

Nitrogen Molecular Orbitals

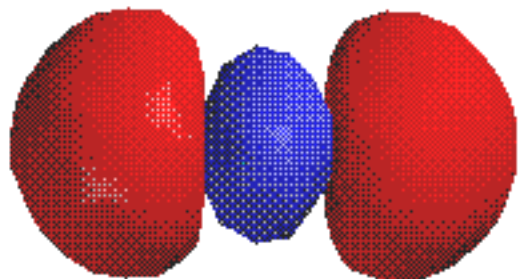
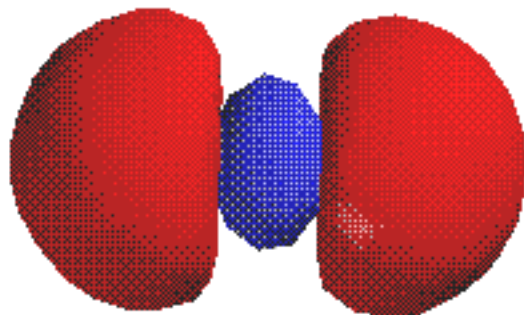
AM1 Level Filled Molecular Orbitals, 1.1056Å exp. bond length.

Nitrogen

MO:		1	2	3	4	5
Eigenvalues:		-41.39274	-21.43030	-16.19188	-16.19188	-14.32296
	(kcal/mol)					
		$\sigma(2s)$	$\sigma^*(2s)$	$\pi(2p_y)$	$\pi(2p_x)$	$\sigma(2p_z)$
1 N	1 S	-0.62096	-0.64963	0.00000	0.00000	-0.33824
2 N	1 PX	0.00000	0.00000	0.01887	0.70685	0.00000
3 N	1 PY	0.00000	0.00000	0.70685	-0.01887	0.00000
4 N	1 PZ	-0.33824	0.27924	0.00000	0.00000	0.62096
5 N	2 S	-0.62096	0.64963	0.00000	0.00000	-0.33824
6 N	2 PX	0.00000	0.00000	0.01887	0.70685	0.00000
7 N	2 PY	0.00000	0.00000	0.70685	-0.01887	0.00000
8 N	2 PZ	0.33824	0.27924	0.00000	0.00000	-0.62096
% p character		22.8%	15.6%	100%	100%	77.1%

$$\%p \text{ character} = \frac{\sum p \text{ coefficients}^2}{s \text{ coefficient}^2 + \sum p \text{ coefficients}^2}$$

N₂ $\sigma(2p_z)$



O₂ $\sigma(2p_z)$