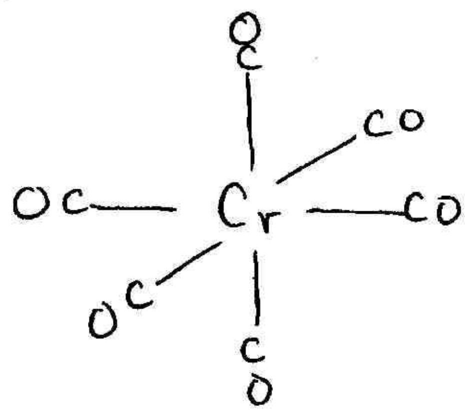
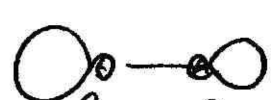
Lecture 37. $Cr(CO)_6$

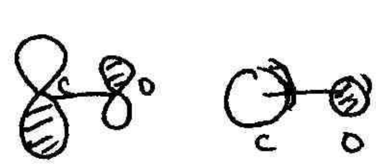
① In this molecule we again have an octahedral molecule



② Cr is d^6 (Note again 3d orbitals fill before 4S orbitals) So HOMO & LUMO are d-orbitals for this fragment.

③ For CO we have

HOMO 

LUMO 

We have 12 CO LUMO's & 6 CO HOMO's.

④ To derive $Cr(CO)_6$ MO we need to:

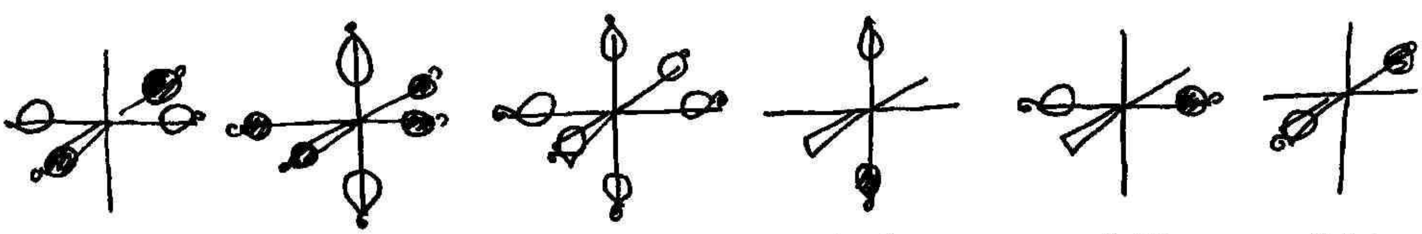
(i) Symmetry adapt CO HOMO's & LUMO's

(ii) Find the CO combinations of the same symmetry set best suited to interact (or not interact) with the d-orbitals.

(iii) Generate MO diagram.

⑤ For simplicity of drawing, we will draw only the C atom of CO's HOMO and LUMO's.

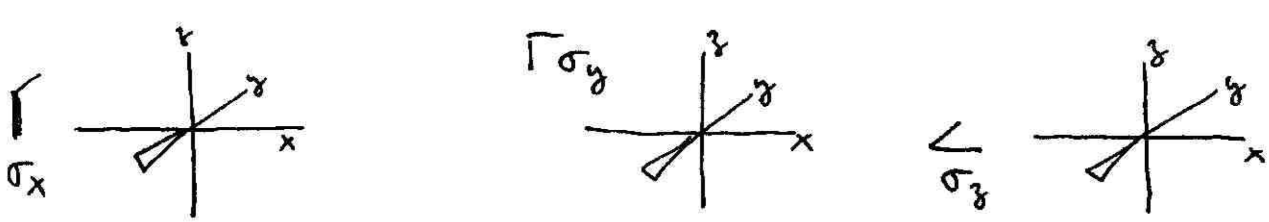
⑥ For HOMO's, the answer should be the same as in the $Cr(NH_3)_6^{3+}$ problem:



