

The MO orbitals in the Hückel approximation for ozone are:

$$\varphi_1 = \frac{1}{2}(p_1 + \sqrt{2}p_2 + p_3)$$

$$\varphi_2 = \frac{\sqrt{2}}{2}(p_1 - p_3)$$

$$\varphi_3 = \frac{1}{2}(p_1 - \sqrt{2}p_2 + p_3)$$

A single-determinant MO wavefunction of ozone based on the Hückel orbitals would look as follows:

$$\psi_{\text{Hückel}} = |\varphi_1 \bar{\varphi}_1 \varphi_2 \bar{\varphi}_2| = \left| \frac{1}{2}(p_1 + \sqrt{2}p_2 + p_3) \frac{1}{2}(p_1 + \sqrt{2}p_2 + p_3) \frac{\sqrt{2}}{2}(p_1 - p_3) \frac{\sqrt{2}}{2}(p_1 - p_3) \right|$$

Developing it into the basis atomic orbitals we get:

$$\begin{aligned} \psi_{\text{Hückel}} = & \frac{1}{8} (|p_1 \bar{p}_1 p_3 \bar{p}_3| - \sqrt{2}|p_1 \bar{p}_2 p_3 \bar{p}_1| + \sqrt{2}|p_1 \bar{p}_2 p_3 \bar{p}_3| - |p_1 \bar{p}_3 p_3 \bar{p}_1| - \\ & \sqrt{2}|p_2 \bar{p}_1 p_1 \bar{p}_3| + \sqrt{2}|p_2 \bar{p}_1 p_3 \bar{p}_3| + 2|p_2 \bar{p}_2 p_1 \bar{p}_1| - 2|p_2 \bar{p}_2 p_1 \bar{p}_3| - 2|p_2 \bar{p}_2 p_3 \bar{p}_1| + 2|p_2 \bar{p}_2 p_3 \bar{p}_3| + \\ & \sqrt{2}|p_2 \bar{p}_3 p_1 \bar{p}_1| - \sqrt{2}|p_2 \bar{p}_3 p_3 \bar{p}_1| - \\ & |p_3 \bar{p}_1 p_1 \bar{p}_3| + \sqrt{2}|p_3 \bar{p}_2 p_1 \bar{p}_1| - \sqrt{2}|p_3 \bar{p}_2 p_1 \bar{p}_3| + |p_3 \bar{p}_3 p_1 \bar{p}_1|) \end{aligned}$$

We will now reorder and gather the components:

$$\begin{aligned} \psi_{\text{Hückel}} = & \frac{1}{8} (4|p_1 \bar{p}_1 p_3 \bar{p}_3| + 2|p_1 \bar{p}_1 p_2 \bar{p}_2| + 2|p_2 \bar{p}_2 p_3 \bar{p}_3| \\ & + 2\sqrt{2}|p_1 \bar{p}_1 p_2 \bar{p}_3| - 2\sqrt{2}|p_1 \bar{p}_1 \bar{p}_2 p_3| \\ & + 2\sqrt{2}|p_1 \bar{p}_2 p_3 \bar{p}_3| - 2\sqrt{2}|\bar{p}_1 p_2 p_3 \bar{p}_3| \\ & + 2|p_2 \bar{p}_2 \bar{p}_1 p_3| - 2|p_2 \bar{p}_2 p_1 \bar{p}_3|) = \end{aligned}$$

$$\begin{aligned} \psi_{\text{Hückel}} = & \frac{1}{2} |p_1 \bar{p}_1 p_3 \bar{p}_3| + \frac{1}{4} (|p_1 \bar{p}_1 p_2 \bar{p}_2| + |p_2 \bar{p}_2 p_3 \bar{p}_3|) + \\ & + \frac{\sqrt{2}}{4} (|p_1 \bar{p}_1 p_2 \bar{p}_3| - |p_1 \bar{p}_1 \bar{p}_2 p_3|) + \frac{\sqrt{2}}{4} (|p_1 \bar{p}_2 p_3 \bar{p}_3| - |\bar{p}_1 p_2 p_3 \bar{p}_3|) + \\ & + \frac{1}{4} (|p_2 \bar{p}_2 \bar{p}_1 p_3| - |p_2 \bar{p}_2 p_1 \bar{p}_3|) \end{aligned}$$

Since:

$$\begin{aligned}
|p_1 \bar{p}_1 p_3 \bar{p}_3| &= \phi_a & ; & & |p_1 \bar{p}_1 p_2 \bar{p}_2| &= \phi_b & ; & & |p_2 \bar{p}_2 p_3 \bar{p}_3| &= \phi_c \\
\frac{\sqrt{2}}{2} (|p_1 \bar{p}_1 p_2 \bar{p}_3| - |p_1 \bar{p}_1 \bar{p}_2 p_3|) &= \phi_d & ; & & \frac{\sqrt{2}}{2} (|p_1 \bar{p}_2 p_3 \bar{p}_3| - |\bar{p}_1 p_2 p_3 \bar{p}_3|) &= \phi_e \\
\frac{\sqrt{2}}{2} (|p_2 \bar{p}_2 \bar{p}_1 p_3| - |p_2 \bar{p}_2 p_1 \bar{p}_3|) &= \phi_f
\end{aligned}$$

We get:

$$\psi_{\text{Hückel}} = \frac{1}{2} \phi_a + \frac{1}{4} (\phi_b + \phi_c) + \frac{1}{2} (\phi_d + \phi_e) + \frac{\sqrt{2}}{4} \phi_f$$