Release note for PhotochemCAD 2.1
November 9, 2007

What's New:

In General

(1) A PDF file called "Getting Started" is available as a brief guide for new users on how to use PhotochemCAD.

(2) The data for newly created spectra (e.g., the result of an energy-transfer simulation, the result of spectra manipulation) can be exported as a tab-delimited text file for further use in other graphing software programs.

(3) Spelling and grammatical errors in a number of the windows have been fixed.

(4) Video instructions (AVI files) have been removed from the installer, which makes the size of the software much smaller. Users can separately download such video instruction files from www.photochemCAD.com as optional files.

(5) A number of calculations (oscillator strength, fluorescence lifetimes, etc.) now can be calculated sequentially for a compound using different parameters. (In version 2.0, spectra needed to be closed to use different parameters in subsequent calculations.)

Modules

Graph Setting:

The bugs regarding the scale for graph settings that related to wavenumber and energy (eV, Kcal, and KK) have been fixed.

Energy Transfer Simulation:

(1) A bug regarding calculation of absorption coefficients has been fixed.

(2) The original emission spectra now are displayed together with the simulated emission spectrum, which facilitates visual comparison.

Oscillator Strength Calculation:

Users can choose a region of the spectrum for calculation: (a) an arbitrary spectral region, selected manually, or (b) automatic integration of the fwhm region of the largest peak within the range.

Transmission

A new function has been added to enable control over the intensity of the radiation (absorption spectrum) by multiplying by a factor (1 to 0).

Add/Subtract spectra

(1) Multiple spectra now can be manipulated mathematically at the same time (in version 2.0, it was limited to 2 spectra).

(2) A bug regarding the absence of datapoints in the background region (typically above 800 nm) has been fixed. Now when the spectrum does not have datapoints in some regions, it is regarded as the base line, thus the data will be treated as 0.

Known issues

Note that when the result of spectra manipulation includes a negative region in the y-axis, the negative region of the spectra cannot be seen automatically. The y-axis of the graph needs to be set manually to an appropriate region to display the negative region of the spectra. This issue should be addressed in a subsequent release.