

Figure captions

Figure 1S. Interaction energies of the H-bonded trimer (top) (**I**-fragment1) and the C–H··· π bonded trimer (bottom) (**I**-fragment2) of **I**_{mon} (Å).

Figure 2S. Interaction energy of the H-bonded trimer (**I'**-fragment1) of **I**_{mon} (Å).

Figure 3S. Interaction energy of the H-bonded and π stacked **I'**-fragment2 of **I'**-fragment1.

Figure 4S. Stabilization energy of **I'**_{net} compared to **I'**-fragment2.

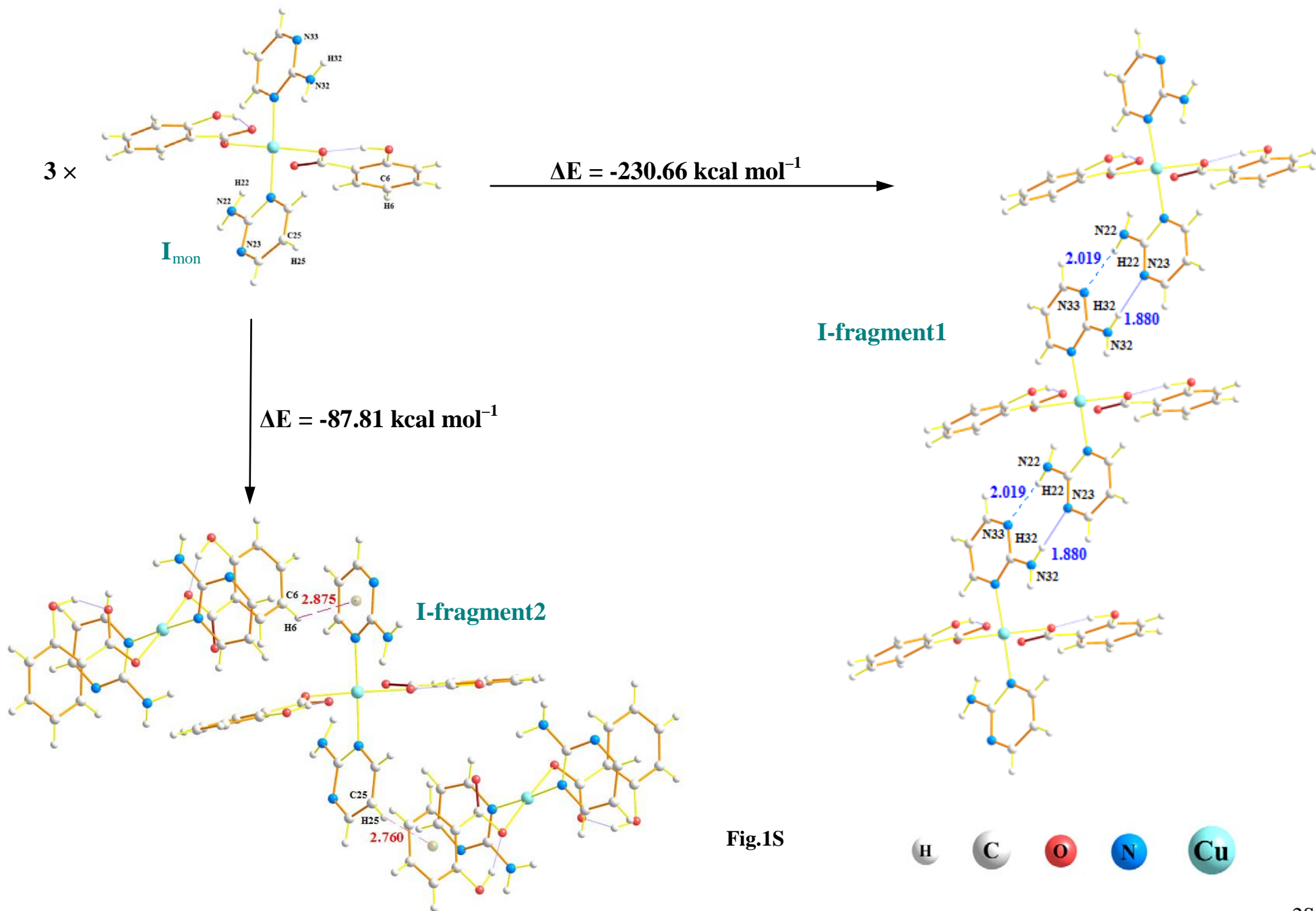


