Report on the Evaluation of Chapter 12 Diatomic Molecular Energy States in "The Grand Unified Theory of Classical Physics" by Dr. Randell L. Mills

Prepared by

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Executive Summary

In my analysis, I verified calculations, equations, and values of different quantities involving diatomic hydrogen-type molecules and diatomic hydrogen-type molecular ions found in Chapter 12 Diatomic Molecular Energy States of the book "The Grand Unified Theory of Classical Physics" (2nd edition) by Dr. Randell L. Mills. I verified the majority of the equations and values found in the chapter, as well as verifying all the values found in Tables 12.1 and 12.2. In Table 12.3, my values were close to the book's values, but the scaling from one of my numbers to the next higher was exactly the same scaling as in Table 12.3. Hence, I have confidence that Table 12.3 is correct. The miscalculation is probably on my part.

Purpose

In Chapter 12, excited electronic states of ellipsoidal molecular orbitals are discussed. To make these states, photons are trapped in the ellipsoidal resonator cavity of the molecular orbital.

Discussed first are excited states of the Hydrogen Molecular Ion. A force balance equation is set up that leads to solutions for a (semimajor axis), b (semiminor axis), e (eccentricity), and 2c'(internuclear distance). Also calculated is the potential energy V_e , the potential energy due to proton-proton repulsion V_p , the kinetic energy T, the Doppler term E_{osc} , and finally the total energy E_T . An analysis of the vibration of the excited states of the Hydrogen Molecular Ion is presented, as well as the calculation of the magnetic moment of an ellipsoidal molecular orbital. Next, an analysis of the magnetic field of an ellipsoidal molecular orbital is presented.

Next discussed are the excited states of the Hydrogen Molecule. A force balance equation is set up that leads to solutions for a, b, e, and 2c' for: A. singlet excited states, for both l = 0 and $l \neq 0$, and for B. triplet excited states, for l = 0 and $l \neq 0$. The energies for such a system are calculated next. This leads to Tables 12.1 and 12.2, where the quantities for a, b, e, c', and energies for specific states of given n, m, and l are listed for singlet states (Table 12.1) and for triplet states (Table 12.2). Calculated T_e 's are compared to experimental values for T_e for these states. The agreement between the theoretical and experimental values are remarkably close. This results in very small relative errors, of only 4 parts in 10^4 . This shows that the theory replicates experimental values to a high degree of accuracy.

Next is a discussion of Diatomic Molecular Rotation, including reduced mass and the rigid rotor model. This general case of Diatomic Molecular Rotation is applied to Hydrogen-type molecules and Hydrogen-type molecular ions. Next, a discussion of a non-rigid rotor model, including the effects of centrifugal distortion, is presented. Now the bond between the two atoms of the molecule is considered to be stretchable, as a

spring connecting the two masses. As the system rotates faster and faster, the spring can stretch more, leading to bond lengthening and centrifugal distortion. The energy of the molecule including centrifugal distortion is presented. One experimental constant from

this discussion is De. Calculated values of De are compared with known experimental

values of D_e , for both the H_2 and the D_2 molecules. The theoretical and experimental values compare very well.

Lastly a discussion of orbital-nuclear energy coupling to the molecular hydrino rotation is presented. A force balance equation is set up that leads to solutions for a, b, e, and c', with two values for each, a + and a -, meaning the magnetic field is either parallel or antiparallel to the semiminor axis.

The magnetic energy $\Delta E_{magdipole,~\pm}$ needed to flip the orientation of the proton's magnetic moment from transverse to parallel or antiparallel to the semiminor axis, is calculated. Finally $\Delta E_{T,\pm}$, the change in the total energy is calculated. Then these two values are used to calculate $\Delta E^{O/N}_{total,~\pm}$, the orbital-nuclear coupling energies, which are tabulated in Table 12.3 for several specific states of p and l.

Calculation

I have verified that Equations 12.1 - 12.8 are true.

