What's New in GaussView

Anharmonic Frequency Analysis

GaussView 6 can display results for both harmonic and anharmonic frequency analysis for IR, Raman, VCD and ROA spectra. The predicted anharmonic peaks and intensities are reported along with the harmomic peaks and intensities. Overtone and combination bands are included.

The spectra can also be viewed graphically, either separately or on the same plot. For example, below we see the harmonic VCD spectrum on the left side of the graph, the anharmonic VCD spectrum in the middle, and the combination of both spectra on the right.

PCM Solvation Cavity

GaussView 6 can display the solvation cavity used for an SCRF calculation. It can display the surface as a solid, a mesh, or as a series of points. The solvation cavity display can be customized.

ORD

GaussView 6 can now plot the results of an Optical Rotary Displacement calculation. The ORD results for every molecule in a molecule group can be displayed in a single plot.

Vibronic Spectra

GaussView 6 can now display the results of vibronic analysis, including vibronic spectra and Duschinky matrices.

Enhanced Calculation Summary

GaussView 6 provides an extensive summary of calculation results:

1. The **Overview** tab displays the key information from the calculation. New items inlcude the solvation model and the polarizability.

2. The **Thermo** tab is active for frequency jobs, and it lists the various thermochemical quantities predicted by the calculation.

3. The **Opt** tab is active for optimization jobs, and it lists the progress towards convergence for the current optimization step, including the maximum and RMS force and displacement. The predicted energy change is also included.

Saving Movies

You can use GaussView6 to save movies of normal mode animations and vibrational normal modes as MP4 video files. When saving normal mode animations, you can specify how often the sequence repeats, whether it plays in forward or in reverse, and adjust the speed and fluidity of the animation. Vibration animations offer options for changing the magnitude of the displacement as well as displaying vectors for the displacement and dipole derivatives.

Combined Plots

GaussView 6 now allows you to view data from multiple sources as a combined plot. The customization options allow you to:

1. Change the lines are represented: as lines, sticks, or a combination of the two.
2. Specify line/stick characteristics, such as thickness and color.
3. Plot a combination line and specify its appearance.
4. Assign weights to the component data sets, including Boltzmann averaging.

One Step Multi-Job Setup

With GaussView 6, you can set up a Gaussian job for a group of molecules in just a few steps.

Symmetry

GaussView's point-group symmetry feature allows you to increase the symmetry of the current molecule. A molecule can be constrained to a specific point group, and all future modifications to the structure will maintain that symmetry.

GaussView 6 now allows you to reduce the symmetry of a molecule you are working on. Preserving some molecular symmetry is useful for setting up calculations that involve Jahn-Teller distortions. The graphic below shows the current point group being modified from D_{3h} to D_3.

New Job Setup Features

The Gaussian Calculation Setup dialog in GaussView6 contains many new features, some are highlighted below:

A: The **Job Preview** panel from the **Gaussian Calculation Setup** dialog shows the generated input file.

B: New controls enable retrieving data from checkpoint files and specifying the **%OldChk** directive.

C: You can specify the maximum disk usage for the job.

D: New job types include predicting polarizabilities and ORD.

E: There is an expanded panel for specifying population analysis.

F: New Gaussian 16 capabilities are supported: e.g., anharmonic IR/Raman, VCD annd ROAcalculations.

G: View the contents of the **Default.Route** file