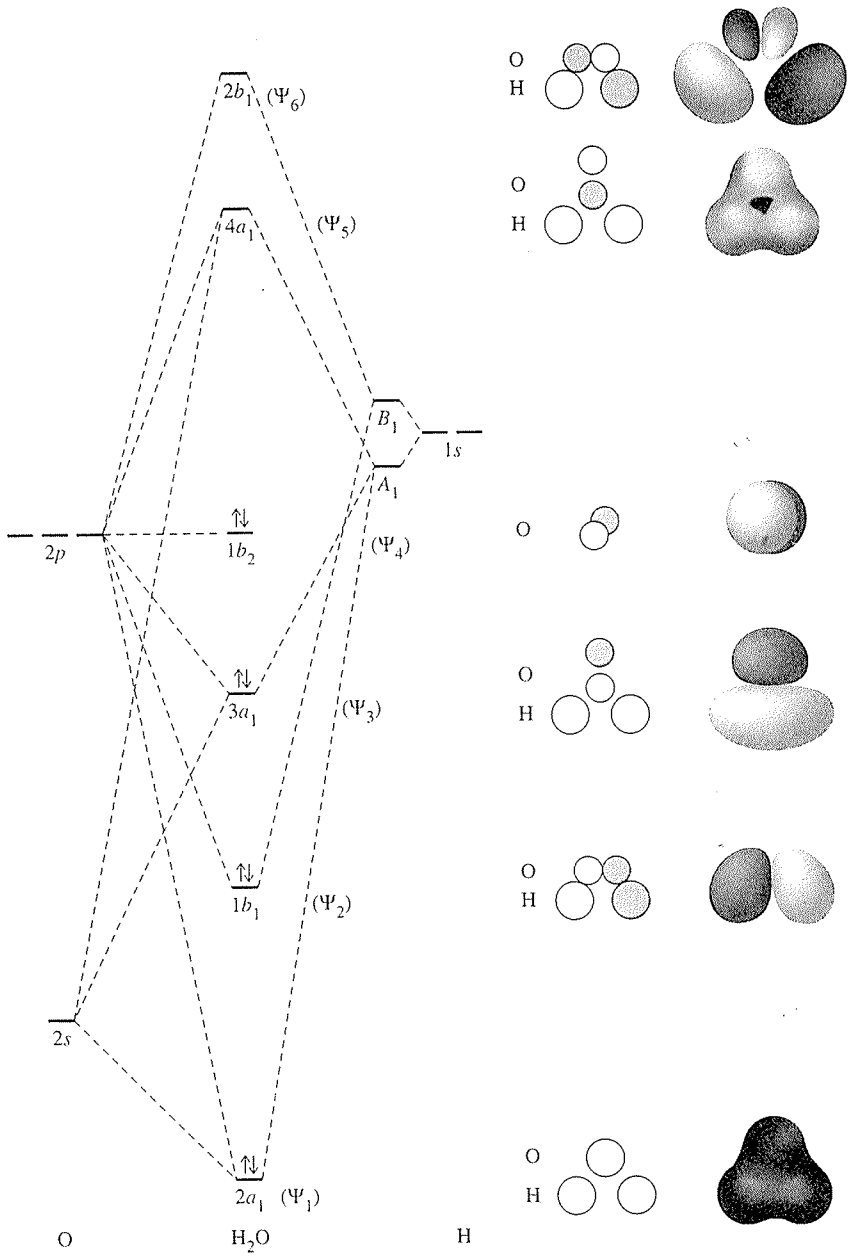

FIGURE 5-27 Molecular Orbitals of H_2O.

5-5-5 NH_3

VSEPR arguments describe ammonia as a pyramidal molecule with a lone pair of elec trons and C_{3v} symmetry. For the purpose of obtaining a molecular orbital picture of NH_3 it is convenient to view this molecule looking down on the lone pair (down the C_3, or z axis) and with the the yz plane passing through one of the hydrogens. The reducible rep resentation for the three hydrogen 1s orbitals is given in Table 5-4. It can be reduced b the methods in Chapter 4 to the A_1 and E irreducible representations, with the orbita combinations in Figure 5-29. Since three hydrogen 1s orbitals are to be considered, ther must be three group orbitals formed from them, one with A_1 symmetry and two with symmetry.

