Use of PCLOBE

I. Copying files

1. Insert the PCLOBE compact disk into your CD drive and locate its three files. One is a zipped file of illustrative examples and another is the ''setup.exe'' file.

2. Transfer the zipped file to your computer and extract the compressed files into a new folder, which you could name ''PCLOBEXAMPLES''

3. Double click on ''setup.exe'' on the CD—this will install PCLOBE on your own drive. You will find the program in your programs list; you may construct a shortcut so to start PCLOBE from your desktop.

II. Running PCLOBE

1. Start (click on) PCLOBE either from the shortcut or from the programs list. If all goes well, you will see a Visual Basic display with selection buttons to define PCLOBE calculations.

2. Define a job, using structures supplied in PCLOBEXAMPLES
   a. Click the Browse button at the top left of the display panel.
   b. Find and click the ''name.XYZ'' file of your choice (open it).
   c. Select the desired basis from the list at center left.
   d. Enter an integer to define the gradient threshold (''3'' $= 10^{-3}$). Selecting the default ''0'' defines a single-point energy calculation. This is required for certain tasks, and enforced by the interface. A gradient threshold of 4 or 5 will invoke calculation of vibrational frequencies. The default of 30 steepest descent iterations is best reset to ''99'' for geometry optimization.

3. Click on ''Launch PCLOBE'' to start the program. You should immediately see a black foreground output window showing progress through the task.

4. When the run finishes, click on the ''View Output'' button at the lower right part of the Visual Basic panel to look at the total output. If you wish to retain the output, save it with a unique file name.

Use of the VISTA operating system

Windows VISTA requires that you explicitly allow PCLOBE to read, write, and delete temporary files by setting permissions within the folder.

Special requirements on input files

Some options require special care that input files be prepared in accordance with certain conventions. For instance, the point group symmetry option requires that the input structure possesses the specified symmetry, and requires that the high order symmetry axis coincide with the ''z'' Cartesian direction. The examples for this input with names xxxsym.XYZ obey these requirements. Consult the ''READpclobe.txt'' file for more detail and an exception with the non-conventional Cnvx symmetry.

Use of the Rydberg basis requires that the file ''rydberg.dat'' contain a non-zero value of scaling for each atom to which a 3sp shell is to be added, remember to reset the value to ''0.0'' for the next run if the Rydberg orbitals are not desired (applies only to CIS in a STO-4G basis).

Preserving data written to placeholder files

From some tasks, PCLOBE produces data files labeled ''uvspectra.txt,'' ''cdspectra.txt,'' ''mcdspectra.txt,'' and ''ordspectra.txt.'' These are intended for use by graphics programs. The file labeled ''lobe.xyz'' is intended to provide input data to an external molecular modeler such as RASMOL. The file ''lobe.draw'' is intended for the external plotting program MOLEKEL. If information in these files is to be retained, they should be saved with more informative names.