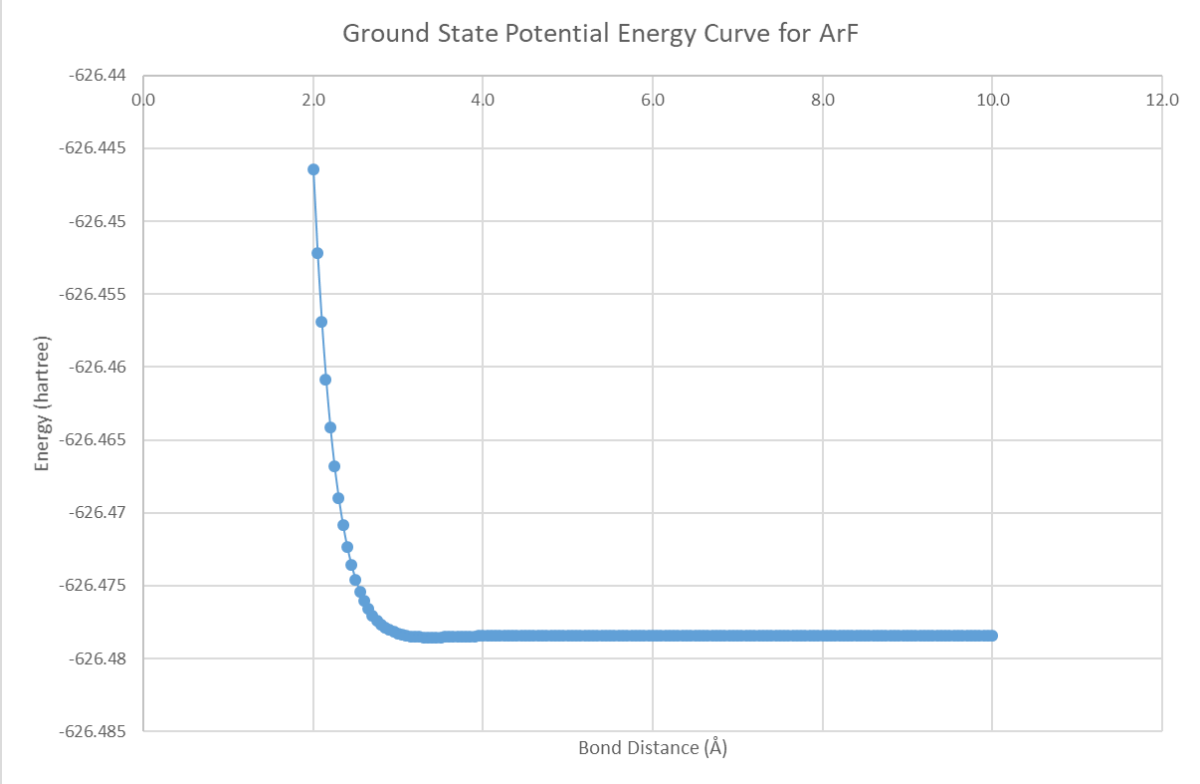
Chem 412 Assignment 2

1. a) Job Number: 172271
   Neutral ArF
   Bond Distance: 3.383 Angstroms ~ 3.4 Angstroms
   Energy: -626.4785415 hartree ~ -626.479 hartree

   Job Number: 172273
   ArF^- (charged)
   Bond Distance: 2.89 Angstroms ~ 2.9 Angstroms
   Energy: -626.51340378 hartree ~ -626.513 hartree

