11月6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:

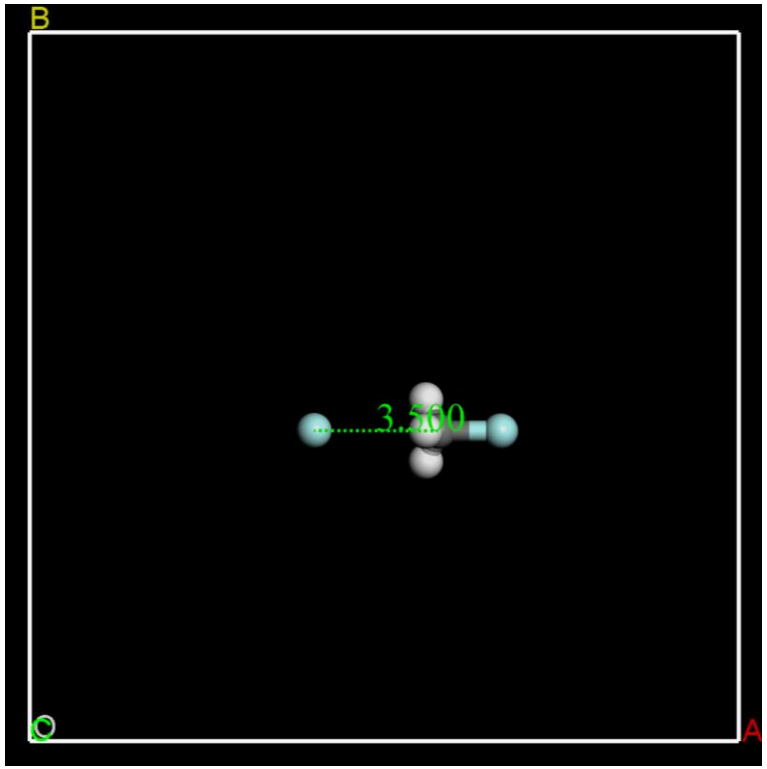
1. Geometry optimizations of **initial state (IS)** and **final state (FS)**
2. Transition state search
3. Transition state confirmation
4. TS further optimization

1. Geometry Optimization of IS

① Put $F^{-}\cdots CH_3F$ as IS into a crystal cell with the volume of 30 Å × 30 Å × 30 Å

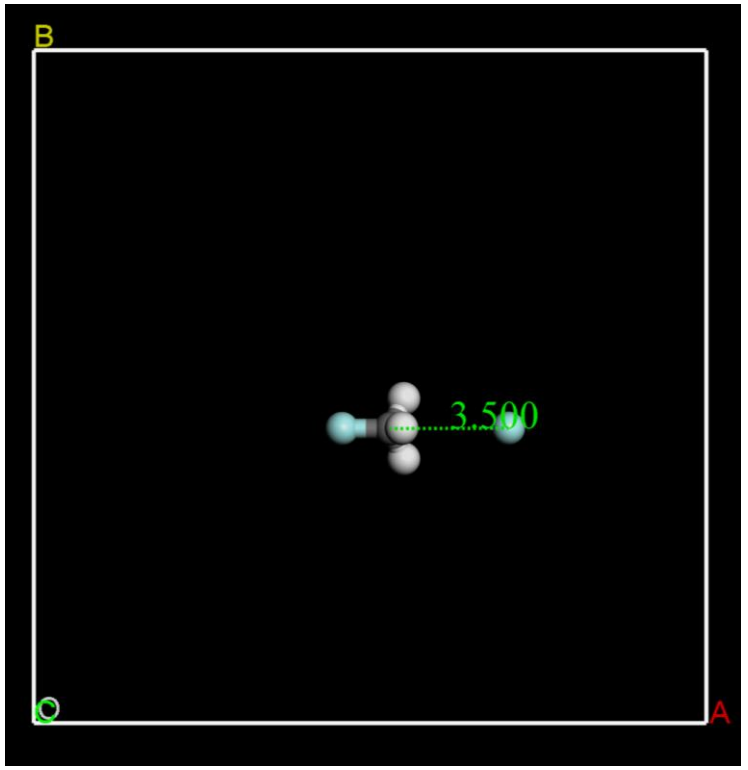
② DMol3 **Geometry Optimization** setting:

- ✓Geometry optimization quality: Fine
- ✓PBE-D (Grimme) functional
- ✓**Charge "–1"**
- ✓Integration accuracy: Fine
- ✓SCF tolerance: Medium (1e−5)
- ✓K points: Gamma
- ✓Core treatment: Effective Core Potentials
- ✓Basis set: DNP (4.4)
- ✓Orbital cutoff: 5.0 Å



1. Geometry Optimization of FS

- Copy IS to new **xsd** file
- Generate FS ($FCH_3 \cdots F^-$) by changing coordinates of C and H atoms of IS
- **Keep the sequence of atomic coordination as the same as IS**



