am sure it can be utilized in productive scientific work. However, it does look like a program created for in-house use and best suited to be employed by those working for the company. I am sure this is a well-designed product from the point of view of somebody who is both a developer and a scientific user. However, given the abundance of other programs on the market that have more versatile molecular modeling capabilities and much more user-friendly interfaces, I personally would not seek to acquire STR3DI32 for my work.

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