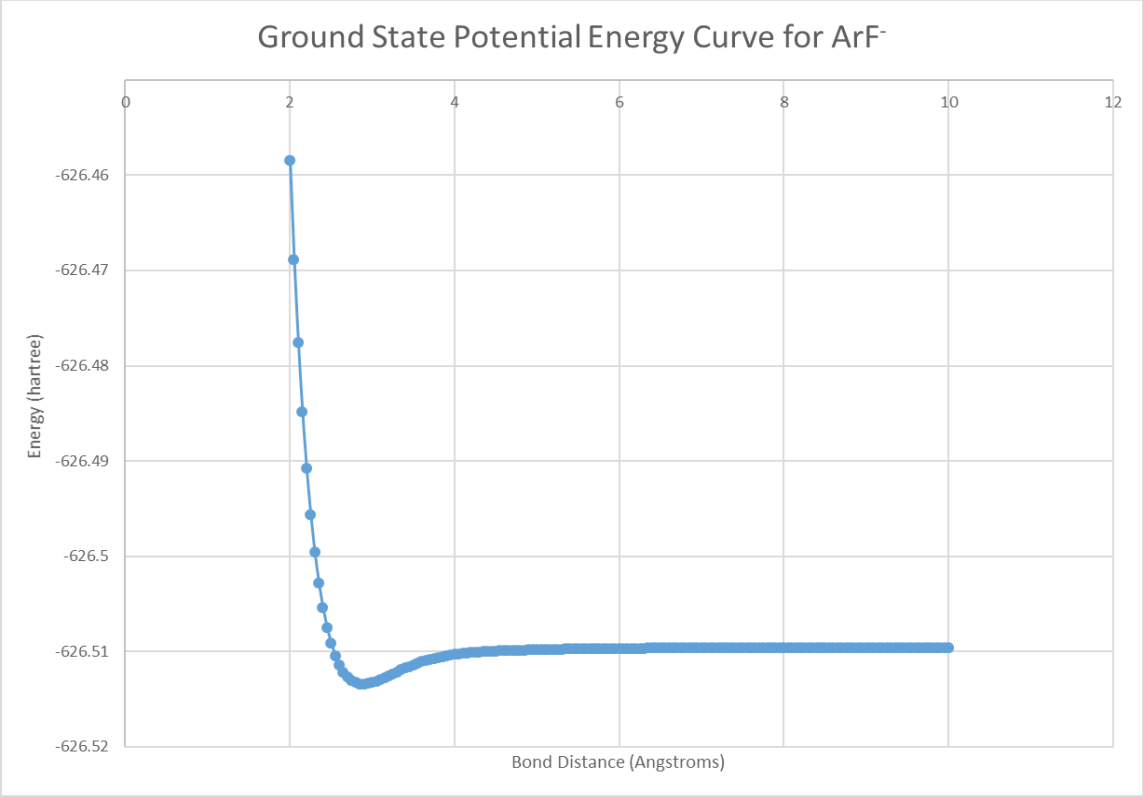
   b) Job Number: 173181
   Neutral ArF



Plot 1: The lowest energy as indicated in this plot is at -626.479 hartree at 3.4 Angstroms, which is the same as in 1) a).

Job Number: 173240

ArF^- (charged)



Plot 2: The lowest energy as indicated in this plot is at -626.513 hartree at 2.9 Angstroms, which is the same as in 1) a) for ArF^{-1}.

c) Job Number: 172271, 173181

For plot 1 neutral ArF: At r = 10.0 Angstroms, the energy in the first plot is -626.478394 hartree, which is -1644819.023 kJ/mol or -137496113.7 cm^{-1}.

Note: 1 hartree = 2,625.500 kJ/mol= 219474.63 cm^{-1}

So -626.478394 hartree = 2,625.500 * -626.478394 = -1644819.023 kJ/mol

And -626.478394 hartree = 219474.63 * -626.478394 = -137496113.7 cm^{-1}

The energy obtained in 1) a) for neutral ArF is -626.478541 hartree = -1644819.411 kJ/mol = -137496146.1 cm^{-1}.

For plot 1, the neutral ArF:

The well-depth is:

-626.478394 hartree – (-626.478541 hartree) = **0.000147 hartree**

-1644819.023 kJ/mol – (-1644819.411 kJ/mol) = **0.388 kJ/mol**

-137496113.7 cm^{-1} - (-137496146.1 cm^{-1}) = **32.4 cm^{-1}**

Job Number: 173240, 172273

For plot 2: charged ArF^-: At r = 10.0 Angstroms, the energy in the second plot is -626.50957

hartree, which is -1644900.86 kJ/mol or -137502955.1 cm^{-1}.

