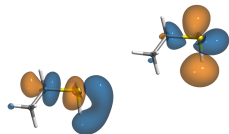
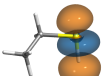
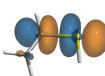
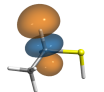




(A) Ethanethiol ϕ_p^1 ϕ_p^2

Percentage of Localized Intrinsic Valence Virtual Orbital Character

	 $\sigma_{S^3-H^9}^*$	 $\sigma_{S^3-C^2}^*$	 $\sigma_{C^2-H^8}^*$	 $\sigma_{C^1-H^6}^*$	 $\sigma_{C^2-H^7}^*$	Total Valence Character
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58

22

0

0

2

84

18

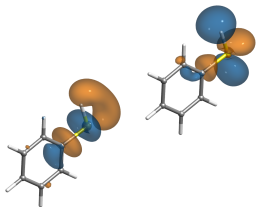
57

0

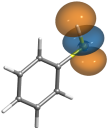
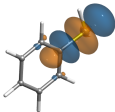
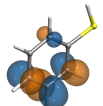
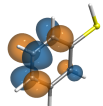
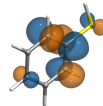
0

0

75

(B) Benzenethiol ϕ_p^1 ϕ_p^2

Percentage of Localized Intrinsic Valence Virtual Orbital Character

	 $\sigma_{S^7-H^8}^*$	 $\sigma_{S^7-C^3}^*$	 $\pi_{C^{4,5,6}}^*$	 $\pi_{C^{1,2,6}}^*$	 $\pi_{C^{2,3,4}}^*$	Total Valence Character
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61

22

0

0

0

88

16

53

0

0

0

71