J|A|C|S
COMPUTER SOFTWARE
REVIEWS

Jaguar 5.5. Schrödinger, Inc., 1500 SW First Avenue, Suite 1180, Portland, OR 97201. www.schrodinger.com. See Web site for pricing information.

Jaguar 5.5 is the latest version of the electronic structure software from Schrödinger. Jaguar, which specifically provides tools for ab initio computations, is positioned as part of a suite of software tools to tackle a broad range of computational tasks in chemistry, focusing particularly on issues of drug design. It offers a variety of computational methods, including HF, local MP2, GVB, and 19 flavors of DFT, as well as the option to customize among them. Absent is the ability to do CI, CASSCF, coupled-cluster, and ONIUM computations. All of the popular basis sets are incorporated, including Pople's split-valence sets, Dunning's correlation-consistent sets, and 10 basis sets that include effective core potentials. The program can optimize structures to local minima or transition states, with a number of techniques for the latter including quadratic synchronous transit (QST) and eigenvector following. Optimizations can be performed with a variety of restrictions, enabling the automated creation of potential energy scans. The intrinsic reaction coordinate can be scanned once a transition state has been located, and vibrational frequencies can be computed, analytically in some cases, along with IR intensities. Solvation can be treated through a self-consistent reaction field method using their custom Poisson−Boltzmann solver for HF, DFT, GVB, and local-MP2 wavefuctions. Mulliken populations, analysis of natural bond orbitals, and electrostatic potentials are available for analyzing charges.

Jaguar is served by the Maestro graphical user interface (GUI), which also functions as the GUI for the entire Schrödinger suite. Maestro offers a variety of molecular building tools, beginning with the very simplest approach of adding one atom at a time and extending to joining molecular fragments that include common organic, bioorganic, and inorganic groups. Distances, angles, and dihedrals can be changed by selecting appropriate atoms or bonds and then entering values; however, a dial or slide would make this manipulation more straightforward. Once the molecule is designed, a computation using molecular mechanics readily cleans up the structure. A particularly strong feature is the series of easily managed windows for selecting the type of computation to perform. One may never need to learn the rather archaic keywords that are actually used to create the input file, because these windows automatically generate the appropriate keywords and defaults. Computations can be directly submitted and monitored through the Maestro interface, and output can be readily displayed for analysis. Maestro manages related computations through what is called the project table, enabling the chemist to organize and maintain results.

Jaguar and Maestro are available on SGI IRIX-mips4, AIX-pwr3, and Linux-x86 platforms. This reviewer tested the package on a Dell PC with a 3.2 GHz Pentium 4 CPU, 1 GB RAM, 120 GB disk running RedHat 9.0. The installation was painless and uneventful. A license server is necessary, but the Help Desk was quick to supply the key and installation was error-free, other than a complaint from the installer utility about the level of perl; however, this did not impede the successful installation and execution of the program. Jaguar and Maestro can be installed on multiple computers, even mixed platforms, under the single license so long as the license server can be reached for authentication.

Creation of input files is very easy once the Maestro interface is learned. Because Maestro is the common interface for all of the applications developed by Schrödinger, Inc., it has been designed to handle a wide variety of molecules and computations. This necessitates an interface that can seem a bit overwhelming and daunting. I first launched Maestro without opening the manual in an attempt to see how intuitive the interface is. I was unsuccessful in creating a molecule, let alone in setting up a calculation. One is faced with 38 buttons along the left side of the interface, along with 7 drop-down menus along the top. Fortunately, the Maestro manual includes a nice set of tutorials to acclimate the user to the interface. Online help manuals are also available with a single mouse click. Nevertheless, I still found myself fumbling about. For example, when trying to rotate a molecule, Maestro uses the middle mouse button (or both the left and the right buttons on the standard PC mouse), whereas the tools for molecular visualization that I have used in other programs all employ the left button for this function. I tend to use Z-matrix representations, and Maestro is more geared toward coordinate representations. Its Z-matrix editor is quite limited relative to the detailed manipulations offered by its major competitor. Maestro offers a number of molecular display modes, and animation of vibrational frequencies and cycling through IRC computations is possible using the ePlayer. I believe one could also use the ePlayer to visualize intermediate geometries along an optimization, but some manipulation of files would be necessary to do this.

Jaguar bills itself as an "extremely fast ab initio structure package". I hesitate to compare times of execution because there are so many variables. Nevertheless, I optimized the structure of the Ser-Leu dipeptide at HF/6-31G** and B3LYP/6-31G** using Jaguar. Each optimization cycle took about 384 seconds for the HF calculation and 411 seconds for the DFT calculation. This performance is outstanding.

Selection of an electronic structure package must be based on a number of factors: cost, ease of use, performance, and selection of features. Jaguar and Maestro provide a nice interface and fine performance. Where it comes up short in comparison to its competitors is in the selection of features, both in terms of tools for visualization and input generation and in terms of computational methodology. Users must balance these criteria relative to their own needs. The Jaguar/Maestro combination certainly deserves serious consideration among the computational packages currently available.

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