The energy obtained in 1) a) for neutral ArF is -626.51340378 hartree = -1644910.94 kJ/mol = -137503797.5 cm^{-1}.

For plot 2, the charged ArF:

The well-depth is:

-626.50957 hartree – (-626.51340378) = **0.00383 hartree**

-1644900.86 kJ/mol – (-1644910.94 kJ/mol) = **10.08 kJ/mol**

-137502955.1 cm^{-1} – (-137503797.5 $^{-1}$) = **842.4 cm^{-1}**

2. a) Job Number: 173302
   Total energy (“CCSD Energy"): -151.18466816 hartree
   Bond distance of O-O: 1.4527 angstroms
   Bond distance of O-H: 0.9694 angstroms
   Bond angle of H-O-O: 99.5723 degrees
   Dihedral angle of H-O-O-H: 116.5092 degrees

   b) Job Number: 173303
   Vibrational modes corresponding to:
   1) O-O stretching: mode 2, with the frequency of 922.1064 cm^{-1}
   2) O-H anti-symmetric stretching: mode 5, with the frequency of 3810.7278 cm^{-1}
   3) Torsional motion of H-O-O-H: mode 1, A with the frequency of 351.6906 cm^{-1}

   c) Job Number: 173250
   Total energy (“CCSD Energy"): -151.18346802 hartree
   Bond distance of O-O: 1.4639 angstroms
   Bond distance of O-H: 0.9682 angstroms
   Bond angle of H-O-O: 97.9686 degrees
   Dihedral angle of H-O-O-H: 180.0 degrees

   d) Job Number: 173253
   Vibrational modes corresponding to:
   1) O-O stretching: mode 2, AG with the frequency of 920.0787 cm^{-1}
   2) O-H anti-symmetric stretching: mode 6, BU with the frequency of 3845.8423 cm^{-1}
   3) Torsional motion of H-O-O-H: mode 1, AU with the frequency of -262.6017 cm^{-1}

   e) Job Number: 172527
   Total energy (“CCSD Energy"): -151.17192085 hartree
   Bond distance of O-O: 1.4614 angstroms

