Beispiel 2: NH_3 (C_{3v})

Orbitale am N-Atom

$\Gamma(1s) = A_1$ Rumpforbital

$\Gamma(2s) = A_1$

$\hat{O}_R$ f	E	$2C_3$	$3\sigma_v$	Irred. DS
N		z.B.	z.B.	
p_x	p_x	$-\frac{1}{2}p_x + \frac{\sqrt{3}}{2}p_y$	p_x	} E
p_y	p_y	$-\frac{\sqrt{3}}{2}p_x - \frac{1}{2}p_y$	$-p_y$	
p_z	p_z	p_z	p_z	A
H		z.B.	z.B.	
s_1	s_1	s_2	s_2	} H-Atome
s_2	s_2	s_3	s_1	
s_3	s_3	s_1	s_3	
$\chi(s_h)$	3	0	1	
A_1	1	1	1	
E	2	-1	0	

Benutze: $n_j = \frac{1}{h}\sum_R \chi^{(j)}(R)^* \chi(R)$

$\Rightarrow$ $n(A_1) = 1/6\,[\,3\cdot1 + 2\cdot0\cdot1 + 3\cdot1\cdot1\,] = 1$

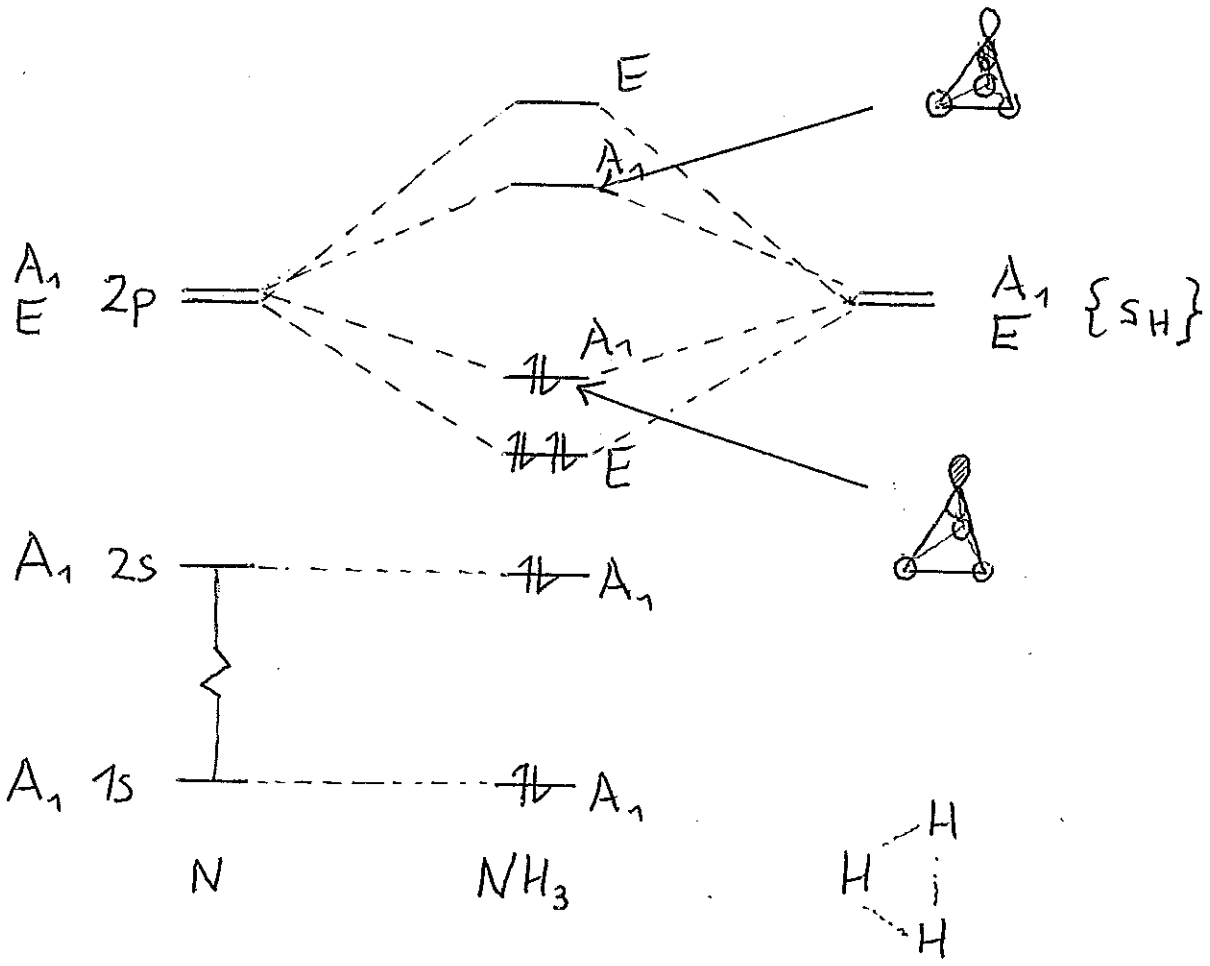
$n(E) = 1/6\,[\,3\cdot2 + 2\cdot0\cdot(-1) + 3\cdot1\cdot0\,] = 1$

