The Mathematical Modeling of the Photo-ionization of Dichloromethane

Stephen Tivenan

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   - Hartree Fock Approximation
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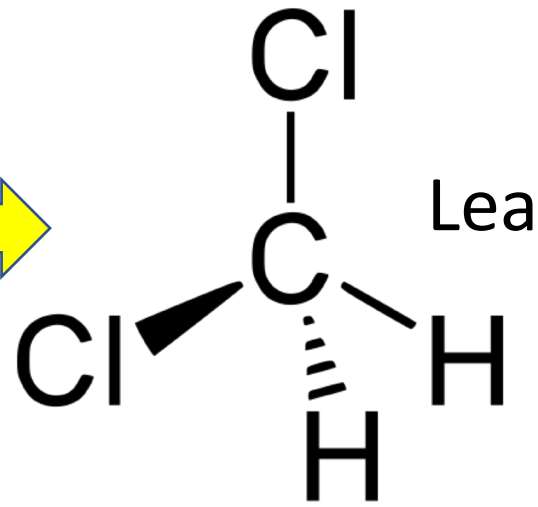
Physical Experiment

$E = h\nu$



[1]

Leads to Fragmentation..

Specific Channels:

$CH_2CL_2 \rightarrow CH_2 + Cl_2^+ + e^-$

$CH_2CL_2 \rightarrow CH_2^+ + Cl_2 + e^-$

Question: Which of these two specific channels is preferred?

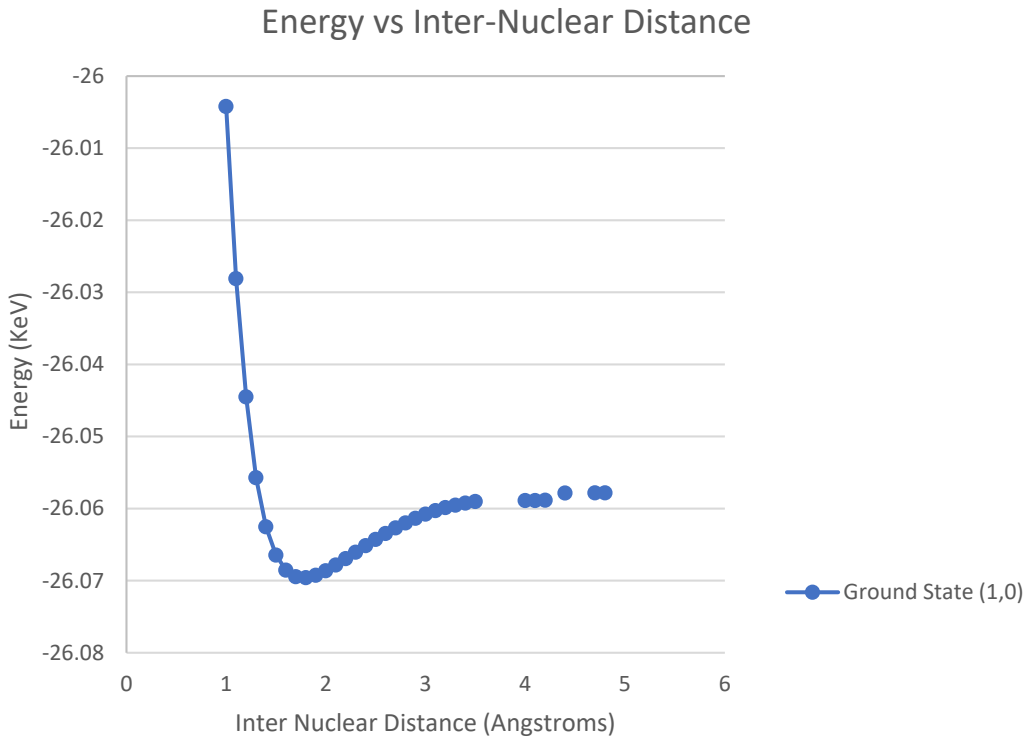
Answer: Examining Multiple Potential Energy Curves

Potential Energy Curves

Inter-nuclear Bond Length

Energy

- The energy of the molecule is the lowest Eigenvalue of our Molecular wavefunction at specific internuclear distance



