Chapter 13 (24): structure and energy levels for polyatomic molecules
Section 5: valence molecular orbitals of water
6 valence electrons from O, 2 from H, 8 total

Chapter 13 (24): structure and energy levels for polyatomic molecules
Section 5: H$_2$O, continued
valence molecular orbitals at optimized geometry

source: Engel, Quantum Chemistry and Spectroscopy, 3rd ed., 2013, Figure 13.10 (24.10).
Chapter 13 (24): structure and energy levels for polyatomic molecules

H₂O Hartree-Fock 6-31G* (GAMESS) constant-R ᵃ slice through the potential energy surface

\[ E \text{ (Hartree)} = C_0(1 - R/R_0)^{1/2} \]

H-0-H angle (degrees)

Chapter 13 (24): structure and energy levels for polyatomic molecules

Section 5: Walsh diagram for H₂O

occupied valence orbital energies at fixed bond length

Figure 13.11 (24.11) from Quantum Chemistry and Spectroscopy by Engel

source: Physical Chemistry by D. A. McQuarrie and J. D. Simon, University Science books, 1997
Chapter 13 (24): structure and energy levels for polyatomic molecules

Section 9: from molecular orbital energies to bands in solids

Example: Mg
- valence electrons fill 2s
- 2p orbitals are empty