Closed shell:

1. In first --Link1-- change: pop=nbo7 to **pop=NBO7read**
2. Add: **$nbo nrt $end**
   1. one line after spin and charge definition in first linked job

Radical/Open shell:

1. Change name of .chk file by adding “\_rad” to end
   1. Example: Het001\_conf-1**\_rad.**chk
   2. Make sure to do this for the geometry optimization and the linked job
2. In first --Link1-- change: pop=nbo7 to **pop=NBO7read**
3. Add: **$nbo nrt $end**
   1. one line after spin and charge definition in first linked job
4. Change spin to doublet
   1. 0 2 (neutral charge, doublet spin state)
5. Delete second linked job that calculated NMR shifts.
   1. Leave two blank lines at end of com file

Anion:

1. Use radical com file, change charge and spin
   1. -1 1 (negative 1 charge, singlet spin state)
2. Change name of .chk file by adding “\_anion” to end
   1. Example: Het001\_conf-1**\_anion.**chk
   2. Make sure to do this for the geometry optimization and the linked job