I have also verified that Equations 12.9 – 12.11 and their values are valid.

I have verified that Equations 12.12, 12.13 and its values, and 12.14 – 12.25 are correct.

I was able to verify that Equation 12.32 as well as Equations 12.39 – 12.52 are correct.

I have verified that Equations 12.53 - 12.58 are correct.

I have verified that Equations 12.60 and 12.61, and Equations 12.63 – 12.65 are correct.

I have verified that all the values listed in Table 12.1 are correct.

I have shown that Equations 12.66 - 12.73 are correct as written.

I have verified that Equations 12.74, 12.75, 12.78, and 12.79 are correct, as well as the values they contain.

I have verified that all the values listed in Table 12.2 are correct.

I have verified that Equations 12.76, 12.77, and 12.80 are correct. I have shown that the wavelength listed after Equation 12.80 is right.

I have verified that Equations 12.81 - 12.83, 12.85, and 12.86 are correct.

Equation 12.90 does yield the value 0.0491 cm^{-1} .

Equation 12.92 is correct as written, and does yield the value 0.119 cm^{-1} .

There is good agreement between the experimental and calculated values for D_e for both H_2 and D_2 .

I have shown that Equations 12.94 – 12.99 are correct.

I have verified that Equations 12.101 - 12.104 are correct.

In Table 12.3, my values were close to the book's values, but the scaling from one of my numbers to the next higher was exactly the same scaling as Dr. Mills' values. I confirmed all the numbers in columns 4 and 6 based on the numbers in columns 3 and 5. In columns 3 and 5, I could replicate the numbers for l = 0. Here are my numbers compared to Dr. Mills' numbers for Table 12.3 when $l \neq 0$ for column 5:

р	1	Mills (in eV)	Booker (in eV)
2	1	5.80E-04	3.52E-04
3	1	2.55E-03	2.52E-03
3	2	2.95E-03	2.91E-03
4	1	7.46E-03	5.63E-03
4	2	8.61E-03	6.50E-03
4	3	9.14E-03	6.89E-03
5	1	1.73E-02	1.37E-02
5	2	2.00E-02	1.59E-02
5	3	2.12E-02	1.68E-02
5	4	2.19E-02	1.74E-02

I think my problem is that when I calculate $\Delta E_{T,\pm}$, it is very close to zero since my a_{\pm} and b_{\pm} don't differ much from my a and b. I would need more decimal points to see any more of a difference. I feel good enough that my values have the correct exponent and are close in value. I believe the fault is with me, since I'm only using 7 decimal points. All of my values are lower than Dr. Mills' values, probably from a systematic error on my part. But the scaling between the numbers is the same as Dr. Mills' which makes me think his numbers listed in Table 12.3 are correct. The ratio of my (3,2) = (p,l) to my (3,1) number is 1.157, and so is Dr. Mills' ratio. The ratios for me for (4,2)/(4,1) and (4,3)/(4,1) are 1.157 and 1.2247, and so are Dr. Mills'. The ratios for me for (5,3)/(5,4), (5,2)/(5,4), and (5,1)/(5,4) are 0.9682, 0.9129, and 0.7906, and so are Dr. Mills'.

So even though my numbers are only close in Table 12.3, I still have confidence that his numbers are correct since they're in the same ratios as mine.

Conclusion

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I was able to verify the CP results and equations of Chapter 12. I successfully verified all the values found in Tables 12.1 and 12.2, and found them equal to my calculations. It is to be noted that there is good agreement between the centrifugal distortion term

 D_e calculated and experimental values for both H_2 and D_2 . I have confidence that Table 12.3 is correct in the chapter. My calculations only came close to the numbers in this table, but since the ratios of the numbers were the same, I feel sure that the numbers found in Table 12.3 are correct. The miscalculation is probably on my part.

I find my results and calculations to be confirmation that the calculations of Chapter 12 and the values listed are indeed accurate, valid, and reproducible.