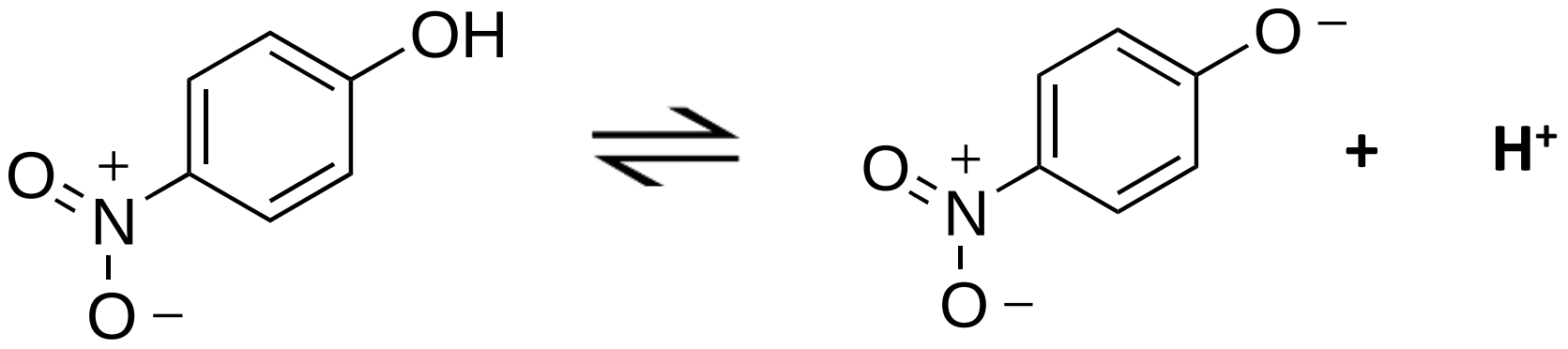
Resonance Energy and Color

What Do You Think?

Paranitrophenol



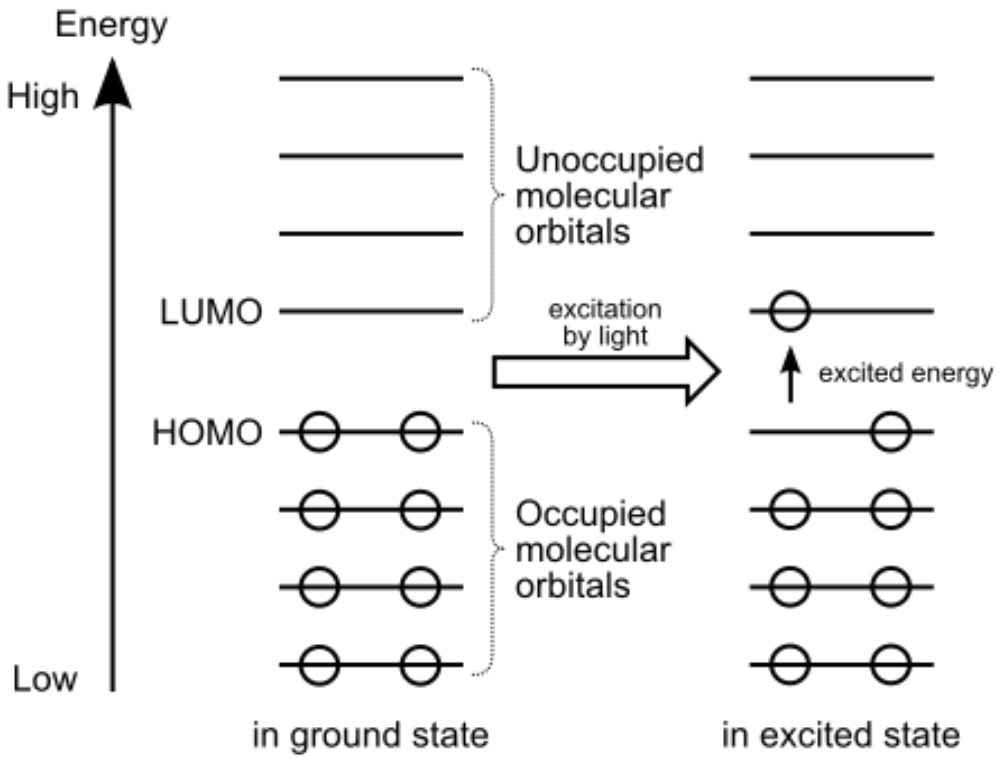
Colorless in Solution

Golden Yellow in Solution

Why is the protonated version clear and the deprotonated version yellow (in solution)?

