about 538.1 eV plus a smaller contribution at 536.6 eV within the tetrahedrally hydrogen bonded bulk [1227]. The 1b2 and 3a1 orbitals are largely responsible for the donation of hydrogen bonding with the 3a1 orbital shown experimentally to contribute the most [411]. Also, the 4a1 and 2b2 antibonding orbitals are reported to be partially occupied in hydrogen bond formation, receiving electron density from donor 1b1 orbitals [814].

An interactive structure with orbitals is available (COW [Plug-in, ActiveX] only, 8 KB).

a. The nomenclature is based upon the symmetry of the orbitals. The figure below shows the planes of symmetry (xz and yz) and the two-fold axis of rotation (C2, z-axis).

If the orbitals are unchanged (that is, symmetric) with respect to the planes of symmetry (xz and yz) and the two-fold axis of rotation (C2) then they are denoted as 'a1' orbitals and numbered from the lowest energy (i.e. 1a1 is the lowest energy a1 orbital). If the sign of the orbital changes with respect to 180° rotation about C2 and reflection through the xz plane it is b1, whereas if the sign of the orbital changes with respect to 180° rotation about C2 and reflection through the yz plane it is b2. An a2 orbital has no change in sign with respect to 180° rotation about C2 but changes sign on reflection through both xz and yz planes (for example, the 9th lowest unoccupied molecular orbital for H2O). [Back]