# Synthesis of Polypyrrole and Azafullerene

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## Poly-pyrrole

- One of a series of heterocyclic polymers which has attracted much attention due to its characteristic electric and electronic properties.
- The structure in the solid state has been studied by means of high resolution solid-state 13C NMR spectroscopy
- The structure, prepared electrochemically, has been analyzed by using high resolution solid-state
- It is found in corn
- It is a flavoring ingredient Pyrrole has very low basicity compared to conventional amines and some other aromatic compounds like pyridine.
- It is a very weak base with a pKaH of about 4. Protonation results in loss of aromaticity,
- It is a heterocyclic aromatic organic compound, a five-membered ring with the formula C4H4NH
- Was used in the microwave fabrication of multi-walled carbon nanotubes, a rapid method to grow CNT's
- Was used to coat silica and reverse phase silica to yield a material capable of anion exchange and exhibiting hydrophobic interactions.
- Has been studied as a material for "artificial muscles", a technology that offers advantages relative to traditional motor actuating elements

## Aza-Fullerene

**Azafullerenes** are a class of heterofullerenes in which the element substituting for carbon is nitrogen.

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Can be in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical azafullerenes resemble the balls used in soccer.

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Member of the carbon nitride class of materials that include beta carbon nitride (β-C3N4), predicted to be harder than diamond.

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Many properties and structures are yet to be discovered for the highly-nitrogen substituted subset of molecules.

irst discovered in 1993 and reported in the California State Science Fair.

## Fullerene

Fullerene

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The first fullerene molecule to be discovered, and the family's namesake, buckminsterfullerene ($C_{60}$), was prepared in 1985 by Richard Smalley, Robert Curl, James Heath, Sean O'Brien, and Harold Kroto at Rice University.

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Composed entirely of carbon, in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical fullerenes are also called buckyballs, and they resemble the balls used in football (soccer).

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Similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal (or sometimes heptagonal) rings.

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The discovery of fullerenes greatly expanded the number of known allotropes of carbon, which had previously been limited to graphite, diamond, and amorphous carbon such as soot and charcoal.

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Fullerenes with a closed mesh topology are informally denoted by their empirical formula $C_n$, often written C*n*, where *n* is the number of carbon atoms. However, for some values of *n* there maybe more than one isomer.

### 15 samples

**Sample 1- Calcium metal mixed with Pyrrole and 0.1M Sodium Hydroxide**

**Sample 2- Calcium metal mixed with Pyrrole and 0.1M HCl**

**Sample 3- Calcium metal mixed with Pyrrole and Bromine**

**Sample 4 - Calcium metal mixed with Pyrrole and RO water**

**Sample 5- Pyrrole**

**Sample 6- Bromine**

**Sample 7- Calcium metal mixed with Pyrrole and 0.1M HCl and RO water**

**Sample 8- Calcium metal mixed with Pyrrole and 0.1M HCl and 0.1M NaOH**

**Sample 9- Calcium metal mixed with Pyrrole, Bromine and 0.1M NaOH**

**Sample 10- Calcium metal mixed with Pyrrole, Bromine and RO water**

**Sample 11- Calcium metal mixed with Pyrrole and Bromine**

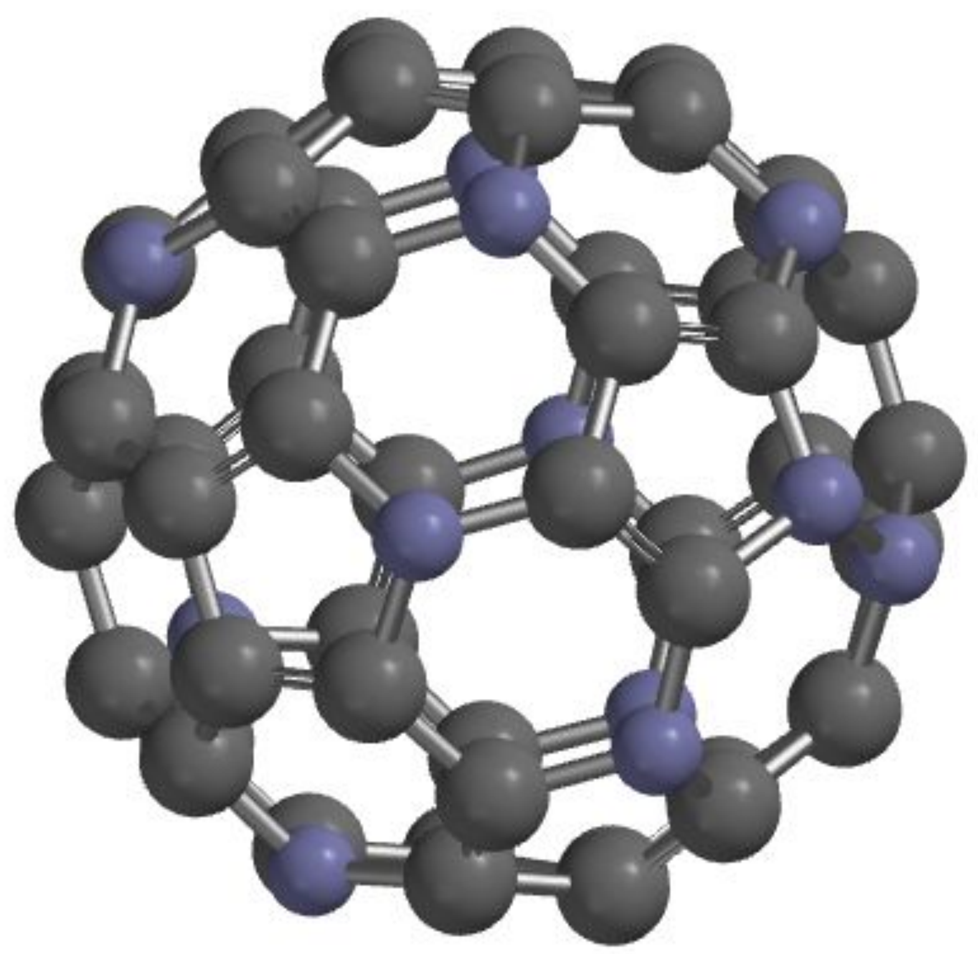
**Sample 12 - Calcium metal mixed with Pyrrole, Bromine and 0.1M NaOH**

