FindSolidAngle package for Mathematica written by Wesley D. Allen
August 28, 2013 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 Solid Angles." *In preparation*.

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, SolidAngleDriver.nb, SolidAnglePackage.m, and SolidAnglePackage.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 SolidAngleDriver.nb), Symbol is the atomic symbol (that atom must be specified in the list of atomic radii in SolidAnglePackage.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. The apex atom (central atom) must be listed first.

SolidAngleDriver.nb

The notebook SolidAngleDriver.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 SolidAnglePackage.m to calculate the cone angle and visualize the results. The variable SolidAngleDirectory must be defined as the location of the folder that contains all of the FindSolidAngle 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]".

Print Options

The output can be controlled by the variable kPrint. All options print the total solid angle, total solid cone angle, and and contributions from each convex and concave loop.

kPrint = 1, Print total solid angle and dissection of loop contributions for each ligand;

kPrint = 2, For each ligand print a (non-shaded) 3D plot highlighting the border arcs and showing the shadow cones intersecting with the unit sphere;
kPrint = 3, For each ligand print a table of atomic radii, vertex angles, and Cartesian coordinates;
kPrint = 4, For each ligand print the aforementioned 3D plot with labels on the arcs and for comparison also tabulate the dissection of loop contributions for each ligand;
kPrint = 5, For each ligand print a 3D plot showing the border arcs and filling gray into the shadow cones intersecting with the unit sphere.

Alternate Atomic Radii

The choice of atomic radii can be changed with the variable kR. When kR = 1 the atomic radii from [Bondi, A. *J. Phys. Chem.* **1964**, *68*, 441-451.] will be used. When kR = 2 the zero energy point radii from [Guzei, I. A.; Wendt, M. *Dalton Trans.* **2006**, 3991-3999] will be used. As of now only H, He, C, N, O, F, Ne, Si, P, S, Cl, Ar, As, Se, Br, Kr, Te, I, and Xe are included. Radii for additional atoms can be added in the SolidAnglePackage.m file (see below).

The implemented Bondi atomic radii are {"H", "He", "C", "N", "O", "F", "Ne", "Si", "P", "S", "Cl", "Ar", "As", "Se", "Br", "Kr", "Te", "I", "Xe"} with corresponding values {1.20, 1.40, 1.70, 1.55, 1.52, 1.47, 1.54, 2.10, 1.80, 1.80, 1.75, 1.88, 1.85, 1.90, 1.85, 2.02, 2.06, 1.98, 2.16}.

The implemented zero energy point radii are {"H", "He", "C", "N", "O", "F", "Ne", "Si", "P", "S", "Cl", "Ar", "As", "Se", "Br", "Kr", "Te", "I", "Xe"}, with corresponding values {1.000, 1.311, 1.539, 1.521, 1.470, 1.413, 1.350, 1.834, 1.801, 1.757, 1.599, 1.649, 1.879, 1.861, 1.845, 1.831, 1.955, 1.941, 1.928}.

Closing a Gap

If a ligand profile contains a small indentation, that gap may not be relevant in quantifying the total sterics. We have added an option to effectively close that gap by placing a dummy atom that overlaps with the two atoms at the start of the gap. The option is controlled by the key word PlugGap, which is set to True or False. To determine the two atoms to use, first find the solid angle with the kPrint option set to 4 and PlugGap set to False. The 3D plot will have each arc labeled. From the labeling, determine which two atoms should be plugged to fill the gap. To find the solid angle with a plugged gap, set PlugGap = True, arc1 = number of first arc in plug, arc2 = second arc in plug, and plugradius = radius of the plug. The plugradius must be determined manually by checking the 3D profile to confirm that the gap is closed.

SolidAnglePackage.nb/ SolidAnglePackage.m

The notebook SolidAnglePackage.nb includes all mathematics used to solve for and visualize the cone angle. A list of standard atomic radii and zero energy point radii are already written into the program but can be changed or added to. To modify the list of atomic 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 atomic radii, and the third list holds the atom colors. The addition of a new atom name/radius/color must occupy the

same position in each list. Once edits have been made to SolidAnglePackage.nb, the file must be saved as a Mathematica Package with the .m extension to allow SolidAngleDriver.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 SolidAngleDriver.nb along with the total run time of the program. To choose various print options see kPrint in the SolidAngleDriver.nb section.