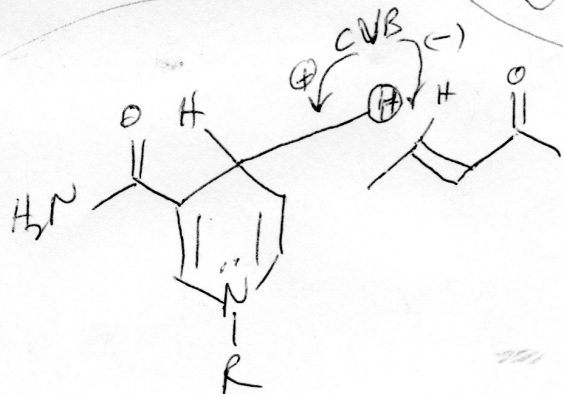


CVB \oplus = make bond
CVB \ominus = break bond

using set pi to aromatize ring and CVB to break bond to ring and make bond to other molecule works for hydride transfer.



this setup should work to go from product to reactants

How can I specify each of these in the same locate-TS command file?

I've even tried to isolate the hydride atom,



but even with a broken bond to the ring, I try to force the aromatic ring with set pi and I can put double bonds correctly, until the last one, and I get error!