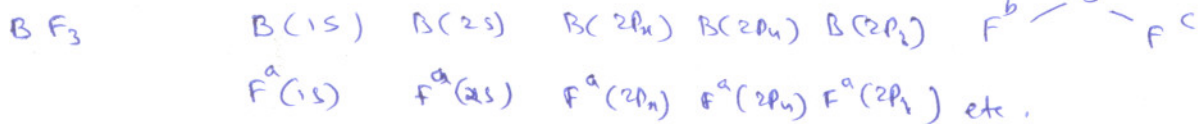


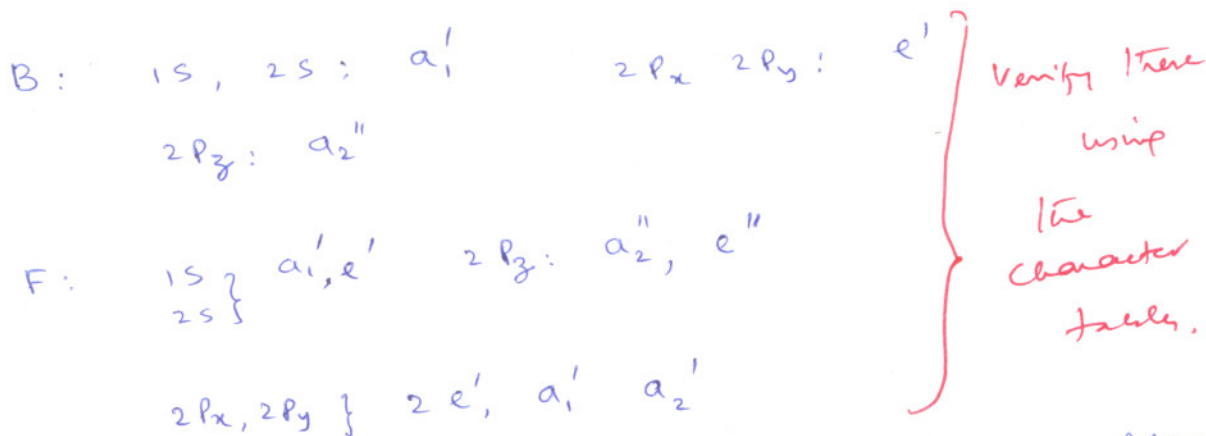
11. List the basis set for a minimal basis set calculation on  $BF_3$ . What simplifications result on application of symmetry.



Total  $5 \times 4 = 20$  basis functions

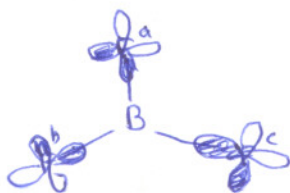
$20 \times 20$  secular determinant, may be symmetric

factored as follows:



Try to construct the SALCs (ref to Cotton; Shriver may help) p. 673

Since  $p_x, p_y$  of F get mixed up by  $C_3$ , it is convenient to relabel them as  $p_\sigma, p_\pi$  - this amounts to using F centred coordinate systems.



$p_\sigma^a, p_\pi^a$  (from  $p_x^a, p_y^a$ )  
 $p_\sigma^b, p_\pi^b$  "  
 $p_\sigma^c, p_\pi^c$  "

$a_1'$ :  $5 \times 5$  determinant       $a_2'$ :  $1 \times 1$        $e''$ :  $1 \times 1$   
 $e'$ :  $5 \times 5$        $a_2''$ :  $2 \times 2$