Experiment 10: Final Review

You are the consultant

> Tip
>
> **At a glance.** Three species, and every choice is yours. **You will show** that you can choose and justify a method, set up the calculations properly, and report the results the way a computational paper would.

The request

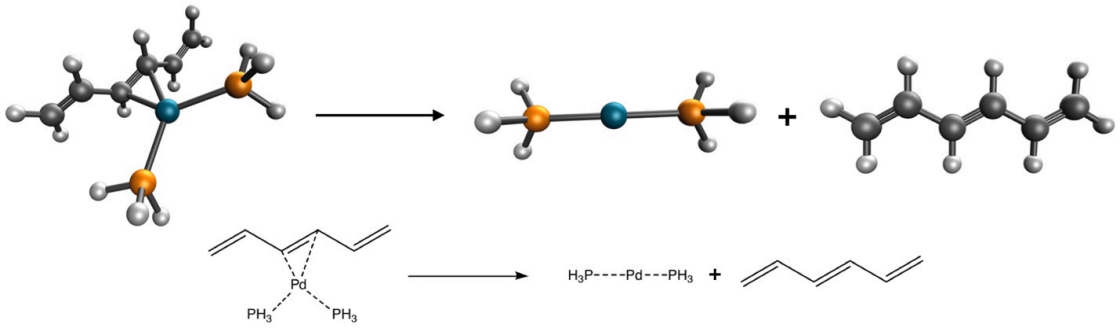


Figure 1: Dissociation of the diphosphinohexatrienepalladium(0) complex. Carbon is black, phosphorus orange, hydrogen white and palladium light blue; dotted lines are dative bonds.

Imagine that a colleague in your department is studying this palladium complex (the structures come from the PdBE2 subset [1] of the Minnesota 2015B database [2]) and asks you to calculate the bond dissociation energy of the reaction above. You are in charge of setting up the calculations.

Choose the functional and basis set based on:

- the published literature, for instance these recent benchmarks [2], [3], [4], [5], [6], [7], [8], [9], [10], [11];
- the functionals available in Q-Chem;
- what you learned in Experiments 1–9: basis-set convergence, dispersion, grids, stability analysis.

Remember that every calculation is a compromise between accuracy and computational cost, and the free server stops jobs after **10 minutes**. Pd needs an effective core potential (`ECP = def2-ECP` with the def2 basis sets).

Your method card

Choose every setting and write down *why*. The card warns you about common pitfalls (double-counting dispersion, grid-sensitive functionals) and estimates whether each job fits in the free server's 10-minute limit. It then gives you the three Q-Chem inputs for your choice.

Enter your results

Record the three total energies, SCF cycles and wall times from your outputs, then your bond dissociation energy $\Delta E = E(Pd(PH_3)_2) + E(C_6H_8) - E(\text{complex})$.

Your report

Write a short report (**about 300 words**) that:

1. has a title;
2. states the method you chose and **why**, citing the literature;
3. describes the computational setup completely (program, functional, basis set, ECP, grid, stability analysis, convergence criteria), enough for someone else to reproduce your numbers;
4. presents your results and compares them with the reference value of **16.20 kcal/mol**;
5. ends with an appropriate reference section.

> **i** Note
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> **Peer review.** Your instructor may ask you to review two classmates' reports on Canvas with a short rubric: is the method justified, is the setup reproducible, is the comparison with the reference honest?

Bibliography

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