Which is the correct molecular orbital energy level diagram?

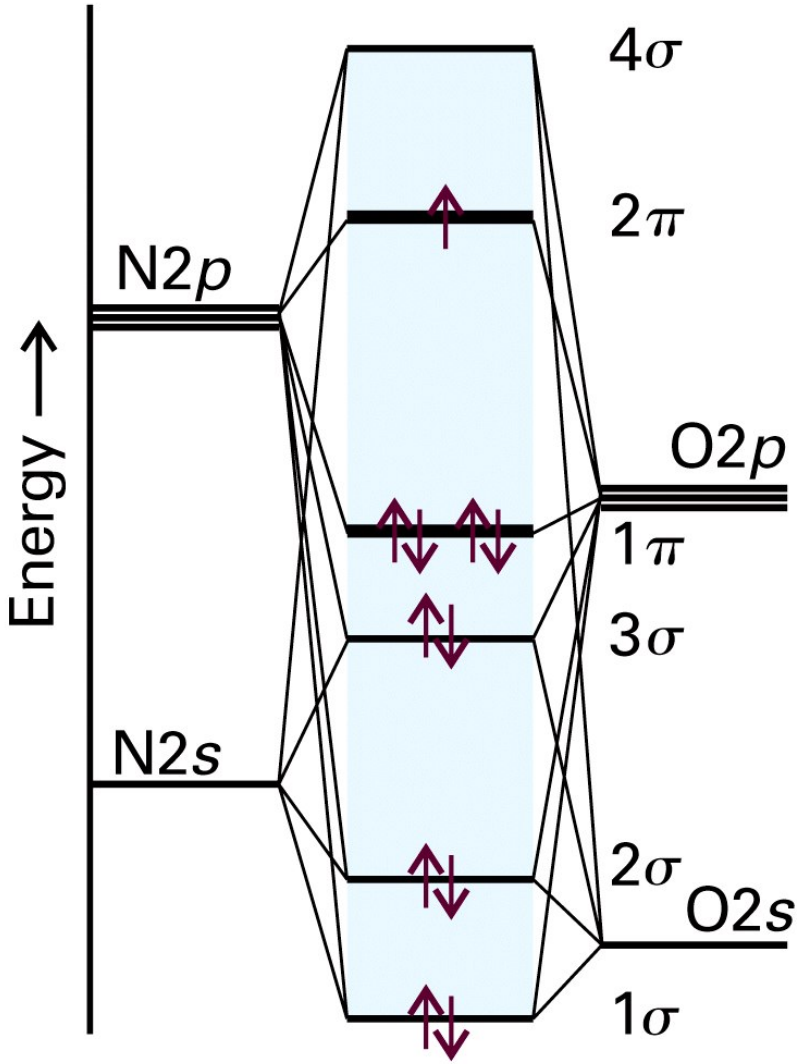
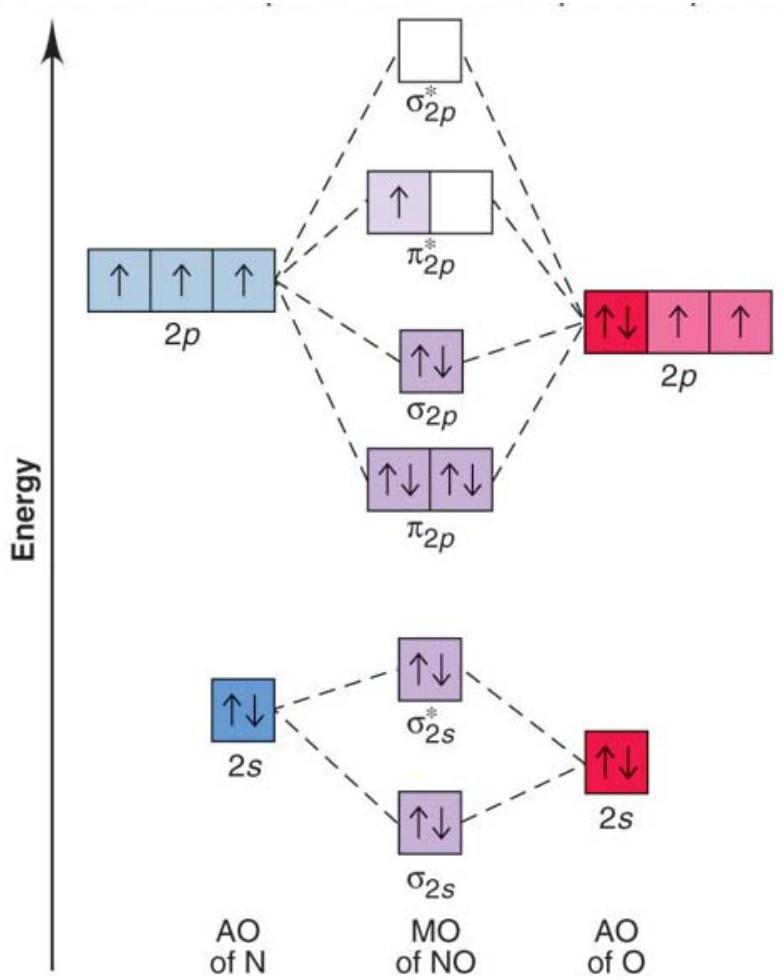


Figure 11-37
Atkins Physical Chemistry, Eighth Edition



Taken from Martin S. Silberberg, *Chemistry*, 4rd Edition, Boston: McGraw Hill, 2003.

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Vibrational spectroscopy of $NO^+(H_2O)_n$: Evidence for the intracluster reaction $NO^+(H_2O)_n \rightarrow H_3O^+(H_2O)_{n-2}$ (HONO) at $n \geq 4$

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Infrared spectra of mass-selected clusters $NO^+(H_2O)_n$ for $n=1$ to 5 were recorded from 2700 to 3800 cm^{-1} by vibrational predissociation spectroscopy. Vibrational frequencies and intensities were also calculated for $n=1$ and 2 at the second-order Møller–Plesset (MP2) level, to aid in the interpretation of the spectra, and at the singles and doubles coupled cluster (CCSD) level energies of $n=1$ isomers were computed at the MP2 geometries. The smaller clusters ($n=1$ to 3) were complexes of H_2O ligands bound to a nitrosonium ion NO^+ core. They possessed perturbed H_2O stretch bands and dissociated by loss of H_2O. The H_2O antisymmetric stretch was absent in $n=1$ and gradually increased in intensity with n. In the $n=4$ clusters, we found evidence for the beginning of a second solvation shell as well as the onset of an intracluster reaction that formed HONO. These clusters exhibited additional weak, broad bands between 3200 and 3400 cm^{-1} and two new minor photodissociation channels, loss of HONO and loss of two H_2O molecules. The reaction appeared to go to completion within the $n=5$ clusters. The primary dissociation channel was loss of HONO, and seven vibrational bands were observed. From an analysis of the spectrum, we concluded that the $n=5$ cluster rearranged to form $H_3O^+(H_2O)_3$(HONO), i.e., an adduct of the reaction products.

$NO^+(H_2O)_2$