

**Report on the Evaluation  
of Chapter 13  
General Diatomic and  
Polyatomic Molecular Ions  
and Molecules  
in  
“The Grand Unified Theory of  
Classical Quantum Mechanics”  
by Dr. Randell L. Mills**

Prepared by

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## Executive Summary

In my analysis, I verified calculations and equations involving the H<sub>2</sub>O water molecule, the CH<sub>3</sub> methyl radical, and the F<sub>2</sub> fluorine molecule found in Chapter 13 General Diatomic and Polyatomic Molecular Ions and Molecules of the book “The Grand Unified Theory of Classical Quantum Mechanics” by Dr. Randell L. Mills. I verified equations and values to a high degree of accuracy that are associated with these three molecular systems. There is a remarkable agreement between the CQM calculated values for the energies, bond distances, and bond angles of these molecular systems and experimental values of those corresponding quantities.

## Purpose

In Chapter 13, the Classical Quantum Mechanics theory is applied to predict results pertaining to several molecules and molecular systems including the H<sub>3</sub><sup>+</sup> Molecular Ion, the OH Hydroxyl Radical, the Water Molecule H<sub>2</sub>O, Hydrogen Nitride NH, Dihydrogen Nitride NH<sub>2</sub>, Ammonia NH<sub>3</sub>, Hydrogen Carbide CH, Dihydrogen Carbide CH<sub>2</sub>, the CH<sub>3</sub> Methyl Radical, the Methane Molecule CH<sub>4</sub>, the N<sub>2</sub> Nitrogen Molecule, the O<sub>2</sub> Oxygen Molecule, the F<sub>2</sub> Fluorine Molecule, the Cl<sub>2</sub> Chlorine Molecule, the Carbon Nitride Radical CN, the Carbon Monoxide Molecule CO, and the Nitric Oxide Radical NO.

I chose to investigate in detail three of these molecules: the Water Molecule, the Methyl Radical CH<sub>3</sub>, and the Fluorine Molecule. The solution to the water molecule is very similar to that of OH except now there are two OH bonds in water. Each of the two OH bonds is a prolate spheroid, except that now the ellipsoidal MO (Molecular Orbital) can't extend into the O-atom to distances shorter than the radius of the 2p shell. The force balance equation is derived for the water molecule from such information. This determines equations for the internuclear separation, the semiminor axis, and the eccentricity of the ellipsoid. Next equations for the different energies in the molecule are derived. Then values for the internuclear distance, the semiminor axis, and the eccentricity are calculated. There is excellent agreement between the CQM-calculated value for the internuclear distance and the experimental result for the internuclear distance. Next, values for the different energies in the molecule are calculated. Then a discussion of vibration in H<sub>2</sub>O is presented. Next the Doppler energy term of the water molecule is derived. This is used to derive expressions for the total energies and bond energies of HOH and DOD. There is remarkable agreement between the CQM-derived bond dissociation energy and the experimental result for both HOH and for DOD. Finally the bond angle for the water molecule is calculated from the CQM theory and is found to be in remarkable agreement with the experimentally measured bond angle.

The solution to the methyl radical  $\text{CH}_3$  is very similar to that of  $\text{CH}_2$  except now there are three CH bonds in  $\text{CH}_3$  instead of just two. The force balance equation is derived for  $\text{CH}_3$ . This determines equations for the internuclear separation, the semiminor axis, and the eccentricity of the molecular orbital ellipsoid. Next equations for the different energies in the molecule are derived, and are found to be three times those of CH due to the three CH bonds in  $\text{CH}_3$ . Then values for the internuclear distance, the semiminor axis, and the eccentricity are calculated. There is excellent agreement between the CQM-calculated value for the internuclear distance and the experimental result for the internuclear distance. Next, values for the different energies in the molecule are calculated. Then a discussion of vibration in  $\text{CH}_3$  is presented. Next the Doppler energy term of the methyl radical is derived. This is used to derive expressions for the total and bond energies of  $\text{CH}_3$ . There is remarkable agreement between the CQM-derived bond dissociation energy and the experimental result. Finally the angle for each CH bond from the z-axis is calculated from the CQM theory.

The bond in the fluorine molecule is similar to that of an  $\text{H}_2$ -type molecular orbital. The force balance equation is derived for  $\text{F}_2$ . This determines equations and values for the internuclear separation, the semiminor axis, and the eccentricity of the molecular orbital ellipsoid. Next, equations for the different energies in the molecule are derived. There is excellent agreement between the CQM-calculated value for the internuclear distance and the experimental result for the internuclear distance. Next, values for the different energies in the molecule are calculated. Then a discussion of vibration in  $\text{F}_2$  is presented. Next the Doppler energy term of the fluorine molecule is derived. This is used to derive expressions for the total and bond energies of  $\text{F}_2$ . There is remarkable agreement between the CQM-derived bond dissociation energy and the experimental result.

