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<nics.py>

This script allows you to generate XYZ coordinates for various NICS calculations by placing Bq's (ghost atoms) at various locations.

HOW THIS SCRIPT WORKS:

1. Rings are located either automatically or randomly (depending on input).
2. The centroid (center) of a random or user specified ring is located by averaging XYZ coordinates of each atom in the ring
3. A ghost atom (Bq) is placed at a location specified by the input
4. A transformed XYZ file is then placed in the same folder

Current known issues:

1. Rings with two heteroatoms that are side by side are not located
2. Central aromatic rings of polycyclic aromatic hydrocarbons are not found

<<These issues can be bypassed by manually inputting rings> (SEE BELOW)>

HELP:

Access all input parameters and file instructions by simply running the nics.py script without any input

USAGE (EASY MODE):

Simply run the script with an input xyz file and a NICS(1)/NICS(1)zz XYZ file will be generated

USAGE (ADVANCED MODE):

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nics.py [filename] [NICS options] [parameters] [displaygraph]

>>>filename:

XYZ files must contain no additional lines (ie headers produced by Cylview, etc). Only raw XYZ data can be read

>>>Parameters:

1. -m : [M]anual ring input. Must be followed by a listing of ALL ring atoms (integer input only
   example > nics.py [inputfile] [NICS option] -m atom1 atom2 atom3 ...
2. -am : [A]utomatic ring search with an additional [M]anually input ring (integer input only
   example > nics.py [inputfile] [NICS option] -am atom1 atom2 atom3 ...
3. -cr : [C]hoose a [R]ing to place in the ZY plane by picking one or more atoms in that ring (integer input only

example > nics.py [inputfile] [NICS option] <parameters> -cr atom#

4. No parameters results in automatic ring search with a random ring selected to place in the ZY plane

>>>NICS options:

1. **-N0** : NICS(0), Places Bq at centroid of all rings (including manually specified rings)
   example > nics.py [inputfile] -N0 [parameters]
2. **-N1** : NICS(1)/NICSzz(1), Places Bq one angstrom above ring centroid, transforms XYZ coordinates
   example > nics.py [inputfile] -N1 [parameters]
3. **-Nx** : NICS(x)/NICSzz(x), Places Bq 'x' angstrom(s) above ring centroid, transforms XYZ coordinates
   example > nics.py [inputfile] -N1 [parameters]
4. **-Nvert** : Places Bq's from the centroid to a specified distance above the ring with specified interval (angstroms
   example > nics.py [inputfile] -Nvert <distance> <interval> [parameters]
   example > nics.py [inputfile] -Nvert 5.0 1.0 [parameters]
   - NOTE: The above example places 5 Bq's at 0, 1, 2, 3, 4, 5 angstroms above the ring.
   - NOTE: Default is to place a Bq at the centroid and at the distance specified.
   - NOTE: if distance = 5 and interval = 3 Bq's will only be placed at 0, 3, and 5 angstroms.

>>>Display graph:

1. **-g** : Displays a 3D graph of the XYZ coordinates after transformation/Bq placement. This allows you to quickly confirm that all all rings were found and all Bqs were roughly placed properly without having to load the XYZ coordinates into a different software. May not be compatible with all terminals.
   example > nics.py [inputfile] [NICS option] [parameters] -g
2. No value omits graph

WHAT IS NICS:

NICS (nucleus independent chemical shift) is a measure of the absolute shielding at a specified location. Formally, it is the isotropic chemical shift at that location. It is usually placed at either the centroid (center) of a ring or one angstrom above the plane of the centroid of the ring. The isotropic shift of these ghost atoms measures the extent to which that location is shielded by the induced magnetic field from the aromatic ring. The negative of the isotropic chemical shift is taken as the NICS value. More negative NICS values typically correspond to increased aromaticity while positive NICS values indicate anti-aromaticity (paratropicity). The isotropic chemical shift is a tensor value and refers to the average of the XX, YY, and ZZ components. When the out of plane value (NICSzz type calculations) is taken instead of the isotropic chemical shift only one of the XX, YY, or ZZ components are considered. This is only reasonable to do if the molecule is in a coordinate plane (ie. the molecule must be in the XY plane in order for the ZZ component to be considered out of plane).

TYPES OF NICS CALCULATIONS:

1. **NICS(0)** : Bq placed at the centroid of the ring. NICS is the negative of the isotropic chemical shift.
2. **NICS(1)** : Bq placed one angstrom above the plane of the ring centroid. NICS is the negative of the isotropid chemical shift.

3. **NICS(1)zz** : Bq placed one angstrom above the plane of the ring centroid. NICS is the negative of the out of plane component (one of XX, YY or ZZ, depending on the plane the ring is in) of the chemical shielding tensor. These values are typically much larger than NICS(0) or NICS(1).
4. **NICS(1)pi-zz** : Bq placed as NICS(1)zz, but only the pi-components of the out of plane component are considered. Requires separating the sigma from pi contributions to each of the out of plane components of the chemical shift. Requires modified input file.
5. **CMONICS(1)** : Bq placed as NICS(1), but only the pi-components of the isotropic chemical shift are considered. Requires separating the sigma from the pi contributions to the chemical shift. Requires modified input file.

NOTE: Placing the aromatic ring in the XY (or XZ, YZ) plane is only important for NICS calculations with "zz" in the name.

RUNNING NICS CALCULATIONS:

1. Generate the XYZ coordinates of the molecule with Spartan/Avogadro/other molecular modelling software
2. Use the nics.py script to transform the XYZ coordinates and append Bqs
3. Run a standard NMR calculation [M062X/6-31+g(d,p) is generally acceptable] with no solvent