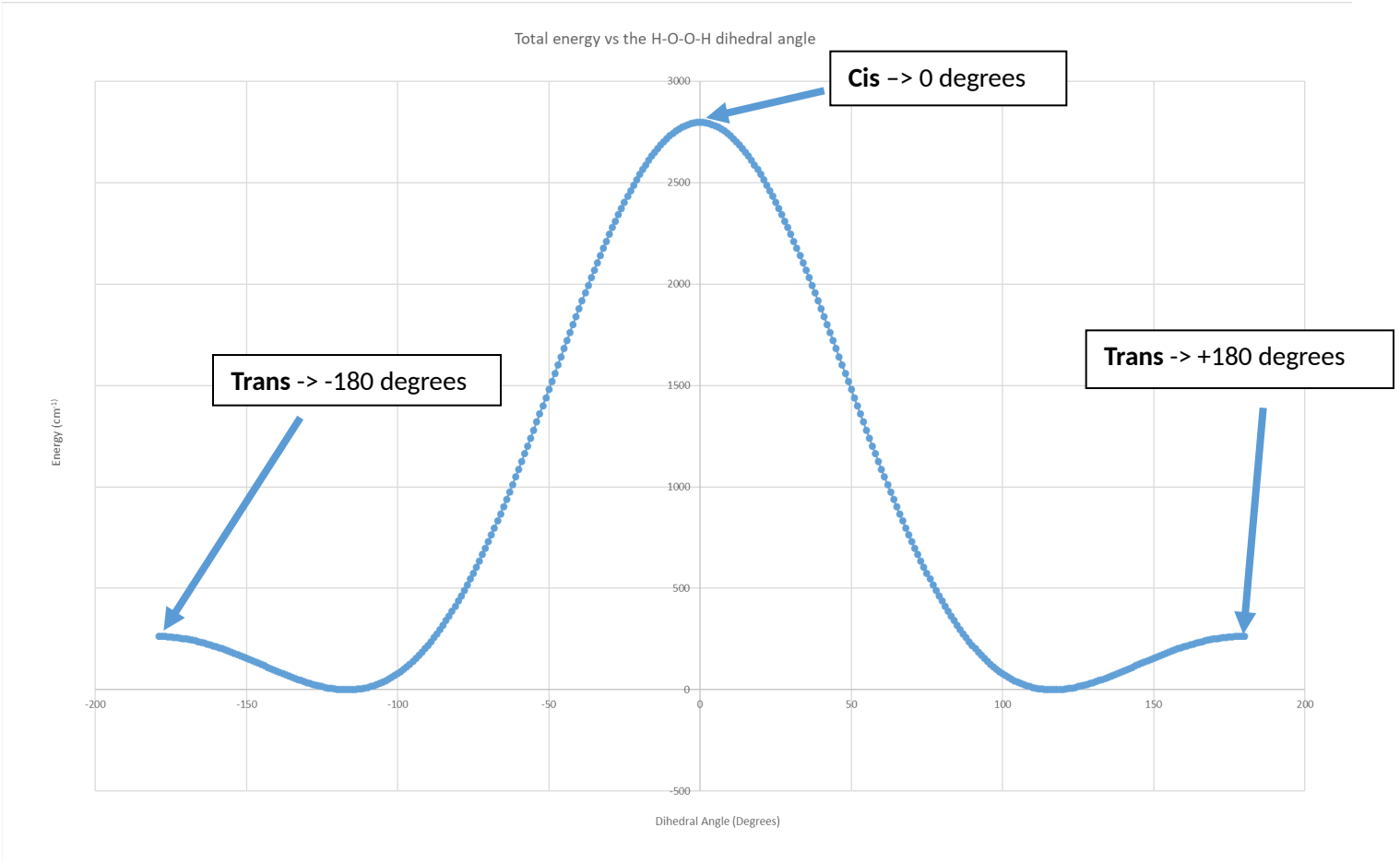
Bond distance of O-H: 0.9694 angstroms
Bond angle of H-O-O: 103.8703 degrees
Dihedral angle of H-O-O-H: 0.00 degrees

f) Job Number: 172531
Vibrational modes corresponding to:
1) O-O stretching: mode 2, A1 with the frequency of 909.1241 cm^{-1}
2) O-H anti-symmetric stretching: mode 5, B2 with the frequency of 3788.3835 cm^{-1}
3) Torsional motion of H-O-O-H: mode 1, A2 with the frequency of -606.6054 cm^{-1}

