Nicotine

“Nicotine and other tobacco alkaloids that possess a basic pyrrolidine nitrogen readily form stable salts with both mineral and organic acids.” (Analytical Determination of Nicotine and Related Compounds and Their Metabolites)

“Complete neutralization of nicotine free base with sulfuric acid will produce nicotine sulfate salt with a 2:1 molar ratio of nicotine to sulfate.” (The Determination of Nicotine and Sulfate in Supermarket Ground Beef Adulterated with Black Leaf 40)

“Nicotine is a Diprotic Base with pKa’s of 3.12 (pyridine ring) and 8.02 (pyrrolidine ring).” (Optimization Study for the Reversed-Phase Ion-Pair Liquid Chromatographic Determination of Nicotine in Commercial Tobacco Products)

The Nicotine Molecule contains two Nitrogen Atoms capable of accepting a Proton
The Pyrrolidine Nitrogen is considerably more basic than the Pyridine Nitrogen

Nitrogen Lone Electron Pairs form Coordinate (Dative) Covalent Bonds with Protons
Nicotine Dissociation in Water
\[ C_{10}H_{14}N_2 + H_2O \rightarrow C_{10}H_{15}N_2^+ + OH^- \]
\[ C_{10}H_{15}N_2^+ + H_2O \rightarrow C_{10}H_{16}N_2^{2+} + OH^- \]

Sulfuric Acid Dissociation in Water
\[ H_2SO_4 + H_2O \rightarrow H_3O^+ + HSO_4^- \]
\[ HSO_4^- + H_2O \rightarrow H_3O^+ + SO_4^{2-} \]

Nicotine Neutralization with Sulfuric Acid
\[ 2 C_{10}H_{14}N_2 + H_2SO_4 \rightarrow C_{20}H_{30}N_4O_4S \text{ (Nicotine Sulfate Salt)} \]

Molar Masses (Molecular Weights)

**Nicotine C_{10}H_{14}N_2**
Carbon Atoms: 10 x 12.0107 = 120.107
Hydrogen Atoms: 14 x 1.00794 = 14.1116
Nitrogen Atoms: 2 x 14.00674 = 28.01348
**Molecular Weight = 162.23164**

**Sulfuric Acid H_2SO_4**
Hydrogen Atoms = 2 x 1.00794 = 2.01588
Sodium Atom = 32.065
Oxygen Atoms = 4 x 15.9994 = 63.9976
**Molecular Weight = 98.07848**

Dilution of Solution – M_1V_1 = M_2V_2
(Molarity 1 X Volume 1 = Molarity 2 X Volume 2)

**Moles of H_2SO_4 (Sulfuric Acid) vs. Moles of Nicotine**

1. 0.12N H_2SO_4 Contains 0.12 Moles of H_2SO_4/Liter.
2. To Calculate Moles of H_2SO_4 in 1 ml of 0.12N H_2SO_4:
   \[ 0.12N \times 1 \text{ ml} = 0.12 \text{ Moles H}_2\text{SO}_4 \]
   \[ 1 \text{ ml} = 0.001 \text{ Liter} \]
   \[ 0.001 \text{ Liter} \times 0.12 \text{ Moles} = 0.00012 \text{ Moles} \]
3. 0.00012 Moles of 0.12N H_2SO_4 will Neutralize 0.00012 Moles of Nicotine.
4. 0.00012 Moles of Nicotine = 19.468 mg (162.23 X 0.00012 = .019468 Grams)
5. 1 ml of 0.12N H_2SO_4 Neutralizes 1 ml of 19.468 mg/ml Nicotine.

**Nicotine Oxidation**
\[ C_{10}H_{14}N_2 + O_2 \rightarrow CO_2 + H_2O + N_2 \]

**Nicotine Oxidation Balanced Equation**
\[ 2 C_{10}H_{14}N_2 + 27 O_2 \rightarrow 20 CO_2 + 14 H_2O + 4 N \]
Sulfuric Acid (H$_2$SO$_4$) is a Diprotic Acid

The dissociation does not happen all at once due to the two stages of dissociation having different $K_a$ values. The first dissociation will occur completely, but the second one will not. Diprotic acids are of particular note in regards to titration experiments, where a pH versus titrant volume curve will clearly show two equivalence points for the acid. This occurs because the two ionization capable hydrogen atoms on the acid molecule do not leave the acid at the same time.

**bromothymol blue**

*Also known as: 3',3''-dibromothymolsulfonephthalein*
*Type: HIn + H$_2$O $\rightleftharpoons$ In$^-$ + H$_3$O$^+$*
*pK: 7.30*
*Approximate pH range for color change: 6.0-7.6*
*Color of acid form: yellow*
*Color of base form: blue*

**pH Scale (pH = -Log$_{10}$ [H+])**