R=1.77 Å

Born-Oppenheimer Approximation

- Assume Nuclei is stationary to electron

$$\hat{\mathcal{H}}\ \psi(r, r_1, r_1, r_2..r_N, R_1, R_2..R_M) \longrightarrow \hat{\mathcal{H}}\psi(r, r_1, r_1, r_2..r_N)$$

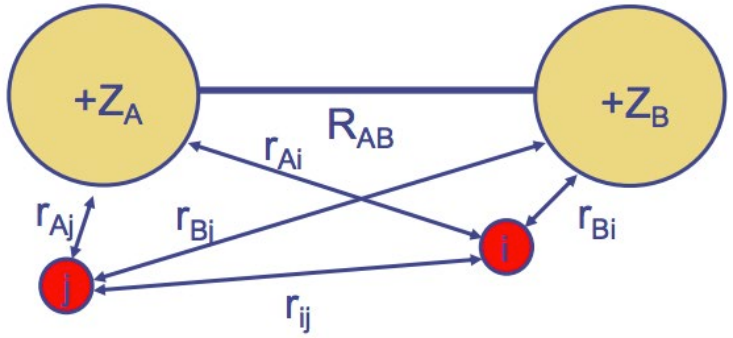
Hartree-Fock Approximation

$$\hat{\mathcal{H}}\ \psi(r, r_1, r_1, r_2..r_N) \longrightarrow \hat{\mathcal{H}}\ \psi(r) = E\ \psi(r)$$

$$\{\psi(r)\} = \{\psi(r), \psi(r), \psi(r) \ldots\}$$

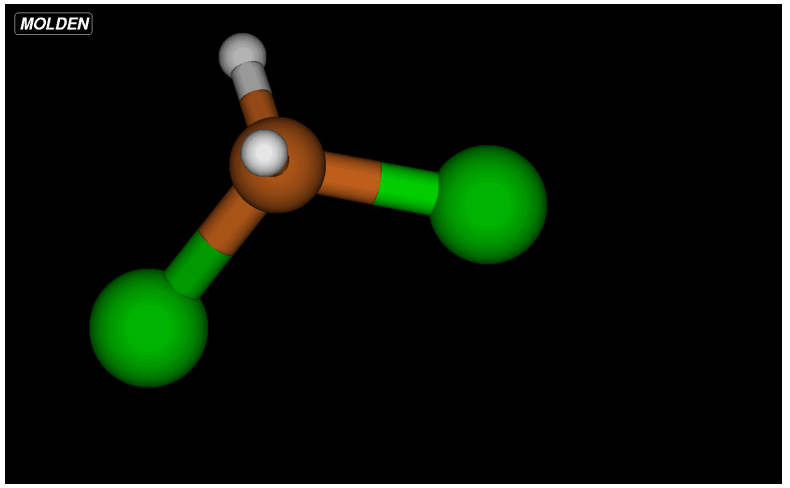
$$\hat{\mathcal{H}}\{\psi(r)\} = E\ \psi(r)$$

- Find Eigen Energy Value of Electron
  - Approximation for Eigen Energy for the Molecule for different Symmetries
  - Symmetries-Orbital and Spin



Calculation

- Set both Carbon Chloride's bond length (distance between nuclei) at specific values.
- Use Hartree-Fock to calculate the optimal Energy Eigenvalues for different symmetries
  - Dichloromethane
  - Methylene
  - Chlorine