g) Job Number: 173183

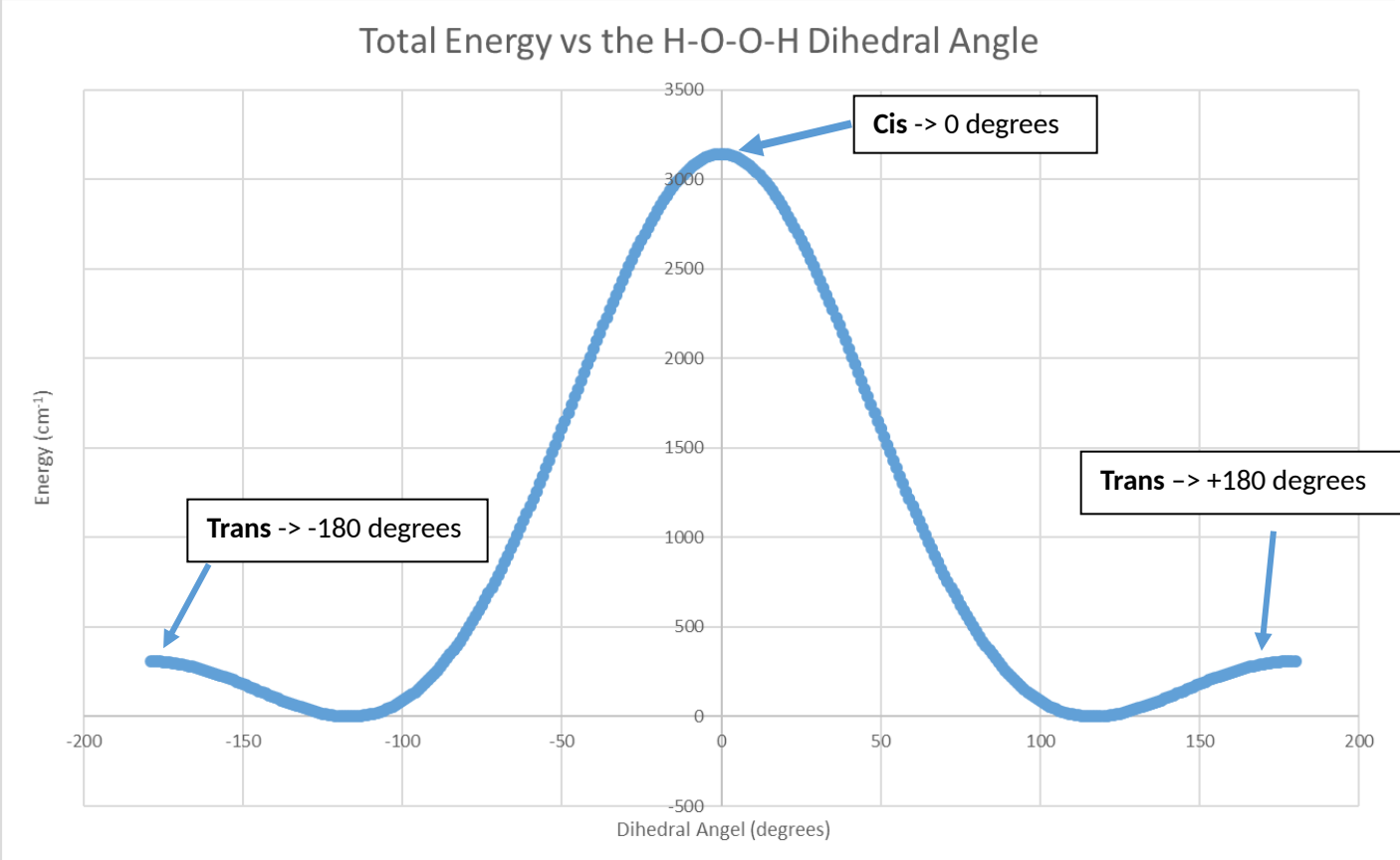
h) Job Number: 173305

i) Job Number: 173183 (from j)



The lowest energy as shown on this plot, at 0 cm^{-1} which corresponds to -151.185 hartree, is reflected by 2 a) also at between 116 ~117 degrees.

i) Job Number: 173305 (from h)



The lowest energy as shown on this plot, at 0 cm^{-1} which corresponds to -151.185 hartree, is reflected by 2 a) also at between 116 ~117 degrees.

j) Job Numbers: 173305, 173183, 173253 and 172531

Barrier Height (g):

Cis: 2797.687004 cm^{-1}
Trans: 263.369556 cm^{-1}

Barrier Height (h):

Cis: 3140.243 cm^{-1}
Trans: 308.6911 cm^{-1}

Tortional Vibration Frequency (d): -262.6017 cm^{-1}
Tortional Vibration Frequency (f): -606.6054 cm^{-1}

Relaxed potential scans has geometry optimization at each point and is requested with Opt at each point/step. On the other hand, structure at each point of scan (like bond length and angles) is kept rigid or fixed in a rigid potential scan, at which it only measures a single point energy (keeps others fixed). A relaxed potential scan is more accurate as it is more informative as to what a real-life dynamic process (all the interactions within the molecule) would look like.