Commands to run acedrg:

1. "acedrg –h" to get a list of command options for acedrg
2. Run "acedrg" to get a dictionary file of mmcif format and a coordinate file of PDB format.
    a. For an input file of SMILES format.
        i. E.g. "acedrg –i DB00201.smiles –o DB00201
        ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)
    b. For an input file of Mol format.
        i. E.g. "acedrg –m DB00201.mol –o DB00201
        ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)
    c. For an input file of mmcif format.
        i. E.g. "acedrg –c DB00201.cif –o DB00201
        ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file).
3. Run "acedrg" to get molecules, atom types, bond lengths and angles in those molecules.
    a. For one single cif file.
        i. E.g. "acedrg -e -b ./inStdcif/1000004.cif -r 1000004 -o 1000004"
        ii. The output for the above examples are (1) Molecule file "1000004_all_mols.txt" and (2) bond and angle file "1000004_unique_bond_and_angles.txt"
    b. For a directory containing several cif files.
        i. E.g. "acedrg -e -d inStdcif"
        ii. All input cif files are in ./inStdcif/.
        iii. The output table is "AcedrgOut_all_atoms_bonds_angles.table" and all other files for each individual molecule are in "AcedrgOut_TMP/"