11月14日上机实习安排

使用MS软件DMol3模块完成：

Locate the transition state (TS) of S_{N2} reaction, F^- (g) + CH_3F (g) → CH_3F (g) + F^- (g) by using LST/QST method:

1. Geometry optimizations of initial state (IS) and final state (FS)
2. Transition state search
3. TS further optimization
4. Transition state confirmation

1. Geometry Optimization of IS

- Put $F^{-}\cdots CH_3F$ as IS into a crystal cell with the volume of 20 Å×20 Å×20 Å
- DMol3 **Geometry Optimization** setting:

✓Geometry optimization quality: Fine

✓PBE-D (Grimme) functional

✓Charge "-1"

✓Integration accuracy: Medium

✓SCF tolerance: Medium (1e-5)

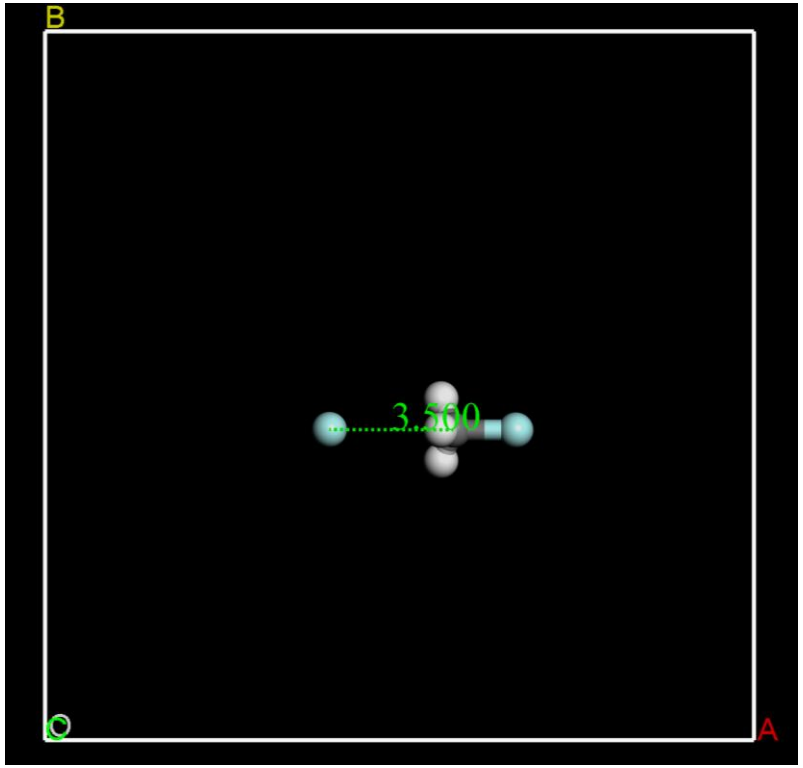
✓K points: Gamma

✓Core treatment: Effective Core Potentials

✓Basis set: DNP (4.4)