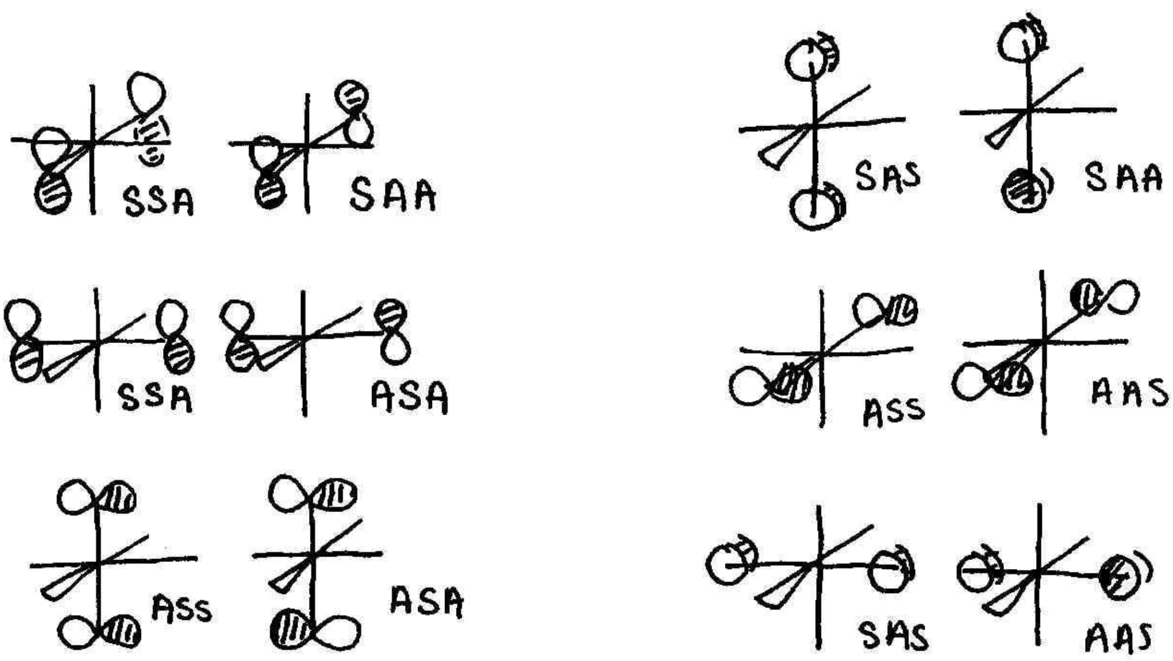
SSS SSS SSS SSA ASS SAS

⑦ For LUMO's we need to follow the regime set out in ④(i)-(iii).

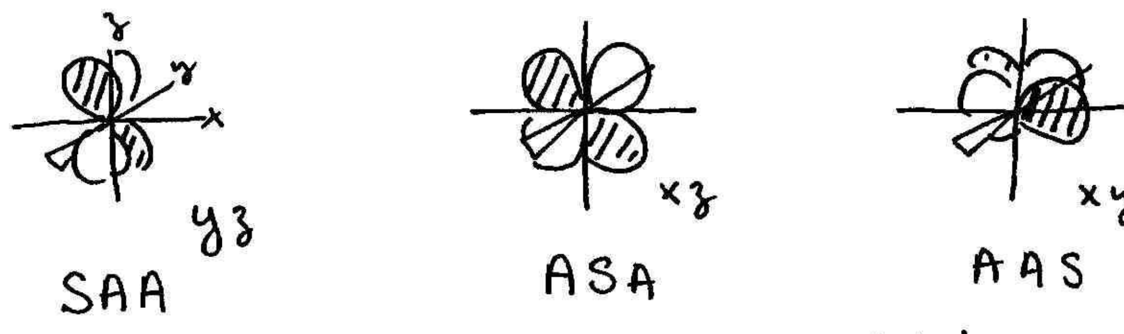
We do so on the next page.



(8)

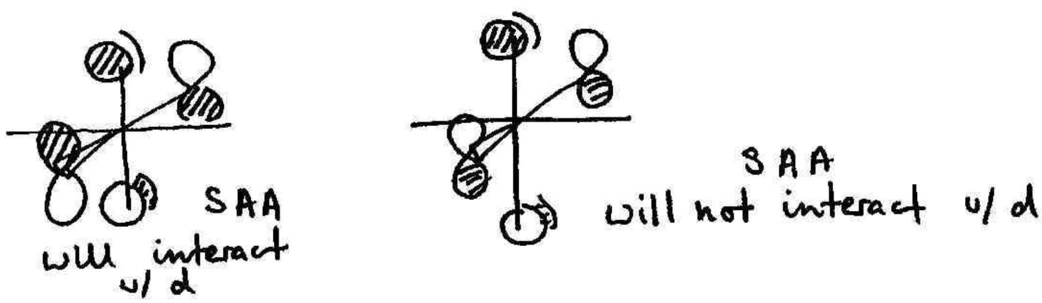


(9) Of these 12 orbitals only the AAS, ASA and SAA sets can interact w/ the d-orbitals. Following step (ii) we need to find AAS, ASA & SAA combinations which interact (or do not interact) with:

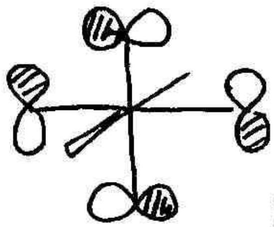


(10) We combine the two CO SAA orbitals:

