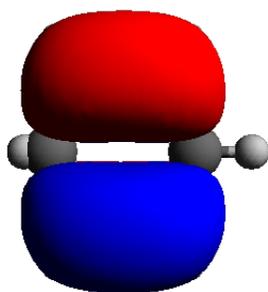
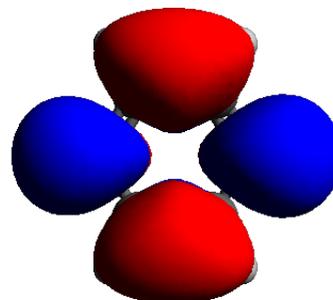


Benzene Bond Stretching PES

Bond Length = 0.5

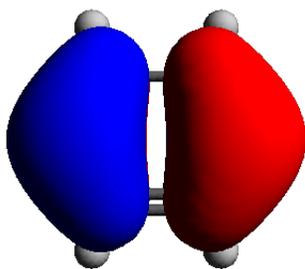


HOMO

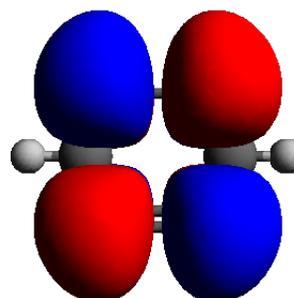


LUMO

Bond Length = 1.1

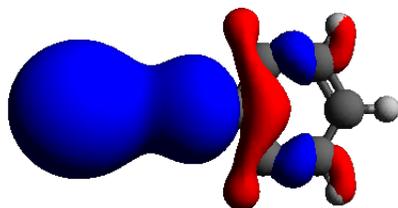


HOMO

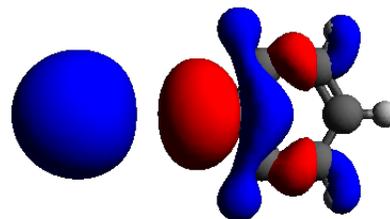


LUMO

Bond Length = 4.0



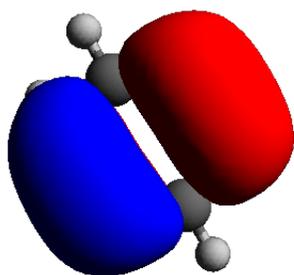
HOMO



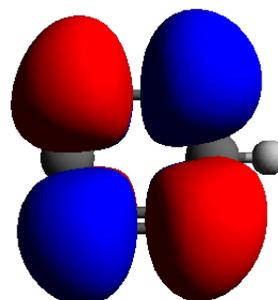
LUMO

Benzene Bond Rotation PES

Bond Angle = -54° from equilibrium

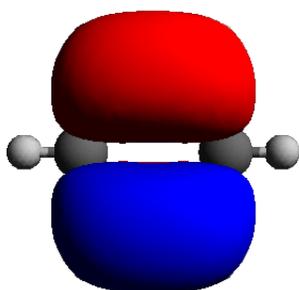


HOMO

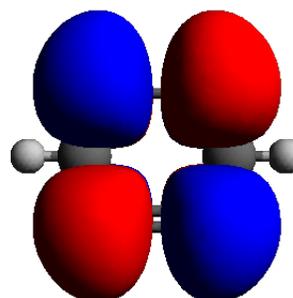


LUMO

Bond Angle = 0° from equilibrium

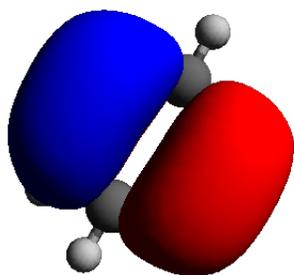


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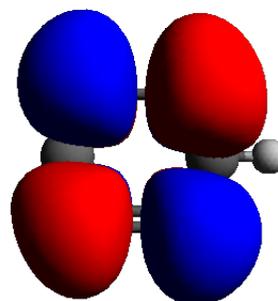