$\Rightarrow$ $\Gamma(s_H) = A_1 \oplus E$

$\Rightarrow$ $\Gamma_{tot} = 4A_1 \oplus 2E = \Gamma_{AO} = \Gamma_{MO}$

Man findet $\Gamma_{bes} = 3\,A_1 \oplus E$

Orbitalenergiediagramm f. NH_3

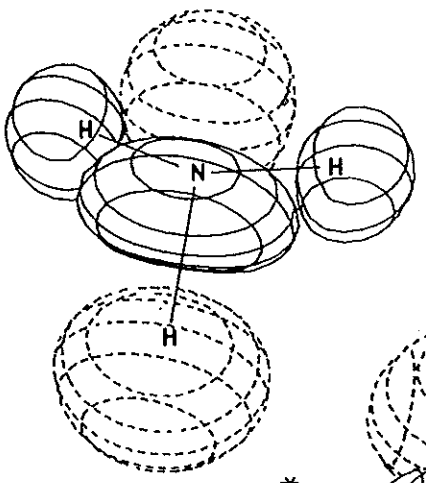


A_1-Orbital (HOMO) bindet stärker für nichtplanare Geometrien ⇒ NH_3 pyramidal.

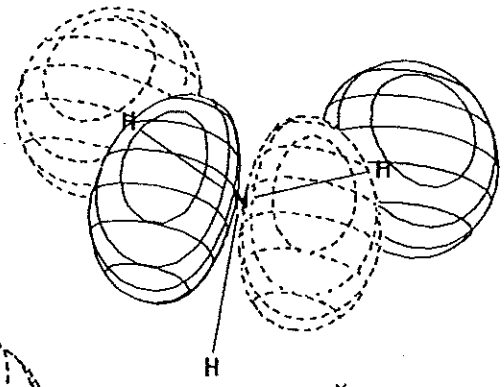
Aber: NH_3^+ im Gt ist planar !

8. Ammonia

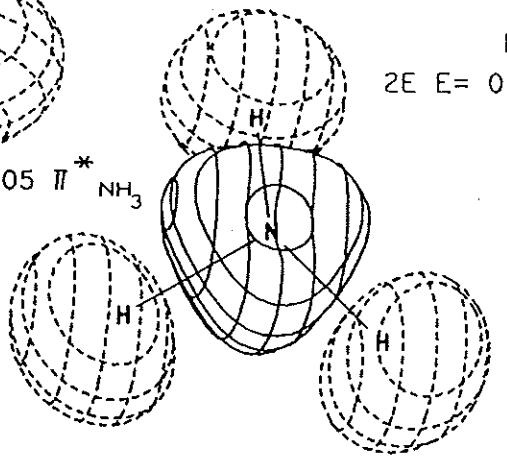
Symmetry: C_{3v}



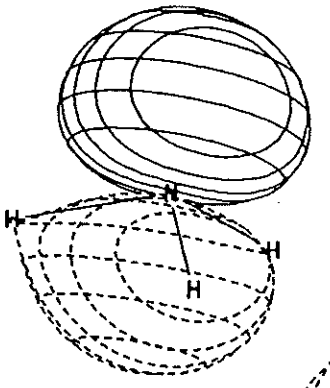
2E E= 0.6905 $\pi^*_{NH_3}$



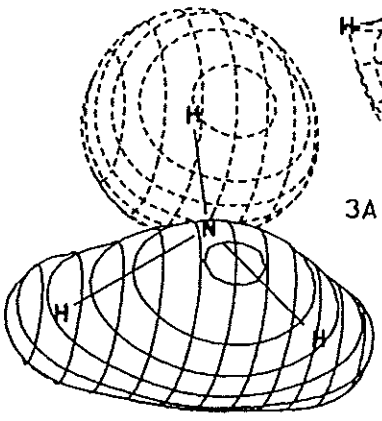
2E E= 0.6905 $\pi^*_{NH_3}$



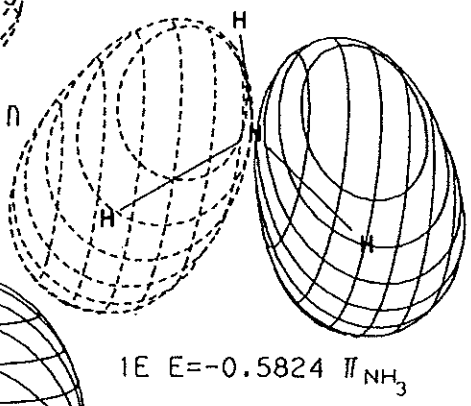
$4A_1$ E= 0.5844 $\sigma^*_{NH_3}$



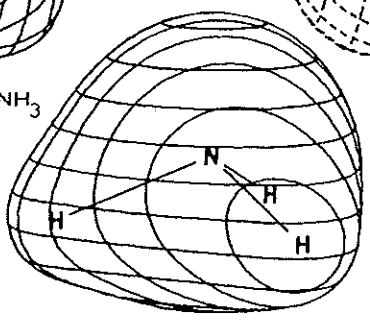
$3A_1$ E=-0.3661 n



1E E=-0.5824 π_{NH_3}



1E E=-0.5824 π_{NH_3}



$2A_1$ E=-1.1014 σ_{NH_3}