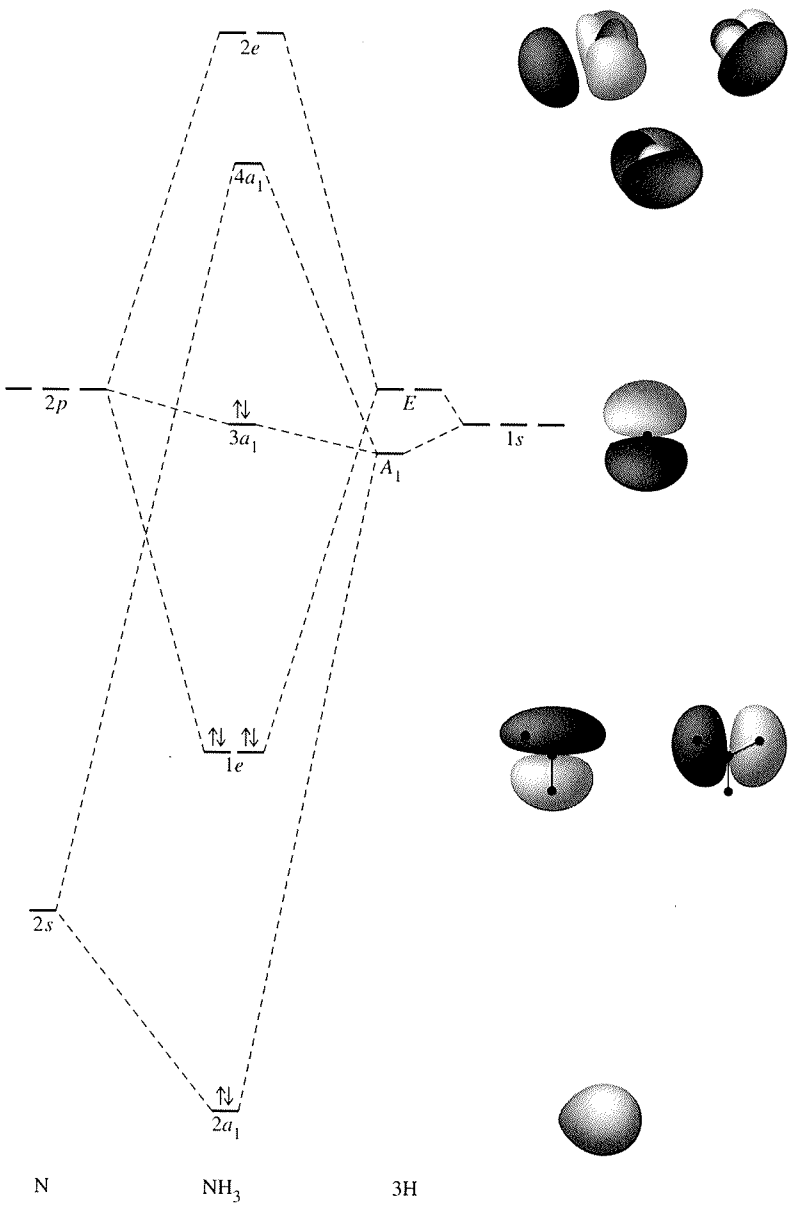

FIGURE 5-29 Molecular Orbitals of NH_3. The $1e$ and $3a_1$ orbitals are shown as transparent orbitals with the ball and stick nuclei to clarify the shapes. The $1e$ orbitals are also shown from directly above the nitrogen; all others are shown from a position between two of the hydrogens and slightly above the molecule.

Although both molecules have three-fold symmetry, the procedure for describing molecular orbitals of BF_3 differs from NH_3, since the fluorine atoms surrounding the central boron atom have $2p$ as well as $2s$ electrons to be considered. In this case, the p_y axes of the fluorine atoms are chosen so they are pointing toward the boron atom and the p_x axes are in the plane of the molecule. The group orbitals and their symmetry in the D_{3h} point group are shown in Figure 5-30. The molecular orbitals are shown in Figure 5-31 (omitting sketches of the five nonbonding $2p$ group orbitals of the fluorine atoms for clarity).

As discussed in Chapter 3, resonance structures may be drawn for BF_3 showing this molecule to have some double bond character in the B—F bonds. The molecular orbital view of BF_3 has an electron pair in a bonding π orbital with a_2'' symmetry delocalized over all four atoms (this is the orbital slightly below the five nonbonding elec-