Energetic Absorption and Electron Promotion

- When an organic compound absorbs energy, electrons are promoted from HOMO to LUMO



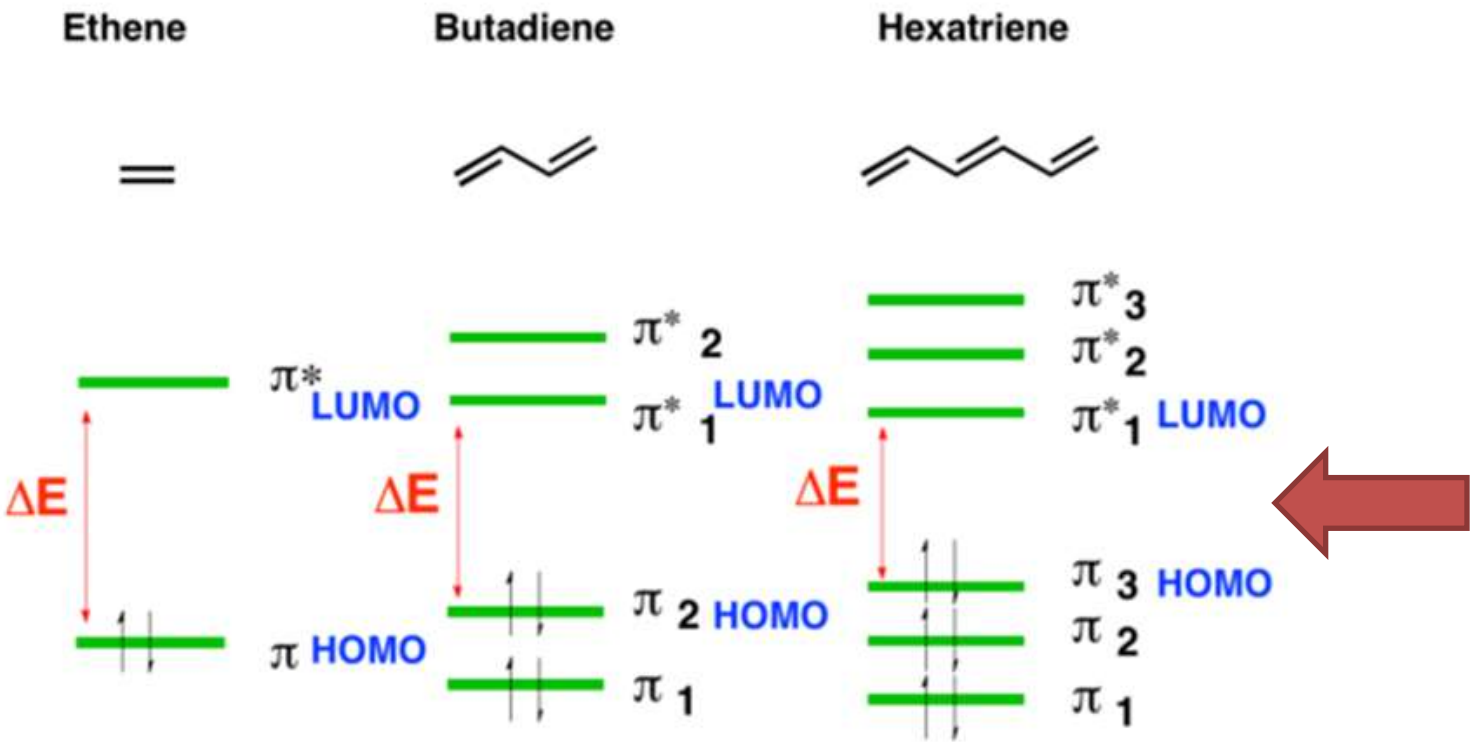
In most organics, this energy gap is in the UV range

