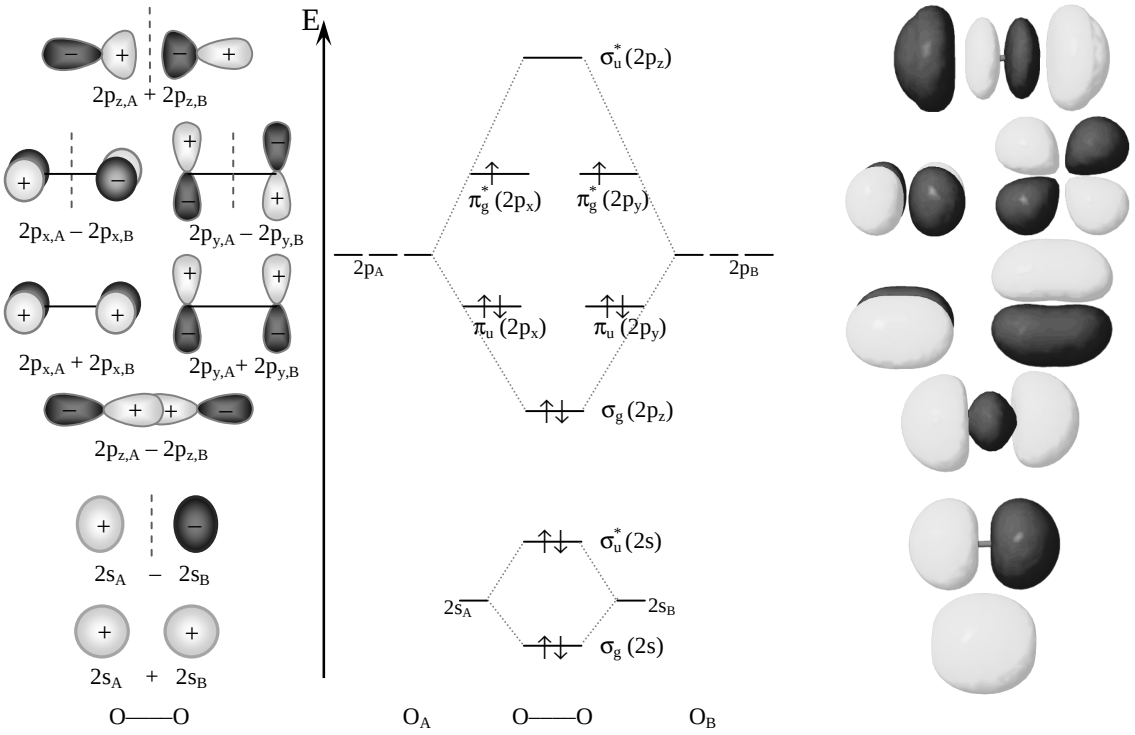
Molecular Orbitals for Diatomics



Nitrogen Molecular Orbitals

AM1 Filled Molecular Orbitals, 1.094 Å experimental bond length.

MO:	1	2	3	4	5
Eigenvalues:(eV)	-41.3927	-21.4303	-16.1919	-16.1919	-14.3230
	$\sigma(2s)$	$\sigma^*(2s)$	$\pi(2p_y)$	$\pi(2p_x)$	$\sigma(2p_z)$
1 N 1 S	-0.6210	-0.6496	0.0000	0.0000	-0.3382
2 N 1 PX	0.0000	0.0000	0.0189	0.7068	0.0000
3 N 1 PY	0.0000	0.0000	0.7068	-0.0189	0.0000
4 N 1 PZ	-0.3382	0.2792	0.0000	0.0000	0.6210
5 N 2 S	-0.6210	0.6496	0.0000	0.0000	-0.3382
6 N 2 PX	0.0000	0.0000	0.0189	0.7068	0.0000
7 N 2 PY	0.0000	0.0000	0.7068	-0.0189	0.0000
8 N 2 PZ	0.3382	0.2792	0.0000	0.0000	-0.6210
% p character	22.8%	15.6%	100%	100%	77.1%

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

Σ over a specific atom

N_2 σ(2pz) **O_2 σ(2pz)** HF/6-31G(d)