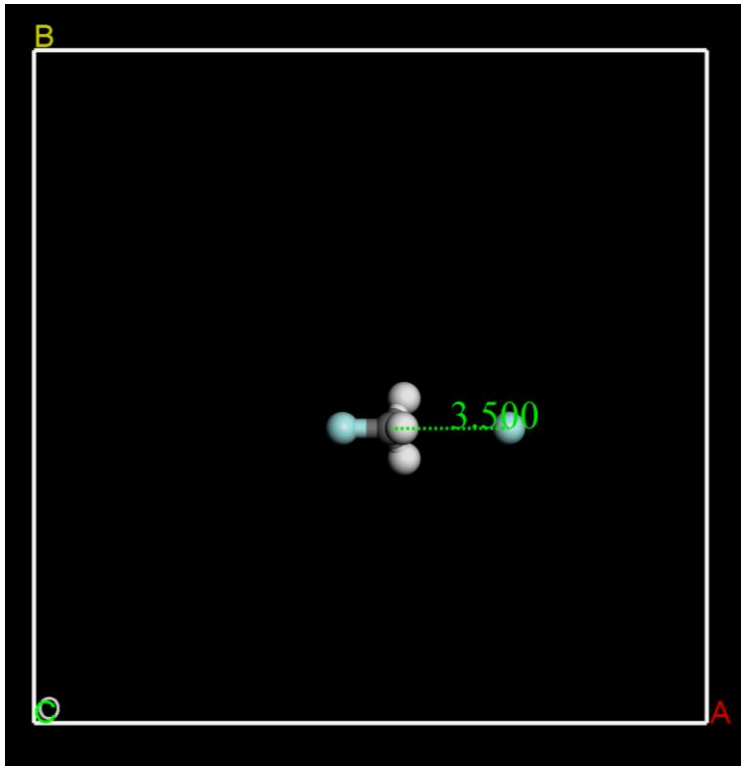
✓Mark **"using smearing (0.01 a.u.)"**

✓Orbital cutoff: 5.0 Å



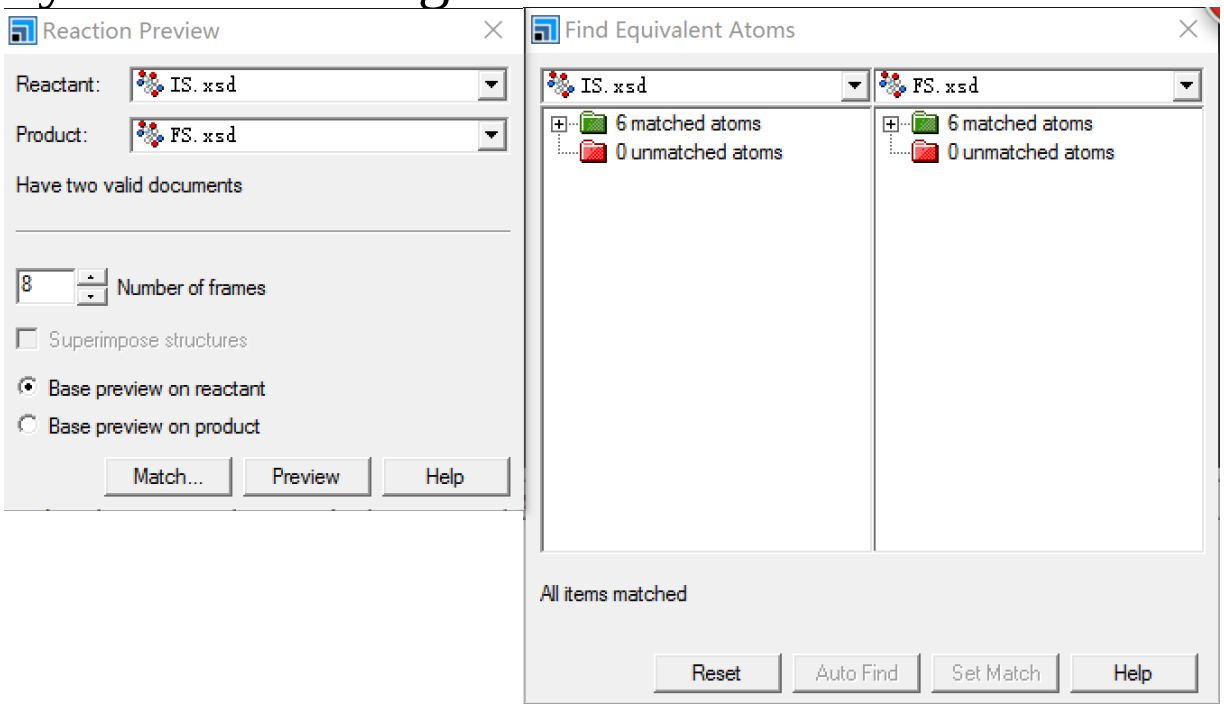
1. Geometry Optimization of FS

- Put $FCH_3\cdots F^-$ as FS into a crystal cell with the volume of 20 Å×20 Å×20 Å
- Keep the sequence of atomic coordination as the same as IS



2. Transition State (TS) Search

- Open **IS.xsd and FS.xsd** files
- Tools → Reaction Preview, import two *.xsd files as IS and FS
- Match atoms
- Determine how many frames to be generated
- Press “Preview”



2. Transition State (TS) Search

- Obtain IS-FS.xtd file and open it
- DMol3 **TS Search** setting:
  - ✓Search protocol: Complete LST/QST
  - ✓Quality: Medium
  - ✓Properties Tab: mark “Frequency”
- After TS search, check *.outmol file for reaction barrier and frequency results or open *.xsd file Tools → Vibrational Analysis → Calculate

3. TS Further Optimization

- Open TS.xsd file
- DMol3 **TS Optimization** setting:

✓Quality: Fine

✓Properties Tab: mark “Frequency”

4. TS Confirmation

- Open TS.xtd file
- DMol3 **TS Confirmation** setting:
  - ✓Quality: Fine
  - ✓Path quality: Coarse (determine the number of MEP (minimum energy path) path)
  - ✓Properties Tab: **Do not mark "Frequency"!!!**
- After TS confirmation, check *.xcd and *.outmol files for further information