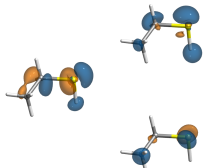


# Percentage of Localized Intrinsic Valence Virtual Orbital Character

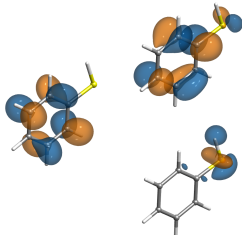
## (A) Ethanethiol



Particle orbitals for Ethanethiol are shown as 3D isosurface plots. The first orbital is a lone pair on sulfur. The second and third are bonding orbitals between sulfur and carbon. The fourth and fifth are bonding orbitals between carbon and hydrogen.

	$\sigma_{S^3-H^9}^*$	$\sigma_{S^3-C^2}^*$	$\sigma_{C^2-H^8}^*$	$\sigma_{C^1-H^6}^*$	$\sigma_{C^2-H^7}^*$	Total Valence Character
$\phi_P^3$	6	0	9	2	7	28
$\phi_P^4$	3	8	5	0	0	18
$\phi_P^5$	0	0	0	6	3	15

## (B) Benzenethiol



Particle orbitals for Benzenethiol are shown as 3D isosurface plots. The first orbital is a lone pair on sulfur. The second and third are bonding orbitals between sulfur and the ring. The fourth and fifth are bonding orbitals within the ring. The sixth is a bonding orbital between a ring carbon and a hydrogen atom.

	$\sigma_{S^7-H^8}^*$	$\sigma_{S^7-C^3}^*$	$\pi_{C^{4,5,6}}^*$	$\pi_{C^{1,2,6}}^*$	$\pi_{C^{2,3,4}}^*$	Total Valence Character
$\phi_P^3$	0	0	15	3	68	87
$\phi_P^4$	0	0	34	48	2	84
$\phi_P^5$	7	0	0	0	0	16

Particle Orbitals

Particle Orbitals