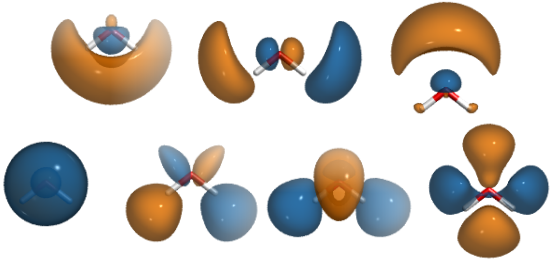
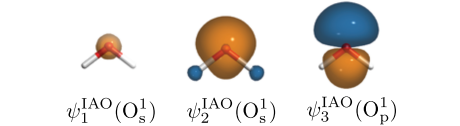
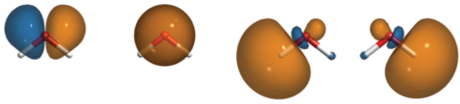
(**A**) Canonical molecular orbitals (CMOs)



(**B**) Intrinsic atomic orbitals (IAOs)



$\psi_1^{\mathrm{IAO}}(\mathrm{O}_\mathrm{s}^1)$ $\psi_2^{\mathrm{IAO}}(\mathrm{O}_\mathrm{s}^1)$ $\psi_3^{\mathrm{IAO}}(\mathrm{O}_\mathrm{p}^1)$



$\psi_4^{\mathrm{IAO}}(\mathrm{O}_\mathrm{p}^1)$ $\psi_5^{\mathrm{IAO}}(\mathrm{O}_\mathrm{p}^1)$ $\psi_6^{\mathrm{IAO}}(\mathrm{H}_\mathrm{s}^2)$ $\psi_7^{\mathrm{IAO}}(\mathrm{H}_\mathrm{s}^3)$

LIVVO Procedure

A) and (**B**)

SVD of overlap matrix

(**C**) Valence virtual orbitals (VVOs)