Laser excitation spectra of yttrium monohydroxide, YOH, have been recorded in the 500-625 nm wavelength region. Rotational analysis of bands of YOH and YOD has shown that the ground state is $^1\Sigma^+$, with the structure $r_D$ (Y–O) $= 1.948\text{ Å}$, $r_D$ (O–H) $= 0.920\text{ Å}$; the bending frequency ($\nu_2$, $\pi$) is 313.73 cm$^{-1}$ (237.43 cm$^{-1}$ in YOD) and the Y–O stretching frequency ($\nu_3$, $\sigma^+$) is 673.83 cm$^{-1}$ (655.34 cm$^{-1}$).

Two excited electronic states have been identified; they are assigned as $^3\Pi$ (16 449 cm$^{-1}$) and $^3\Sigma^+$ (18 509 cm$^{-1}$). Unusually strong vibronic coupling through the bending vibration occurs between these two states, which causes their vibrational structures to be highly irregular; assignments have only been possible following extensive wavelength-resolved fluorescence experiments. The vibronic coupling raises the bending frequency of the $^3\Sigma^+$ state to 457 cm$^{-1}$, and reduces that of the lower Born-Oppenheimer component of the $^3\Pi$ state (which has $A'$ symmetry in the $C_3v$ point group) to the extent that the molecule becomes non-linear, with a potential barrier at the linear configuration of about 120 cm$^{-1}$. The presence of the potential barrier is clearly demonstrated by the level structure of YOD, where the $\Sigma^+$ vibronic component of the 010 vibrational level (linear molecule notation) lies 1.4 cm$^{-1}$ below the 000 level. The upper Born-Oppenheimer component, which has $A''$ symmetry, is unaffected; its bending frequency is similar to that of the ground state. Perturbations occur in both the $^3\Pi$ and $^3\Sigma^+$ states; some of these represent local interactions between the two of them, but others are caused by higher vibrational levels of lower-lying “dark” electronic states. Over 40 ground state vibrational levels have been identified for both YOH and YOD from the wavelength-resolved fluorescence spectra.