In this problem set, you will use CPMD to study the dynamics of a proton transferring among water molecules (H$_9$O$_4^+$). And you can compare what you observe with the literature report (Ref: *Nature*, vol. 397, 1999, 601).

Solution:
The detailed procedure has been described in the problem statement. Here in the solution, we will only present the snapshots from the simulations (5000 steps).

[Left: DynamicBond; Right: Hydrogen Bond]

Snapshot 1 (Frame 1): H$_9$O$_4^+$ has an H$_3$O$^+$ core that donates three hydrogen bonds to its neighboring H$_2$O molecules. (Similar to Fig. 1a in Ref.)

Snapshot 2 (Frame 141): One of the three protons of the H$_3$O$^+$ core migrates along its hydrogen bond and forms an H$_5$O$_2^+$, in which this proton is equally share between two water molecules. (Similar to Fig. 1b in Ref.)
Snapshot 3 (Frame 335): $\text{H}_3\text{O}_4^+$ formed again. And three are three hydrogen bonds in the system again.

Snapshot 4 (Frame 434): Further migration of a different proton in $\text{H}_3\text{O}^+$ forms another $\text{H}_5\text{O}_2^+$ with one hydrogen bond. (Similar to Fig. 1d in Ref.)