

# Atomic and molecular physics

## second written exam

December 11, 2018

1. Determine the ground state electron configuration of  $F_2$  molecule in the MO-LCAO approximation. Draw the orbital correlation diagram with correct electron occupancies. Determine the ground state molecular term symbol.
2. Determine the vibrational normal modes of  $NH_3$  molecule.
3. Hückel molecular orbital theory is used to determine the  $\pi$  molecular orbital energies of  $\pi$ -delocalized molecules. Determine the symmetries of these  $\pi$  molecular orbitals for benzene molecule (which irrep. they belong to).

Table 1: Character table of  $C_{3v}$  point group.

	E	$2C_3 (z)$	$3\sigma_v$	linear, rotations
$A_1$	1	1	1	$z$
$A_2$	1	1	-1	$R_z$
E	2	-1	0	$(x, y), (R_x, R_y)$

Table 2: Character table of  $D_{6h}$  point group. ( $\sigma_d$  is a diagonal mirroring, its plane bisects the angle between a pair of rotational axis  $C_2$ .)

	E	$2C_6$	$2C_3$	$C_2$	$3C'_2$	$3C''_2$	i	$2S_3$	$2S_6$	$\sigma_h$	$3\sigma_d$	$3\sigma_v$	lin.,rot.
$A_{1g}$	1	1	1	1	1	1	1	1	1	1	1	1	
$A_{2g}$	1	1	1	1	-1	-1	1	1	1	1	-1	-1	$R_z$
$B_{1g}$	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	
$B_{2g}$	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1	
$E_{1g}$	2	1	-1	-2	0	0	2	1	-1	-2	0	0	$(R_x, R_y)$
$E_{2g}$	2	-1	-1	2	0	0	2	-1	-1	2	0	0	
$A_{1u}$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	
$A_{2u}$	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	$z$
$B_{1u}$	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	
$B_{2u}$	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1	
$E_{1u}$	2	1	-1	-2	0	0	-2	-1	1	2	0	0	$(x, y)$
$E_{2u}$	2	-1	-1	2	0	0	-2	1	1	-2	0	0	