Most organics absorb UV light and reflect the entire visible spectrum

Most organics appear white (colorless in solution)

Phthalic Acid

Resonance Affects Energetic Absorption



- **More** resonance → **more** overlapping atomic orbitals

- **More** π molecular orbital (MOs) possibilities
- π MOs are **more similar** in terms of constructive vs. destructive interference
- **Smaller** energy gap between HOMO(s) + LUMO(s) → **less energetic light absorbed**

Resonance Affects Energetic Absorption

- **More** resonance in compound

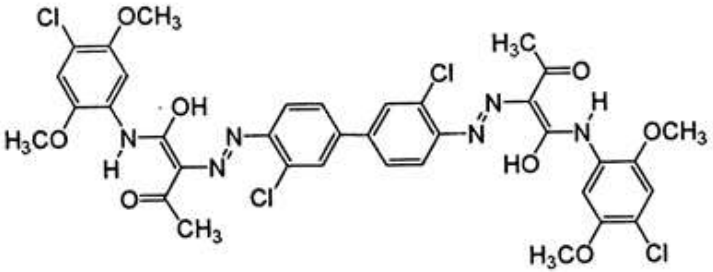
- **Smaller** energy gap between π e^- HOMO(s) + LUMO(s)

- **Less** energetic light absorbed

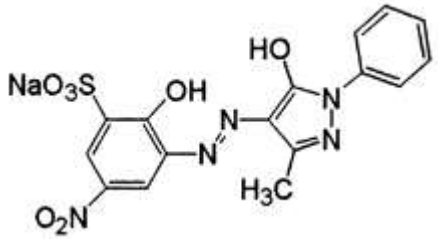
If a compound has **sufficient resonance**:

- Absorbance in **visible spectrum** as opposed to the UV
- No longer reflects entire visible spectrum
- Appears **colored** instead of white

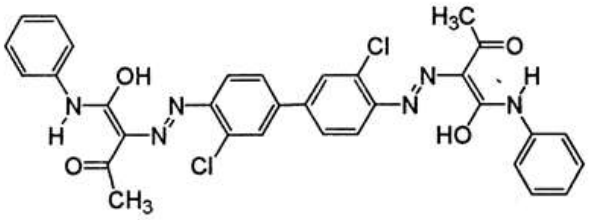
Examples: Organic Dyes and Pigments



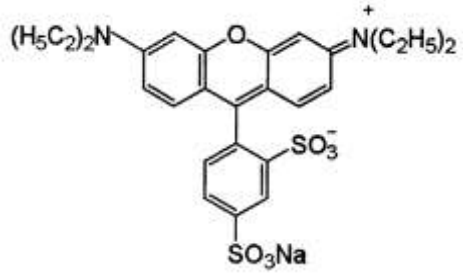
Pigment Yellow 83



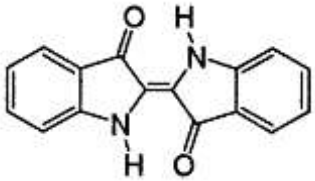
Acid Dye Orange 74



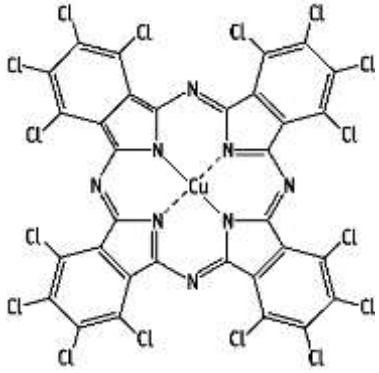
Pigment Yellow 12



Acid Dye Red 52



Indigo
Pigment Blue 66

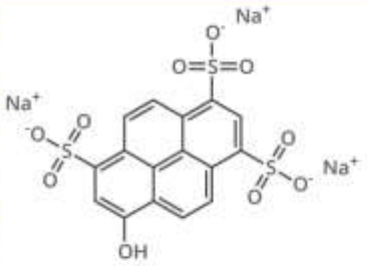


Pigment Green 7

THE CHEMISTRY OF HIGHLIGHTER COLOURS

HIGHLIGHTERS COME IN A RANGE OF COLOURS. THIS GRAPHIC SHOWS A SELECTION OF COMPOUNDS THAT CAN BE USED TO IMPART THESE COLOURS TO THE INK.

