FindConeAngle package for Mathematica written by Wesley D. Allen
December 9, 2012 version

For a detailed derivation of the mathematics and interesting uses of the program see J. A. Bilbrey, A. Kazez, J. Locklin, W. D. Allen. "Exact Ligand Cone Angles." *J. Comput. Chem.*, **2013**. DOI: 10.1002/jcc.23217

INPUT

All Mathematica files provided for the program and the database of ligand Cartesian coordinates should be stored in the same folder on one's computer. These include: ComplexDataBase.m, ComplexDataBase.nb, ComplexDataBase1.txt, ConeAngleDriver.nb, ConeAnglePackage.m, and ConeAnglePackage.nb.

ComplexDataBase1.txt

The Cartesian coordinates for all ligands are stored in ComplexDataBase1.txt. Additional ligands can be added to the list with the following format

(X#) NAME
1 Symbol xval yval zval
2 Symbol xval yval zval
0

where # is the order of the ligand in the database (to be called upon by ConeAngleDriver.nb), Symbol is the atomic symbol (that atom must be specified in the list of van der Waals radii in ConeAnglePackage.nb), and xval, yval, and zval are the x y and z Cartesian coordinates of the atom. A 0 follows each input to separate the ligands. <u>The apex atom (central atom) must be listed first.</u>

ConeAngleDriver.nb

The notebook ConeAngleDriver.nb is the only package the user needs to modify to use the code as is. This interface calls on ComplexDataBase.m to read in Cartesian coordinates from the file ComplexDataBase1.txt and calls on ConeAnglePackage.m to calculate the cone angle and visualize the results. The variable ConeDirectory must be defined as the location of the folder that contains all of the FindConeAngle files on one's computer. ComplexSet enumerates which ligands in the database the cone angle should be found for. The number of the ligand corresponds to the order listed in ComplexDataBase1.txt (X#). For example, if one wishes to find the cone angles of ligands 12-17, the input "ComplexSet = Range[12, 17]" would be used. To find the cone angle of only ligand 12, the input would be "ComplexSet=Range[12,12]".
The output can be controlled by the variable kPrint:

kPrint = 0, No printing within package;
kPrint = 1, Print {ConeAngle, ConeAxis, ConeAtoms} for each ligand;
kPrint = 2, For each ligand print both {ConeAngle, ConeAxis, ConeAtoms} and a 3D plot showing the ligand placed inside the cone;

kPrint = 3, For each ligand print both {ConeAngle, ConeAxis, ConeAtoms} and a table of van der Waals radii, vertex angles, and Cartesian coordinates;
kPrint =4, For each ligand print both {ConeAngle, ConeAxis, ConeAtoms} and a histogram of candidate three-atom cone angles (°) in the range of (θ_{2max},θ_{cm}).

ConeAnglePackage.nb/ ConeAnglePackage.m

The notebook ConeAnglePackage.nb includes all mathematics used to solve for and visualize the cone angle. A list of standard van der Waals radii is already written into the program but can be changed or added to. To modify the list of van der Waals radii, locate the variable "RvdW" near the top of the code. RvdW is a list of three lists. The first list holds atomic symbols whose position in this list correspond with values given in the next two lists, the second list holds van der Waals radii, and the third list holds the colors the atoms appear in the visualization in kPrint=2. Once edits have been made to ConeAnglePackage.nb, the file must be saved as a Mathematica Package with the .m extension to allow ConeAngleDriver.nb to call upon the package.

ComplexDataBase.nb/ ComplexDataBase.m

The notebook ComplexDataBase.nb reads in ligand Cartesian coordinates and formats Apex, Ligands, and XAtoms correctly for ConeAngleDriver.nb. To change the text (.txt) file where the ligands are stored the lingandsIn variable can be edited. To read in a .txt file, for example, within the same folder called NewLigands.txt the lingandsIn variable should read: ligandsIn=OpenRead["NewLigands.txt"]. To solve for cone angles of multiple ligands on a single center, the variable Ligands can be expanded. For example, if atom 1 is the metal center, atoms 2-6 belong to the first ligand, and atoms 7-14 belong to the second ligand, the variable Ligands would read: Ligands={Range[2,6],Range[7,14]}. Once edits have been made to ComplexDataBase.nb, the file must be saved as a Mathematica Package with the .m extension to allow ConeAngleDriver.nb to call upon the package.

OUTPUT

The output of the program will appear in ConeAngleDriver.nb along with the total run time of the program. To choose various print options see kPrint in the ConeAngleDriver.nb section.