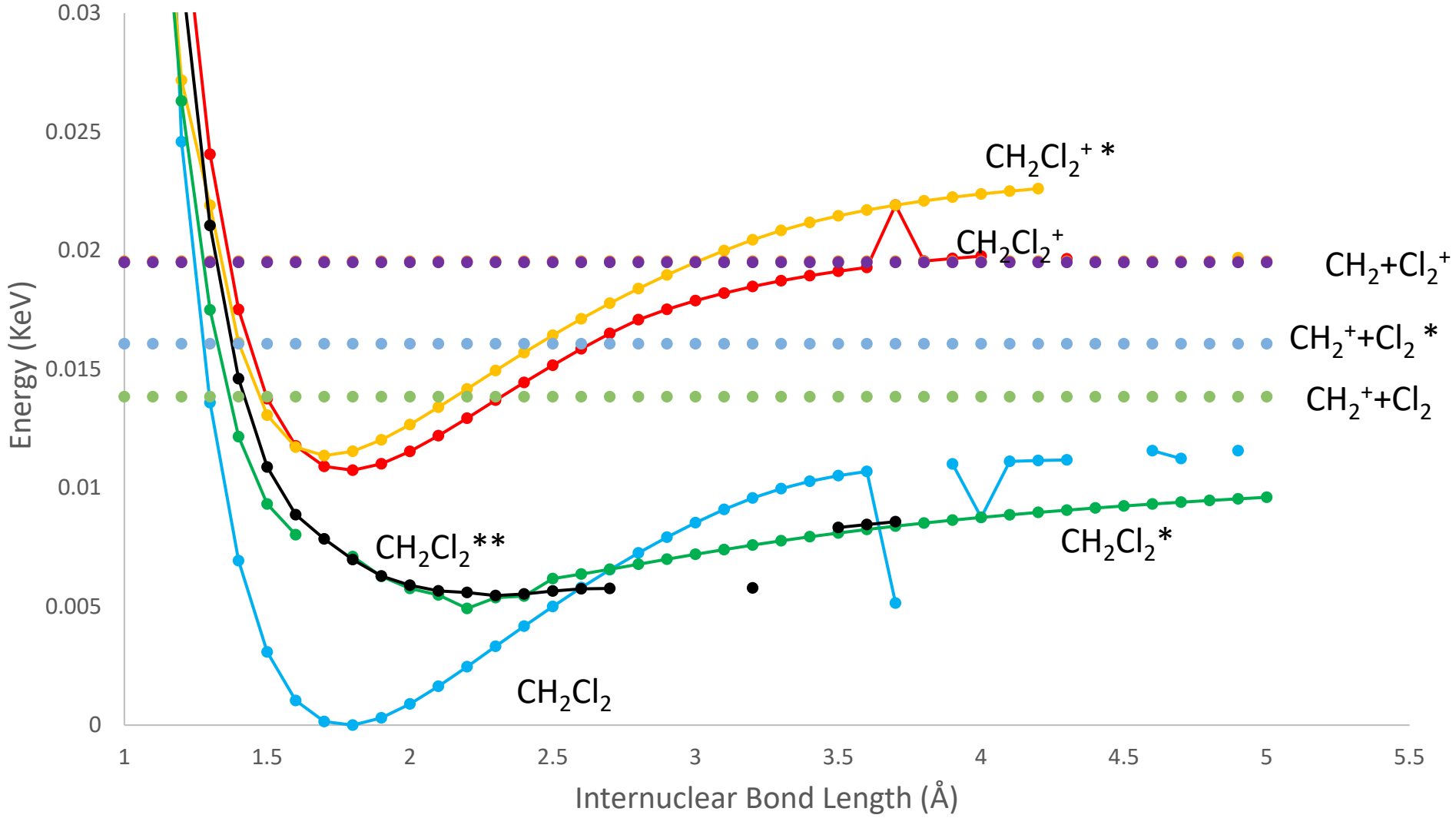
CH_2Cl_2

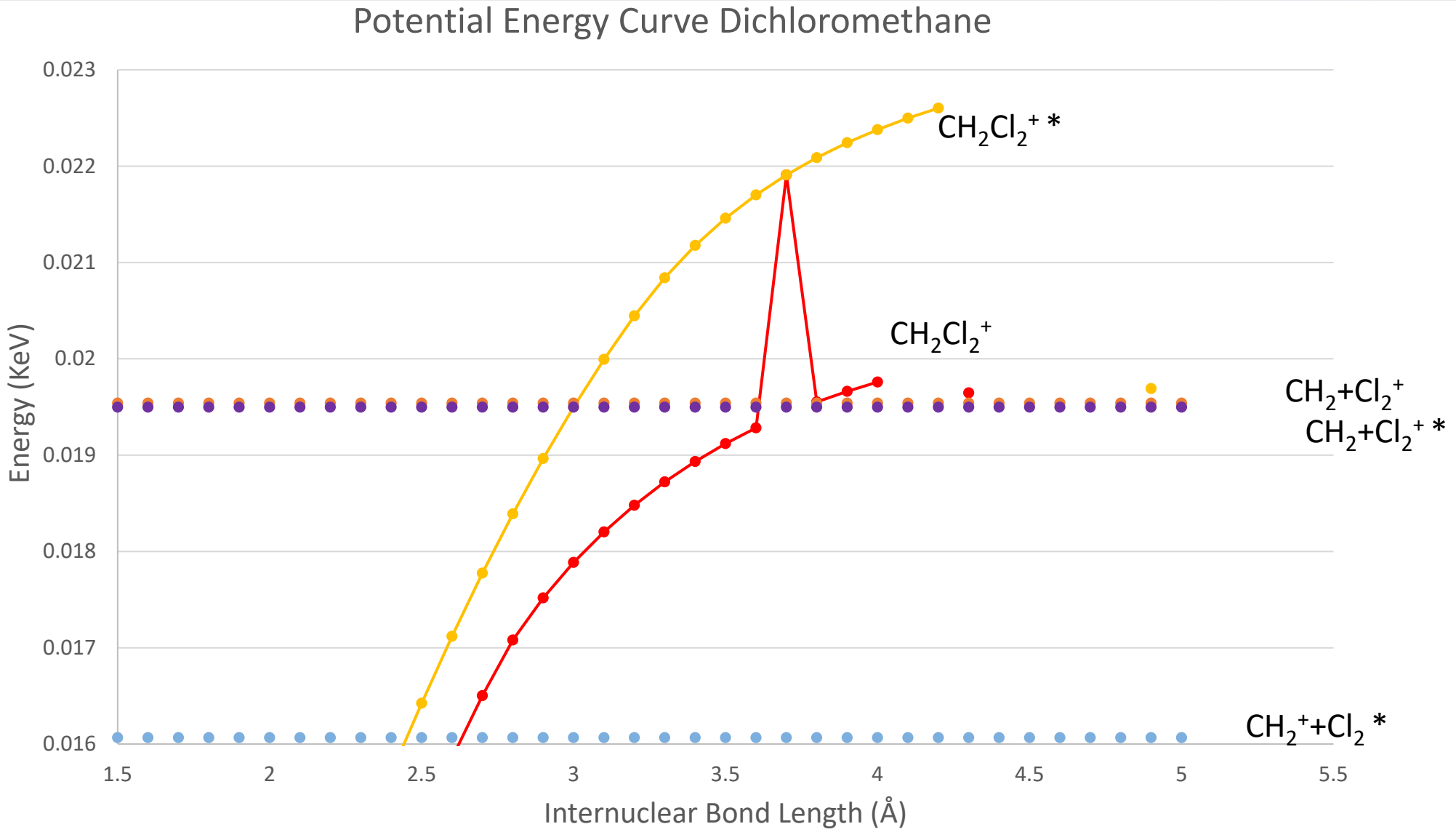
Optimal Potential Energies for Methylene and Chlorine

CH2	CH2+
-1.0498 KeV	-1.0585 KeV

Cl2	Cl2+
-24.8121 KeV	-24.7977 KeV
-24.8098 KeV	-24.7976 KeV

Potential Energy Curve Dichloromethane




Potential Energy Curve Dichloromethane
0.023
0.022
0.021
0.02
0.019
0.018
0.017
0.016
Energy (KeV)
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Internuclear Bond Length (Å)
$CH_2Cl_2^+$ *
$CH_2Cl_2^+$
CH_2+Cl_2^+
CH_2+Cl_2^+ *
CH_2^++Cl_2 *

Conclusion

- For different symmetry, Dichloromethane fragments and ionizes to
  - $CH_2CL_2 \rightarrow CH_2 + Cl_2^+ + e^-$
- Moving Forward produce more Potential Curves varying the symmetry of the molecule, different approximations
- Produce more fragment energy values with different symmetries

Citations

[1] “Organic Chemistry - Caffeine Lab.” *Science Forums*, 30 Sept. 2015, www.scienceforums.net/topic/91351-organic-chemistry-caffeine-lab/.

[2] *The Sherrill Group: Notes*, vergil.chemistry.gatech.edu/notes/index.html.

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