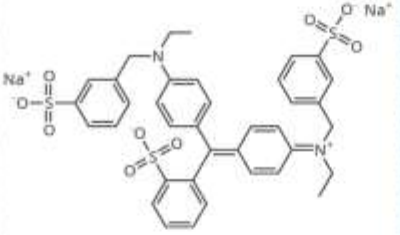
Yellow



PYRANINE - SOLVENT GREEN 7
(Pyrene dye)

Pyranine, a pyrene dye, is the dye commonly used in yellow highlighters. Another compound that can be utilised is fluorescein. By mixing a pyrene dye with a triphenylmethane dye, a green ink can also be obtained.

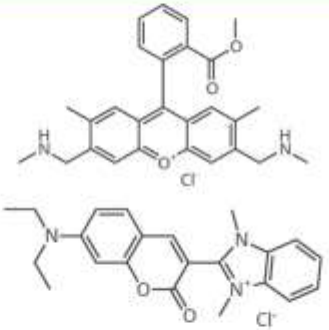
Blue



ACID BLUE 9
(Triphenylmethane dye)

A triphenylmethane dye such as Acid Blue 9 is commonly used to achieve a blue ink colour; it is used in combination with a colour-brightening compound, for example an anionic stilbene derivative.

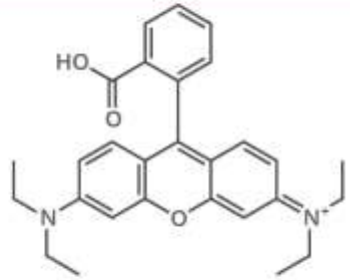
Orange



BASONYL RED 485 (TOP) & BASIC YELLOW 40
(Xanthene dye and Coumarin dye)

A mix of a xanthene dye and a coumarin dye is required to achieve an orange colour.

Pink

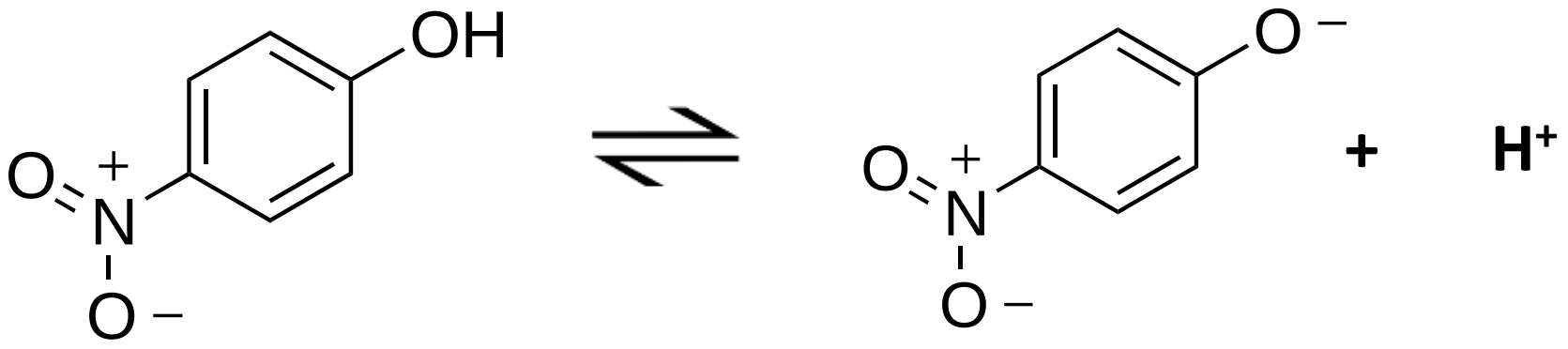


SOLVENT RED 49
(Rhodamine dye)

A rhodamine dye can be used to impart a pink colour to the highlighter ink. A rhodamine dye can also be combined with a triphenylmethane dye in order to produce a purple-coloured highlighter.

What Do You Think?

