**So Much Potential**

**Question 1: What is the reduced mass of the CO molecule in atomic units?**

The reduced mass of the CO molecule in atomic units is as follows:

**µ = = = = = 12589.71 amu**

Since the relative mass of an electron is 1/1836 of that of a proton or neutron, it is very small, and therefore neglected *(1)*. To calculate the reduced mass of the CO molecule in atomic mass units (amu), the atomic mass, or the mass of protons and neutrons, of C and O are multiplied by 1836. The product of these two numbers is the numerator, and the sum is the denominator, resulting in the 12,589.71 amu of the CO molecule.

Answer may be found below “**Question 1 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_1.py**”.

**Question 2: Use your spline fit to the PES of CO to estimate the vibrational frequency of CO. Express your number in atomic units and also convert to a common spectroscopic unit system of your choosing (wavenumbers, nm, microns, Hertz, THz are all acceptable choices).**

My spline fits were two – a quartic one and a pentic one. Using the conversion factor of 1 a.u. = 2.19475 cm-1 *(2)*, code was written to convert the vibrational frequency to wavenumber units of cm-1. This conversion was also done for the cubic spline function, shown below the line below the quartic and pentic spline values:

Quartic spline fit yields the following vibrational frequencies:

* atomic units = **0.016582287155607327 a.u.**
* wavenumbers = **0.03639397473476918 cm-1**

Pentic spline fit yields the following vibrational frequencies:

* atomic units = **0.01601683873961036 a.u.**
* wavenumbers = **0.03515295682375984 cm-1**

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Cubic spline fit yields the following vibrational frequencies:

* atomic units = **0.01619263521082673 a.u.**
* wavenumbers = **0.03553878612896197 cm-1**

Answers for the quartic spline may be found below “**Question 2 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_2.py**”.

Answers for the pentic spline may be found below “**Question 2 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_3.py**”.

**Question 3: What will be the accelation of the bond stretch when C is separated by O by 3 atomic units? You can express your acceleration in atomic units, also.**

The acceleration differed with the order of the spline function.

Cubic Spline:

Acceleration of the bond stretch when C is separated by O by 3 atomic units is **-2.232206235305841 \* 10-5** atomic units.

Quartic Spline:

Acceleration of the bond stretch when C is separated by O by 3 atomic units is **-2.215714021043643 \* 10-5** atomic units.

Pentic Spline:

Acceleration of the bond stretch when C is separated by O by 3 atomic units is **-2.189079674704397 \* 10-5** atomic units.

Answers for the cubic spline may be found below “**Question 3 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_1.py**”.

Answers for the quartic spline may be found below “**Question 3 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_2.py**”.

Answers for the pentic spline may be found below “**Question 3 Answer Below:**” in the output of the code titled, “**So\_Much\_Potential\_CISD\_Reem\_3.py**”.

**References:**

1. Properties of Subatomic Particles. <http://www.kentchemistry.com/links/AtomicStructure/subatomic.htm> (accessed Feb 23, 2019).
2. Weinhold, F.; Landis, C. R. *Discovering chemistry with natural bond orbitals*; Wiley: Hoboken, NJ, 2012.