## Calculation

### Water Molecule

I have verified that Equations 13.163-13.177 and the values they yield are true.

I have verified that Equations 13.178-13.182 along with their associated values are also correct.

The values in Equations 13.183-13.185 are correct as listed in the CQM book.

There is very good agreement between the internuclear distance calculated from the CQM theory and the experimental bond distance. These are compared in Equations 13.185 and 13.186.

I have verified that the values listed in Equations 13.187 and 13.188 are correct as listed.

I have verified that Equations 13.189-13.193 are also valid and correct. I have also verified the value of  $r_8$  in the line after Equation 13.189 as correct.

Likewise, I have verified that Equations 13.195-196, 13.198, and 13.200 are correct.

I have also verified that the CQM values for the values for O1s, O2s, and O2p listed in the 5<sup>th</sup> line from the bottom of page 480 are correct.

I have verified that all the energy equations 13.201-13.205 are correct and yield the values listed.

I have verified that Equations 13.207-13.213 and their values are correct as listed. I have also checked the value for  $E_{\text{vib}}$  listed in the line before Equation 13.212 and it is correct.

Likewise Equations 13.214-215 are correct along with their values that are listed. I have also checked the value for  $E_{\text{vib}}$  listed in the line before Equation 13.215 and it is correct.

I have verified that Equations 13.217-13.222 are valid along with the values listed in those equations.

There is a remarkable agreement between the CQM value calculated for the HOH bond dissociation energy and its experimental result, given in Equations 13.222 and 13.223.

I have verified that Equations 13.224 and 13.225 are valid.

In Equation 13.226, I get 5.175 eV, but Mills gets 5.178 eV.

Again, there is very good agreement between the CQM value calculated for the DOD bond dissociation energy and its experimental result, given in Equations 13.226 and 13.227.

I have verified that Equations 13.228-13.230 are correct as presented. Equation 13.233 has also been verified as correct.

The values listed in Equations 13.234-13.238 and Equations 13.241-13.242 have been verified to be correctly calculated from the CQM theory.

There is remarkable agreement between the internuclear distance of the two H atoms calculated from the CQM theory and its experimental value, listed in Equations 13.236 and 13.243.

There is also excellent agreement between the O-H bond angle calculated from the CQM theory and its experimental result, listed in Equations 13.242 and 13.244.

### Methyl Radical CH<sub>3</sub>

I have verified as correct Equations 13.539 and 13.541-545, and the values they contain.

I have verified as correct Equations 13.546-13.554, and the values they contain (except for Equation 13.548 which is an experimental result).

There is also excellent agreement between the internuclear distance calculated from the CQM theory and its experimental result, listed in Equations 13.547 and 13.548.

I have verified as correct Equations 13.555-13.561 and their associated values.

I verified that Equations 13.562-13.566 and Equations 13.568-13.569 and their values are correct.

I verified that Equations 13.571-13.572 and 13.574 are correct including the values they produce.

There is very good agreement between the CH<sub>3</sub> bond dissociation energy calculated from the CQM theory and the experimental result (Equations 13.572 and 13.573).

### Fluorine Molecule

I have verified that Equations 13.709 and 13.711-13.729 are correct.

I have verified that Equations 13.731-13.732 are correct.

There is a remarkable agreement between the CQM-derived value for the F<sub>2</sub> internuclear distance and the experimental result, given in Equations 13.729 and 13.730.

I have verified that all energy equations and values in Equations 13.733-13.739 are correct.

I have verified as true all the equations and values listed in Equations 13.740-750.

There is good agreement between the CQM-derived value for the F<sub>2</sub> bond dissociation energy and its experimental result, given in Equations 13.750 and 13.751.

The entries in Table 13.1 for all the values for H<sub>2</sub>O, D<sub>2</sub>O, CH<sub>3</sub>, and F<sub>2</sub> are shown to be correct.

## Conclusion

I was able to verify the CQM results of Chapter 13 in excellent agreement with my own calculations for the three molecules  $\text{H}_2\text{O}$ ,  $\text{CH}_3$ , and  $\text{F}_2$ . I successfully reproduced almost all of the equations and their corresponding values for these three molecules found in Chapter 13. There was excellent agreement between many of the calculated results based on the CQM theory and their corresponding experimental values, such as internuclear distances and bond dissociation energies for these molecules. This chapter demonstrates that the CQM theory is successful in not only describing atomic systems as it did in Chapters 1-10, but it is also successful at describing molecular systems, to a high degree of accuracy.

I find my results and calculations to be confirmation that the calculations and equations of Chapter 13 for the Water Molecule,  $\text{CH}_3$  Methyl Radical, and Fluorine Molecule are indeed accurate, valid, and reproducible.