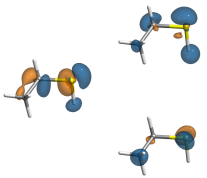
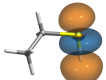
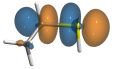
Percentage of Localized Intrinsic Valence Virtual Orbital Character

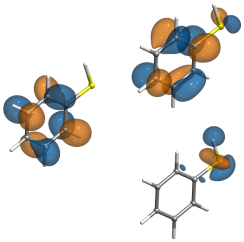
**(A)** Ethanethiol



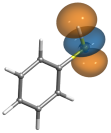
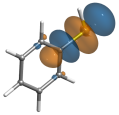
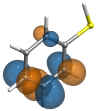
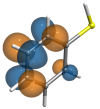
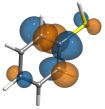
Particle Orbitals

| |  $\sigma^*_{S^3-H^9}$ |  $\sigma^*_{S^3-C^2}$ |  $\sigma^*_{C^2-H^8}$ |  $\sigma^*_{C^1-H^6}$ |  $\sigma^*_{C^2-H^7}$ | Total Valence Character |
|---|---|---|---|---|---|---|
| $\phi^3_p$ | 6 | 0 | 9 | 2 | 7 | 28 |
| $\phi^4_p$ | 3 | 8 | 5 | 0 | 0 | 18 |
| $\phi^5_p$ | 0 | 0 | 0 | 6 | 3 | 15 |

**B)** Benzenethiol



Particle Orbitals

| |  $\sigma^*_{S^7-H^8}$ |  $\sigma^*_{S^7-C^3}$ |  $\pi^*_{C^{4,5,6}}$ |  $\pi^*_{C^{1,2,6}}$ |  $\pi^*_{C^{2,3,4}}$ | Total Valence Character |
|---|---|---|---|---|---|---|
| $\phi^3_p$ | 0 | 0 | 15 | 3 | 68 | 87 |
| $\phi^4_p$ | 0 | 0 | 34 | 48 | 2 | 84 |
| $\phi^5_p$ | 7 | 0 | 0 | 0 | 0 | 16 |