

antibonding molecular orbital

The molecular orbital whose occupation by electrons decreases the total bonding (as usual, increases the total energy) of a molecule. The energy level of an antibonding MO lies higher than the average of the valence atomic orbitals of the atoms constituting the molecule.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1923