pyOptking
a robust, flexible optimizer for Psi4

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Objectives of pyOptking

- improve power and flexibility by ‘inverting’ the optimization process
  - old way: successive calls to optimizer(gradient-value)
  - new way: one call to optimizer(gradient-function)
- produce an optimizer readily compatible with other atom-based optimization programs
Desired characteristics

- Efficiency
- Robustness
- Predictability
auxiliary bonds
steeped-descent

What is the symmetry of this \((4n+2)\) \(\pi\)-electron system? \(D_{6h}, D_{3h}, C_i, C_2, \ldots\)?
Code Status

- virtually all capabilities of C++ code
  - RFO, NR, P-RFO (TS)
  - internals (frozen and fixed), cartesians
  - Hessian guesses, updates, transformations
  - flexible convergence criteria

- current tasks
  - debugging fixed cartesians; IRC; “run-levels”

- new capabilities
  - automated line-searching
  - return trajectory
# class method to make an optking system from a psi4 molecule

```
mol = core.get_active_molecule()
OptMol = optking.molsys.MOLSYS.fromPsi4Molecule(mol)
```

# Takes and returns a numpy array

```
def setGeometry_func( newGeom ):
    psi_geom = core.Matrix.from_array( newGeom )
    mol.set_geometry( psi_geom )
mol.update_geometry()
return np.array( mol.geometry() )
```
calcName = 'ccsd'

# Returns energy and gradient. In- and out- formats are numpy.
def gradient_func(xyz):
    xyz[:] = setGeometry_func(xyz)
    psi4gradientMatrix, wfn = driver.gradient(calcName, molecule=mol, return_wfn=True)
    gradientMatrix = np.array(psi4gradientMatrix)
    E = wfn.energy()
    return E, np.reshape(gradientMatrix, (gradientMatrix.size))

optking.optimize( OptMol, optking_user_options, setGeometry_func, gradient_func, hessian_func, energy_func)
Discussion Points

- Keep the current C++ optking?
- Should Psi4 check keywords?
- Easiest tool to visualize trajectories (minimization or IRC)?
- Desired future features?
Other projects

- Raman optical activity
  - Alex Heide and Kate Rynders

- absorption spectra of photovoltaic donor polymer candidates
  - Mitchell Lahm

- optical activity of solvated species
  - Sarah Greteman-Leo, Kendra Folsom

- partitioning of contributions to optical activity
  - Sarah Elliott