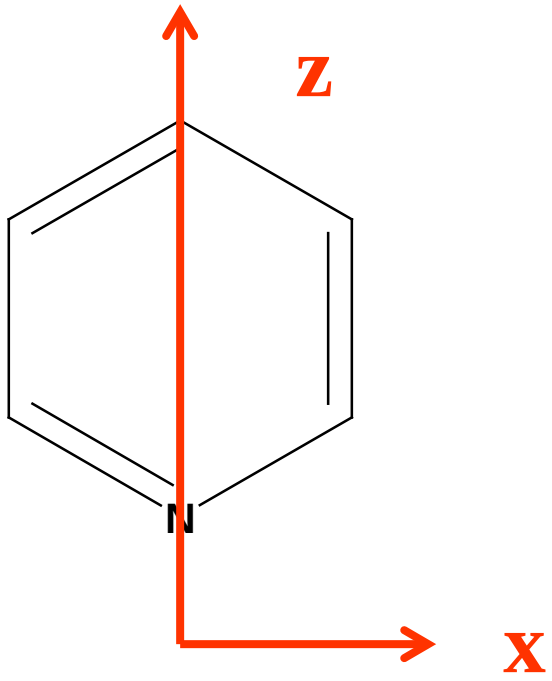
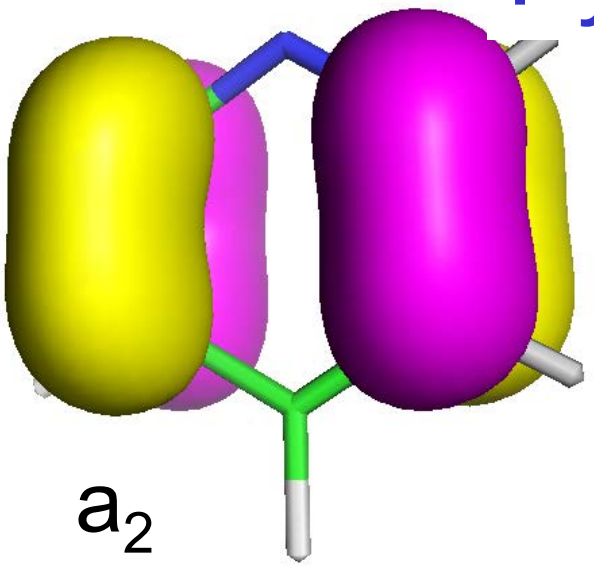
Pyridine

Pyridine has many of the spectroscopic characteristics of Benzene. However, pyridine has the lone pair of the N atom, Which leads to the possibility of n-π^* transitions in addition To the π-π^* transitions of benzene. Pyridine belongs to the C_{2v} point group.

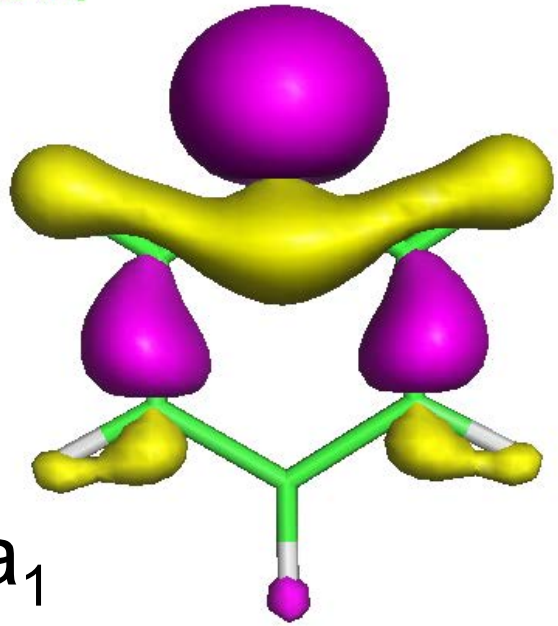


C_{2v}	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v(yz)}$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