Paranitrophenol



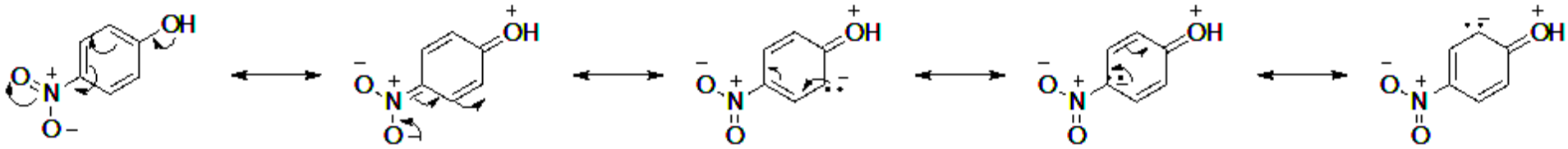
Colorless in Solution

Golden Yellow in Solution

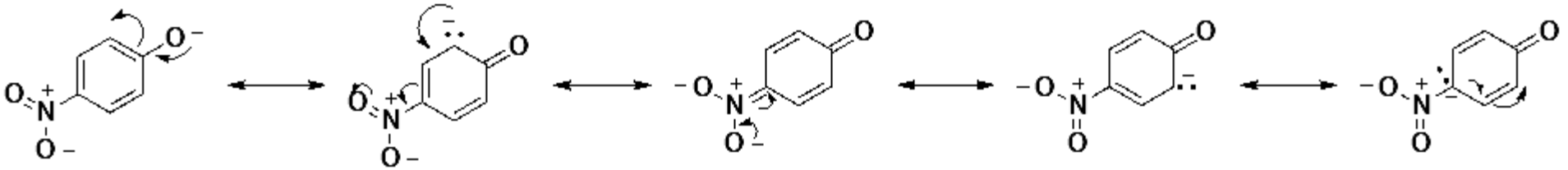
Why is the protonated version clear and the deprotonated version yellow (in solution)?