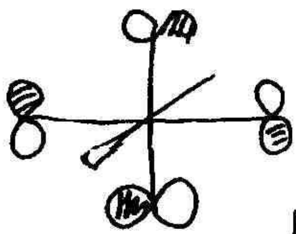
SAA



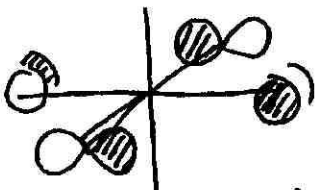
(11) In the same way we generate:



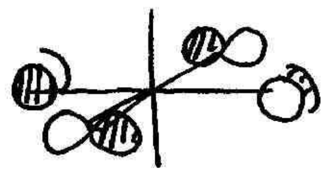
ASA will interact w/ d-orbital



ASA will not interact w/ d-orbital



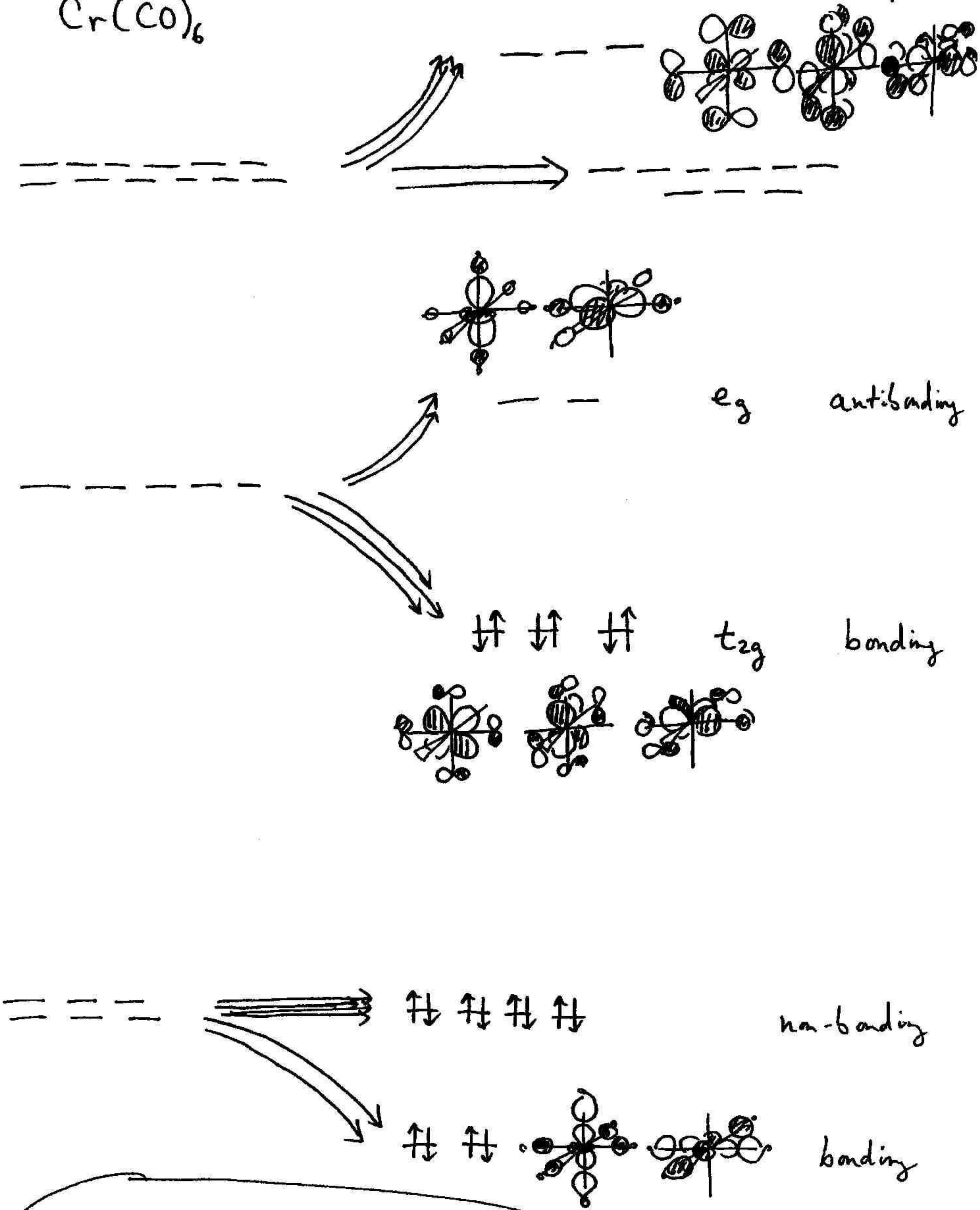
AAS will interact w/ d-orbital



AAS will not interact w/ d-orbital.

This completes step (ii). We now derive the complete MO diagram. See next page.

$Cr(CO)_6$



$Cr(CO)_6$ is a stable molecule