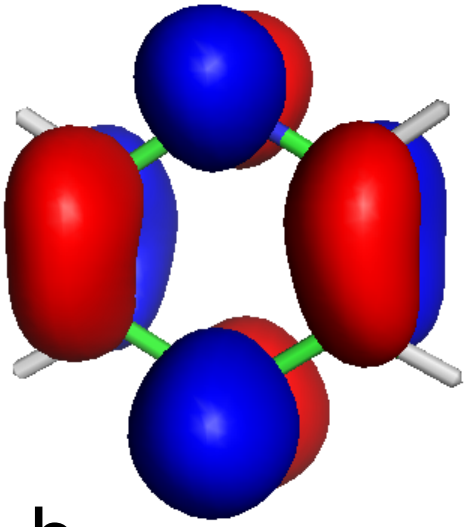
Pyridine



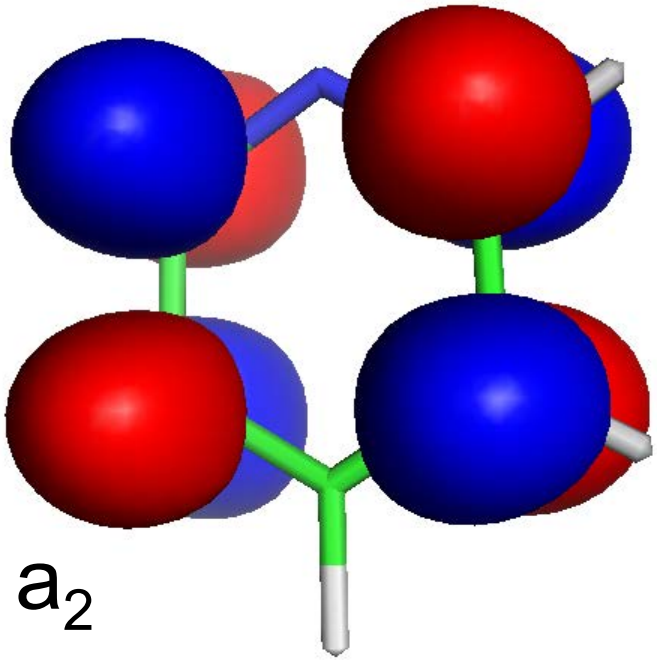
20 a_2



21 a_1



22 b_2



23 a_2

Pyridine transitions

The n-π^* is:

21 a_1 -> 22 b_2

Weak absorption 280 nm

The π-π^* transitions are similar to benzene:

19 b_2 -> 22 b_2 or 23 a_2
20 a_2 -> 22 b_2 or 23 a_2

Moderate absorption 274 nm, 230 nm
Strong absorption 169 nm

MO	Irrep	eV	Occupation
11	a_1	-15.520	2.000
12	a_1	-13.042	2.000
13	b_1	-11.820	2.000
14	a_1	-11.487	2.000
15	b_1	-10.459	2.000
16	b_2	-9.824	2.000
17	a_1	-9.816	2.000
18	b_1	-8.800	2.000
19	b_2	-7.222	2.000
20	a_2	-6.623	2.000
21	a_1	-5.896	2.000
22	b_2	-1.778	0.000
23	a_2	-1.412	0.000
24	a_1	1.519	0.000
25	b_2	2.421	0.000

Product table for the C_{2v} point group

We can see that there are numerous possibilities for transitions. Using the method that

$$\Gamma_{homo}\Gamma_{lumo} = \Gamma_{x,y\ or\ z}$$

for an allowed transition, and recalling that x, y and z transform as b_1, b_2 and a_1, respectively, we can quickly determine the allowed transitions and polarizations using a C_{2v} product table.

	A_1	A_2	B_1	B_2
A_1	A_1	A_2	B_1	B_2
A_2	A_2	A_1	B_2	B_1
B_1	B_1	B_2	A_1	A_2
B_2	B_2	B_1	A_2	A_1