

Data types:

type atom

! Setting the element in this project only C (carbon) or H (hydrogen)

character(1) :: element = 'E'

! The xyz coordinates of the atom in the molecule

real(realkind) :: cords(3) = 0.

end type

type bond

! Setting the indices of the atoms that are bonding

integer :: link(2) = 0

! Setting the type of bond in this project only CC or CH

character(2) :: type = 'EE'

! Setting the calculated distance of the bond in A

real(realkind) :: length = 0.

! Setting the vector for the bond

real(realkind) :: vector(3) = 0

end type

type bond\_angle

! Setting the types of bonds over which the angle is calulated

character(2) :: bonds(2) = (/'EE', 'EE'/)

! Setting the indicies of the atoms over wich the angle is calcualted

integer :: atom\_indicies(3)

! The actual angle of the bonds

real(realkind) :: angle = 0.

end type

type molecule

type (atom), allocatable :: atoms(:)

type (bond), allocatable :: bonds(:)

type (bond\_angle), allocatable :: angles(:)

end type

is it better to make a type called molecule under which the different data types are placed (atom, bond?

What does R0AC2 mean

What does lower case omega mean (angular frequency)

Non bonding interactions

How to minimize? By changing coordinates

Metropolitan with random distribution?