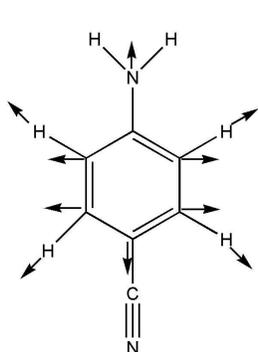
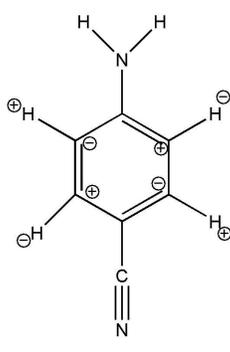


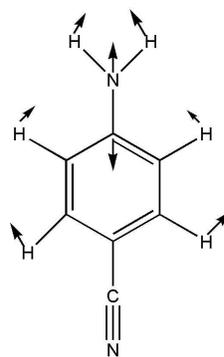
4ABN B3LYP/6-311G(d,p)



821 cm^{-1}
ring breathing mode
calculated IR intensity: 3.0
calculated Raman intensity: 35.3

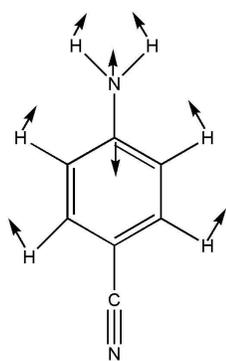


934 cm^{-1}
CH out of plane
bend mode
calculated IR intensity: 0.0028
calculated Raman intensity: 0.0675

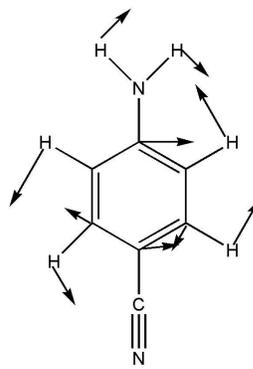


1286 cm^{-1}
C-NH₂ stretch mode
calculated IR intensity: 81.9
calculated Raman intensity: 7.4

4ABN complexed with a silver ion B3LYP/LANL2DZ



Ag⁺
1330 cm^{-1}
C-NH₂ stretch mode
with silver ion
calculated IR intensity: 109.0
calculated Raman intensity: 4.4



Ag⁺
1344 cm^{-1}
ring deformation/
NH₂ bend mode
with silver ion
calculated IR intensity: 0.7145
calculated Raman intensity: 3.4

176x234mm (300 x 300 DPI)