Resonance Affects Energetic Absorption

Protonated Paranitrophenol

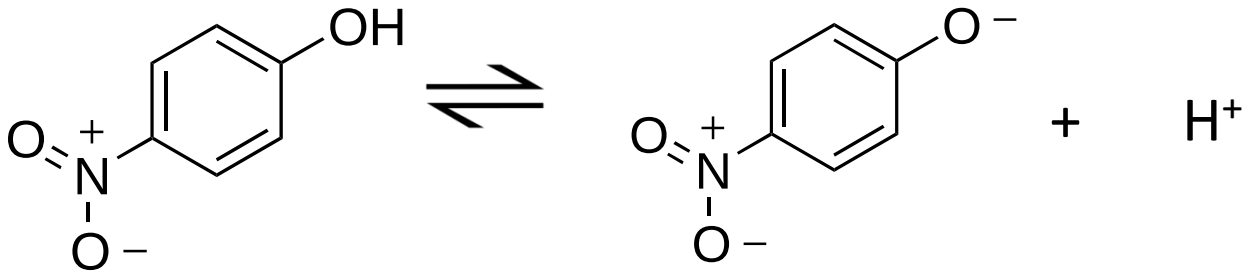


Deprotonated Paranitrophenol

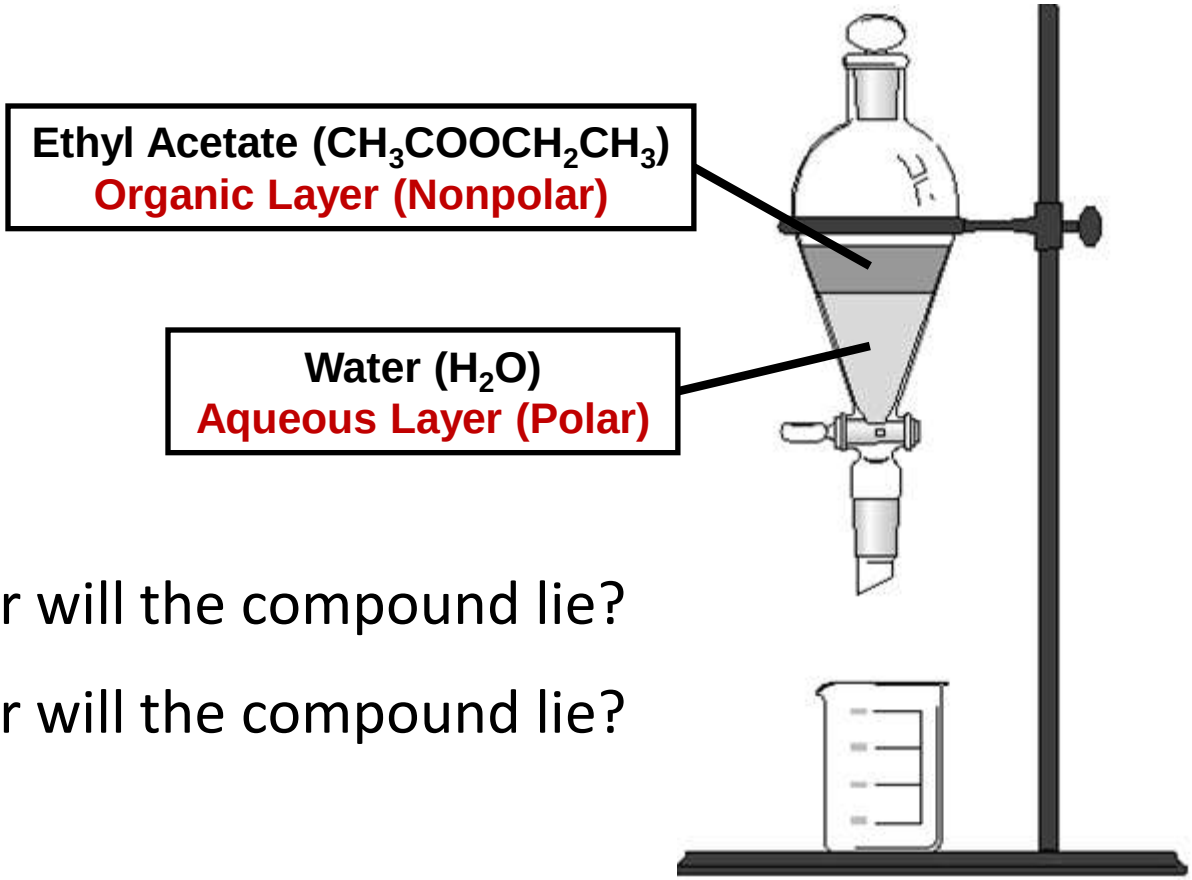


- Deprotonated has more stable resonance contributors
- Deprotonated has greater degree of electron delocalization
- **LESS** of energy gap between the π electron **HOMOs** and **LUMOs**
- **LESS** energy required to promote π electron from **HOMO** to **LUMO**
- **LESS** energetic light absorbed→ visible range as opposed to UV

Demo: Extraction of Paranitrophenol



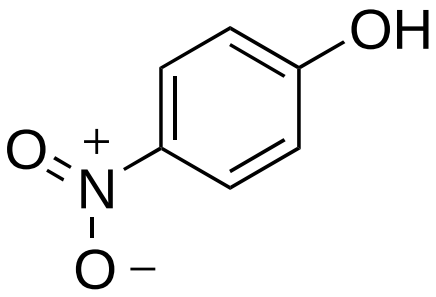
Colorless Solution **Golden Yellow Solution**



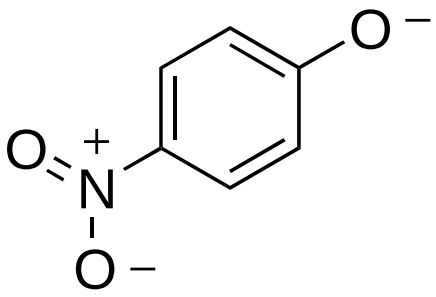
- At **pH 5**, in which layer will the compound lie?
- At **pH 9**, in which layer will the compound lie?

Demo: Extraction of Paranitrophenol

pH 5



pH 9



+ H^+

- **More H^+ in solution**
- Equilibrium shifts to favor **neutral** protonated form
- Compound in nonpolar organic layer
- Colorless (cloudy) solution color

- **Less H^+ in solution**
- Equilibrium shifts to favor deprotonated **ionic** form
- Compound in polar aqueous layer
- Yellow solution color

Acid/Base Indicators and Resonance Energy

- **Example:** Phenolphthalein