LUMO

Bond Angle = 54° from equilibrium



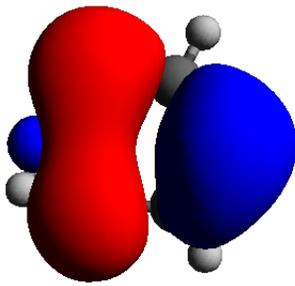
HOMO



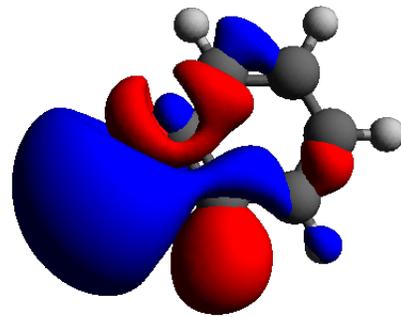
LUMO

Phenol OH Group Bond Stretching PES

Bond Length = 0.5

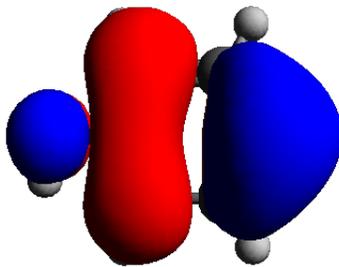


HOMO

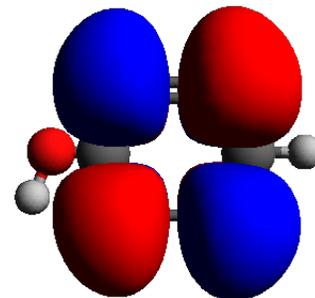


LUMO

Bond Length = 1.0

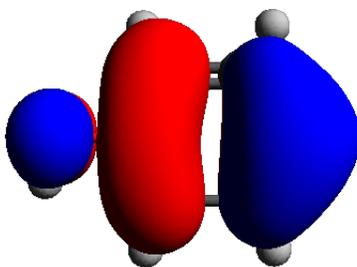


HOMO

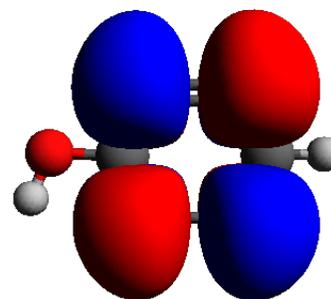


LUMO

Bond Length = 1.4

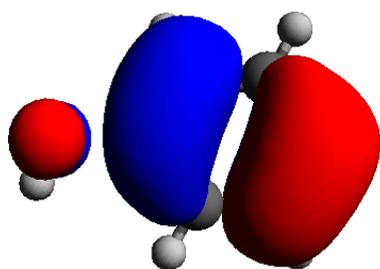


HOMO

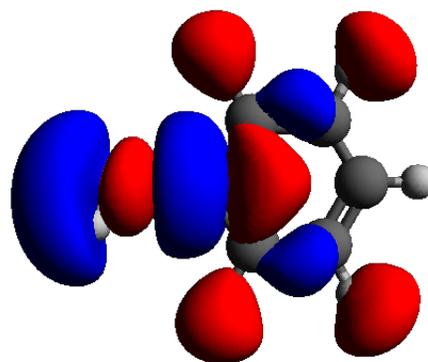


LUMO

Bond Length = 2.0

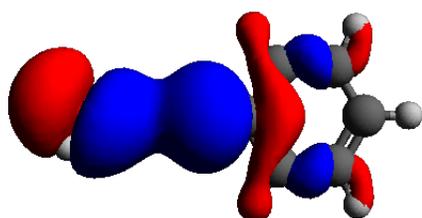


HOMO

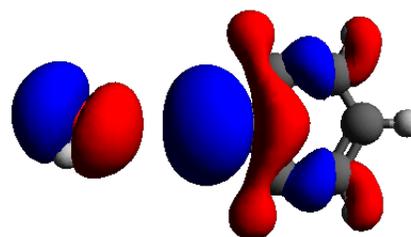


LUMO

Bond Length = 4.0



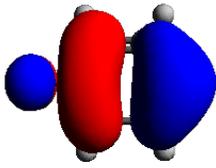
HOMO



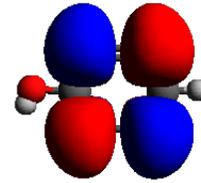
LUMO

Phenol Bond Stretching PES

Bond Length = 0.5

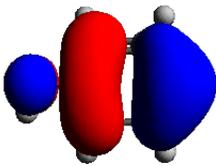


HOMO

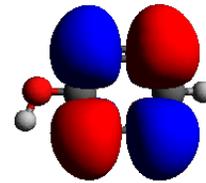


LUMO

Bond Length = 1.0

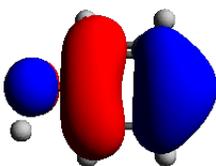


HOMO

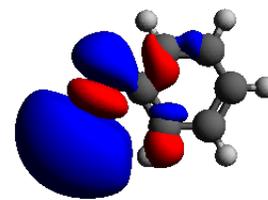


LUMO

Bond Length = 1.5

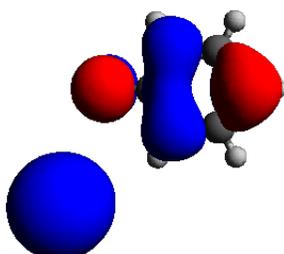


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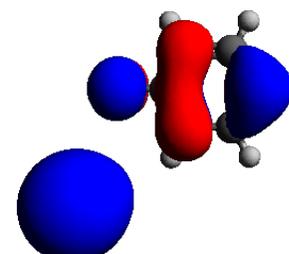


LUMO

Bond Length = 4.0



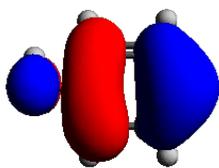
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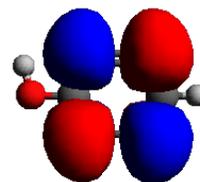
LUMO

Phenol Bond Rotation PES

Bond Angle = -144° from equilibrium

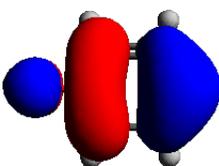


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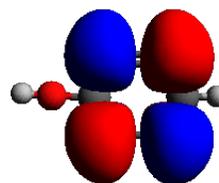


LUMO

Bond Angle = -72° from equilibrium

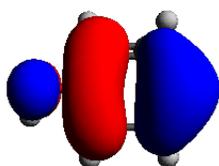


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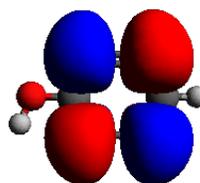


LUMO

Bond Angle = 0° from equilibrium

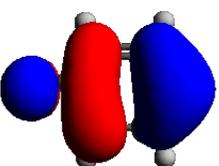


HOMO

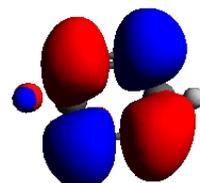


LUMO

Bond Angle = 126° from equilibrium



HOMO



LUMO