2. Transition State (TS) Search

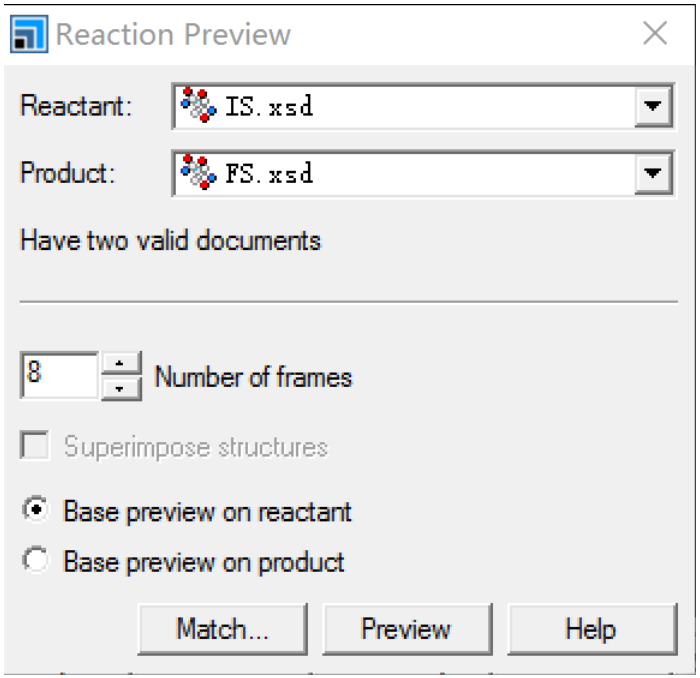
① Open **IS.xsd and FS.xsd** files

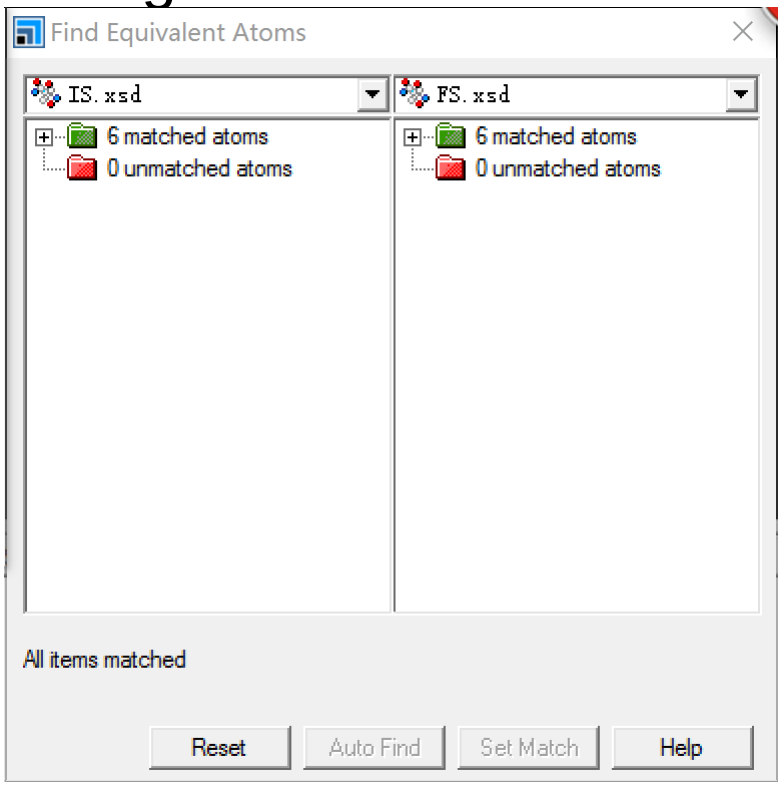
② Tools → Reaction Preview, import two *.xsd files as IS and FS

③ Match atoms

④ Determine how many frames (8) to be generated

⑤ Press “Preview”





2. Transition State (TS) Search

① Obtain IS-FS.**xtd** file and open it

② DMol3 **TS Search** setting:

- ✓Search protocol: Complete LST/QST
- ✓Quality: Fine
- ✓Properties Tab: mark “Frequency”

③ After TS search, check *.outmol file for reaction barrier and frequency results or open *.xsd file Tools → Vibrational Analysis → Calculate

3. TS Confirmation

① Open TS.**xtd** file

② DMol3 **TS Confirmation** setting:

- ✓Quality: Fine
- ✓Path quality: Medium
- ✓Max. images: The number of intermediate NEB images used during the transition state confirmation.
- ✓Properties Tab: **Mark "Frequency"!!!**

③ After TS confirmation, check *.xcd and *.xtd files for further information

4. TS Further Optimization

① Open TS.**xsd** file

② DMol3 **TS Optimization** setting:

- ✓Quality: Fine
- ✓Properties Tab: mark “Frequency”