Fig.1S

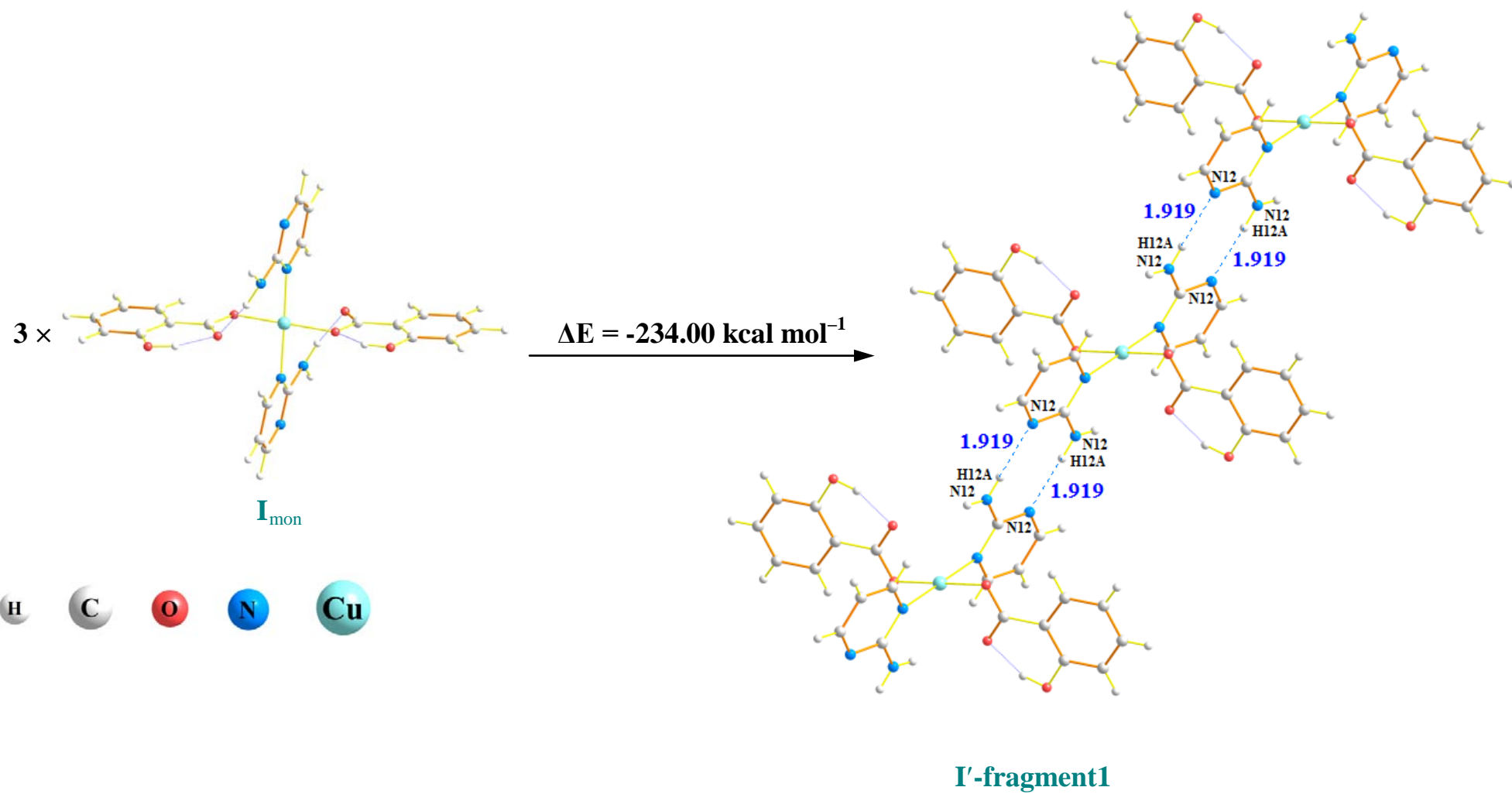


Fig. 2S

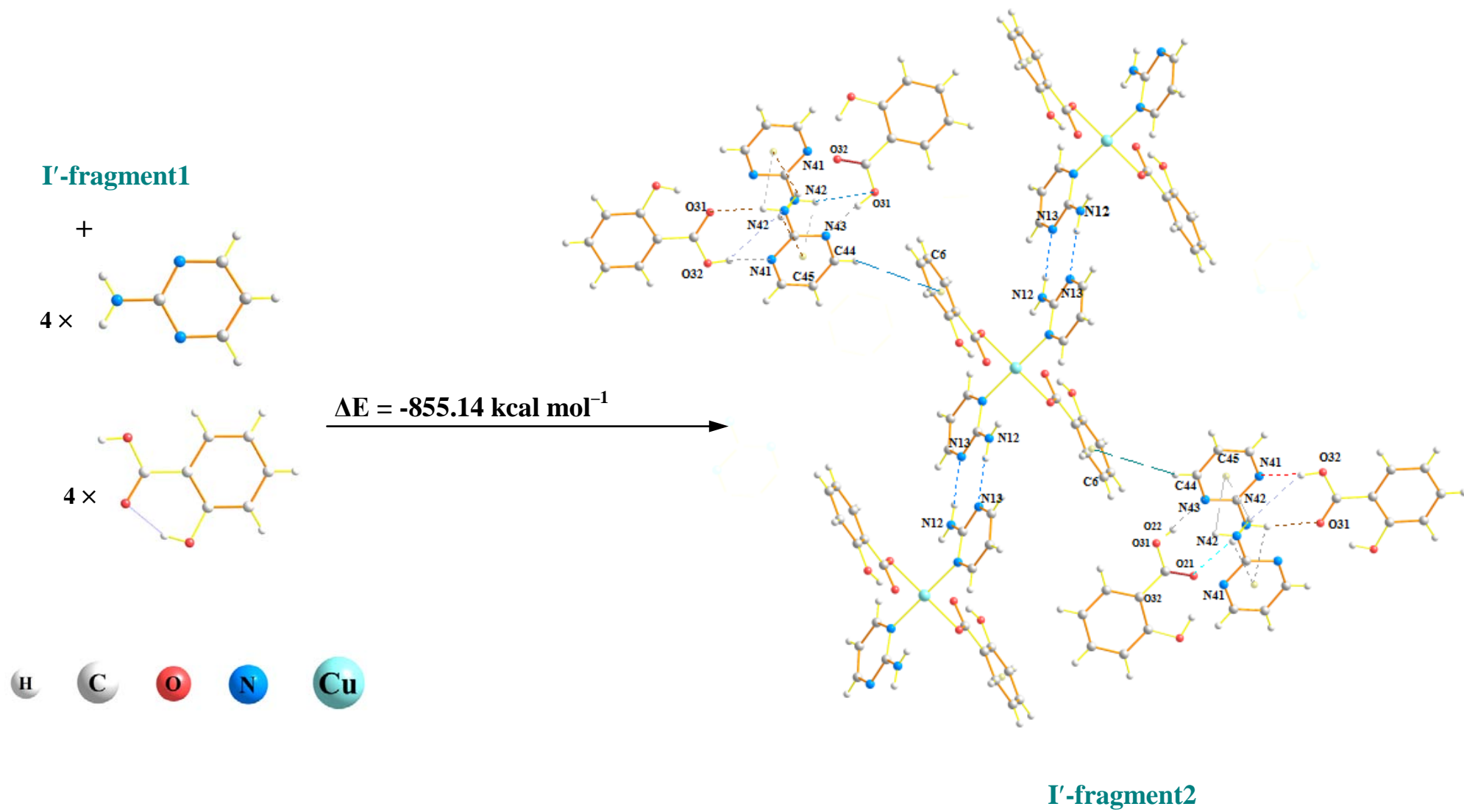


Fig. 3S

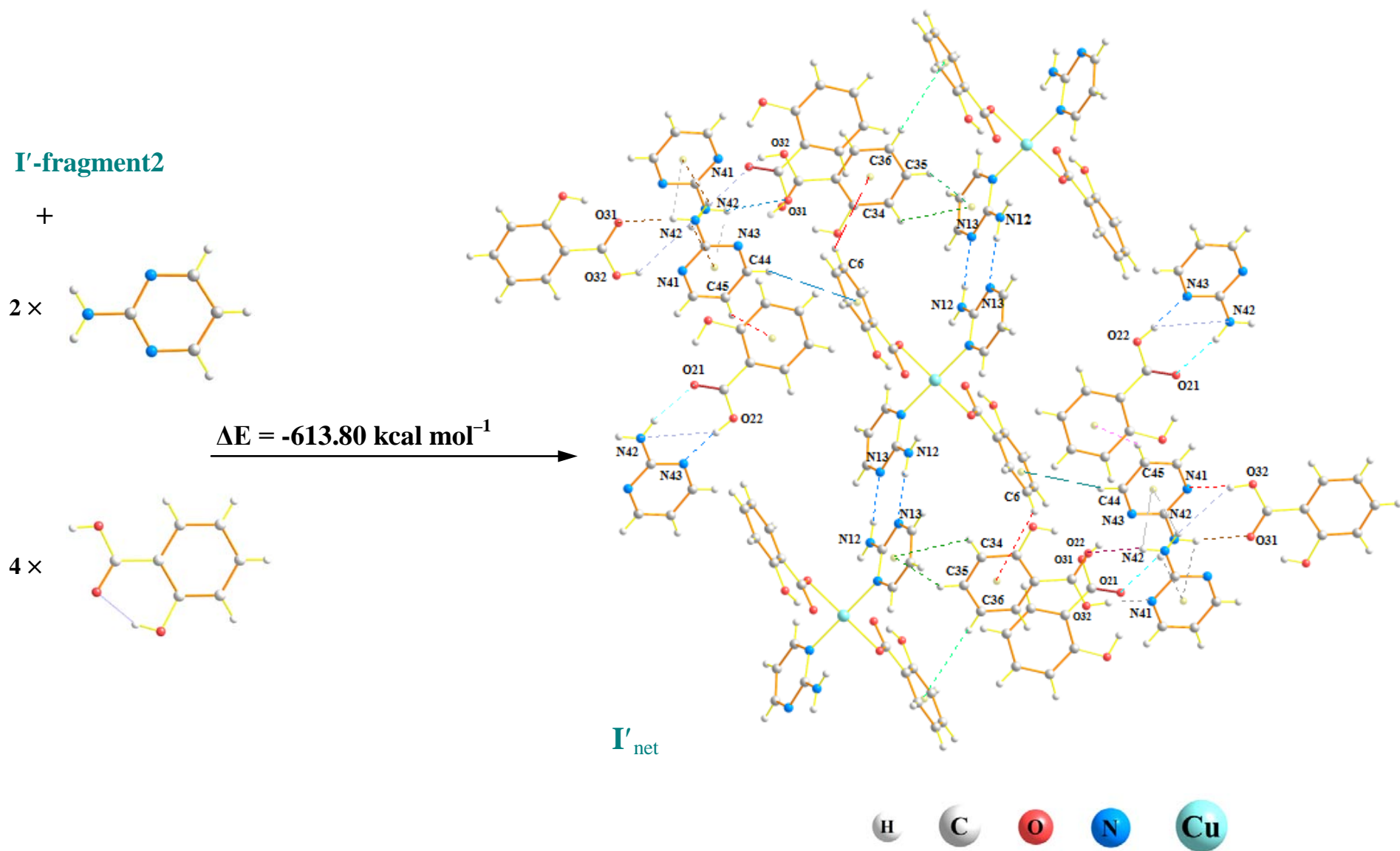


Fig. 4S