# Worksheet 1: Quantum mechanical approaches: Hückel approximation and DFT methods

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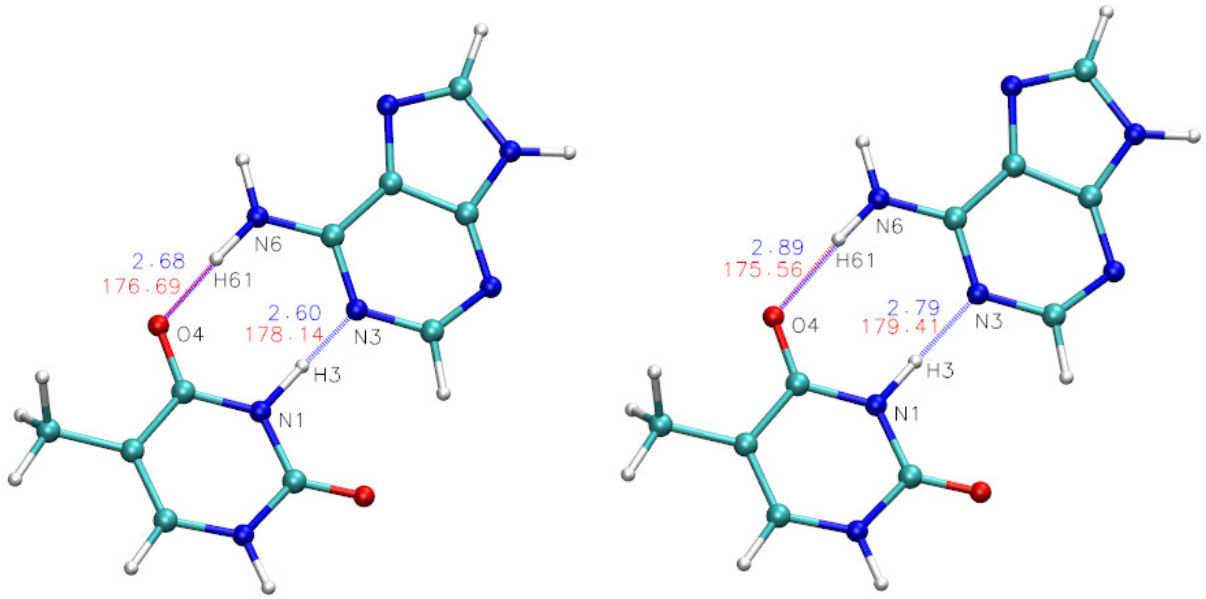
## Contents

# 1 Computational Task: DFT calculations with Siesta

## 1.1 Geometry optimization of adenine

| Distance | Here | Ref [20] | Ref [7] | Exp | Angle | Here | Ref [20] | Ref [7] | Exp |
|---|---|---|---|---|---|---|---|---|---|
| C2-N3 | • | • | • | • | • | • | • | • | • |
| N1-C2 | • | • | • | • | • | • | • | • | • |
| C6-N1 | • | • | • | • | • | • | • | • | • |
| C5-C6 | • | • | • | • | • | • | • | • | • |
| C4-C5 | • | • | • | • | • | • | • | • | • |
| N3-C4 | • | • | • | • | • | • | • | • | • |

## 1.2 Theoretical Prediction of Watson-Crick Hydrogen-bond length in adenine-thymine base pair




*(a)* LDA *(b)* GGA

*Figure 1:* Results for two flavours of XC functional. Blue numbers show bond lengths and red ones show bond angles.

| Angle in Å | LDA | GGA | Literature [1] |
|---|---|---|---|
| O4-H61-N6 | 176.7 | 175.6 | 175.8 |
| N1-H3-N3 | 178.1 | 179.4 | 178.1 |

*Table 1:* Bond angles

| Distance in Å | LDA | GGA | Experiment 1 [1] | Experiment 2 [1] |
|---|---|---|---|---|
| O4-N6 | 2.68 | 2.89 | 2.95 | 2.93 |
| N1-N3 | 2.60 | 2.79 | 2.82 | 2.85 |

*Table 2:* Bond lengths

TODO: Write some text. Write down number of steps.

[1] source: Attachment1b.pdf