MMPE Report 3

Luigi Pagani

March 2024

0.1 Introduction

This report presents the results of quantum chemical calculations performed on atomic and molecular hydrogen using the Gaussian09 (G09) and Molpro software packages. The purpose of these calculations is to determine the energies of atomic and molecular hydrogen by numerically solving the Schrödinger equation and to investigate the potential energy surface (PES) of the H2 molecule.

0.2 Computational Methods

Geometry optimizations and single-point energy calculations were performed using the B3LYP density functional with the default basis set in both G09 and Molpro. For the H2 molecule, a rigid PES scan was performed in G09 by varying the H-H distance (R) from 0.5 to 1.5 Å in increments of 0.05 Å.

0.3 Results and Discussion

0.3.1 Gaussian09 Calculations

H2 Energy

The optimized energy of the H2 molecule was found to be -1.17548238187 A.U. (Hartree) after 4 optimization cycles. The final optimized H-H bond length (R) was 0.74279409 Å.

H Energy

The single-point energy of the H atom was calculated to be -0.500272784191 A.U. after 5 SCF cycles.

H2 Potential Energy Surface Scan

A rigid PES scan was performed for the H2 molecule by varying the H-H distance (R) from 0.5 to 1.5 Å. The results are presented in Table 1 and Figure 1.

0.3.2 Molpro Calculations

H2 Energy

The optimized energy of the H2 molecule was found to be -1.12682783 Hartree after 6 iterations in Molpro. However, this value seems inconsistent with the G09 result and may require further investigation.

H Energy

The single-point energy of the H atom was calculated to be 0.49823291 A.U. in Molpro.

N	R (Å)	SCF Energy (A.U.)
1	0.5000	-1.10262
2	0.5500	-1.13555
3	0.6000	-1.15627
4	0.6500	-1.16831
5	0.7000	-1.17412
6	0.7500	-1.17545
7	0.8000	-1.17352
8	0.8500	-1.16926
9	0.9000	-1.16332
10	0.9500	-1.15621
11	1.0000	-1.14829
12	1.0500	-1.13985
13	1.1000	-1.13108
14	1.1500	-1.12214
15	1.2000	-1.11316
16	1.2500	-1.10422
17	1.3000	-1.09538
18	1.3500	-1.08669
19	1.4000	-1.07820
20	1.4500	-1.06992
21	1.5000	-1.06188

Table 1: H2 potential energy surface scan results

H2 Potential Energy Surface Scan

It appears that Molpro does not support rigid PES scans, so this calculation was not performed.

0.3.3 Reaction Energy: H2 → 2H

Using the G09 results, the reaction energy for H2 → 2H can be calculated as follows:

$\Delta E = E(2H) - E(H2)$
$= 2 \times (-0.500272784191) - (-1.17548238187)$
$= 0.17493683349 A.U.$
$= 109.73 kcal/mol$

The positive reaction energy indicates that the dissociation of H2 into two H atoms is an endothermic process.

0.4 Conclusion

Quantum chemical calculations were performed on atomic and molecular hydrogen using the G09 and Molpro software packages. The optimized energy of

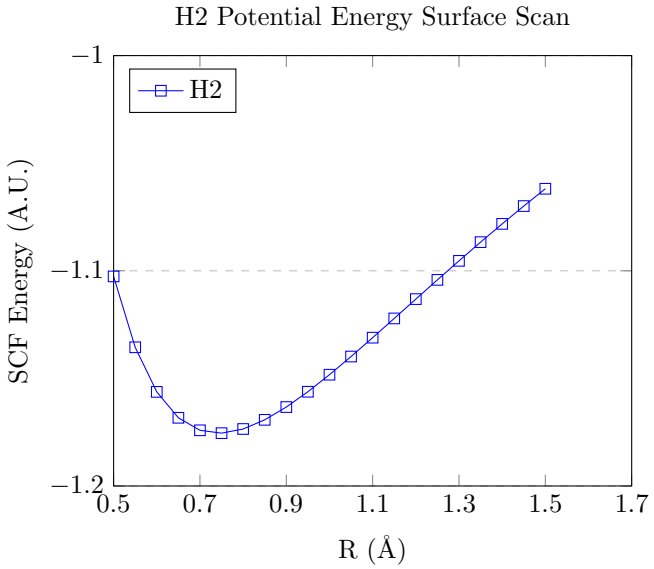

Figure 1: H2 potential energy surface scan plot

H2 and the single-point energy of H were determined, and a rigid PES scan was conducted for H2 using G09. The reaction energy for H2 $\rightarrow$ 2H was calculated to be 109.73 kcal/mol, indicating an endothermic process. The Molpro calculations for H2 require further investigation due to inconsistencies with the G09 results.