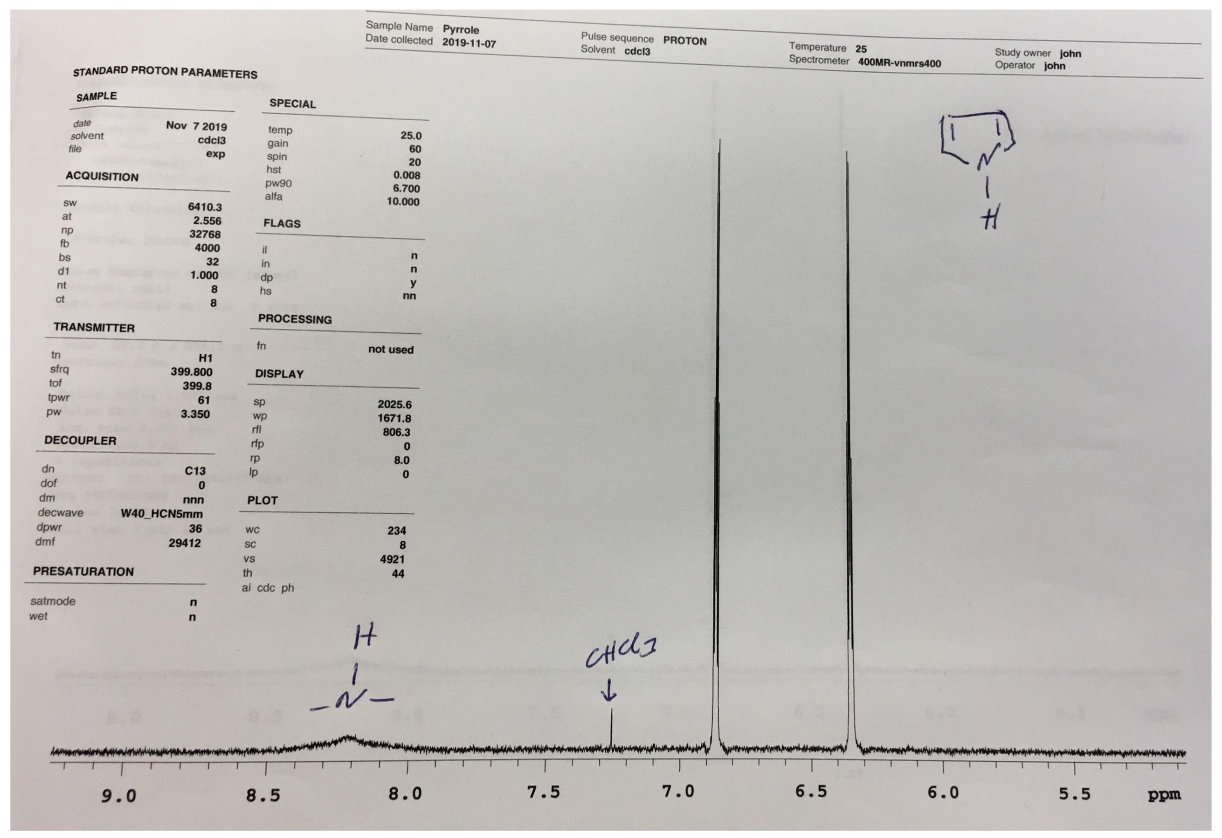
**Sample 13 - Calcium metal mixed with Pyrrole, Bromine and RO water**

**Sample 14- Calcium metal mixed with Pyrrole and 0.1M HCl**

**Sample 15- Calcium metal**

**All samples were then microwaved for 2 mins and methanol was added to them as a solvent.**






NMR of pure pyrrole - lots of materials in different samples prevented NMR spectra (need pure sample for NMR)

### Redox Reactions

Ca (s) + NaOH (aq) → Ca(OH) (aq) + Na (s) E°= -6.51 V

Ca (s) + 2HCl (aq) → $CaCl_2$ (aq) + $H_2$ (g) E°= -2.76 V

Ca (s) + $Br_2$ (l) → $CaBr_2$ (s) E°= -1.69 V

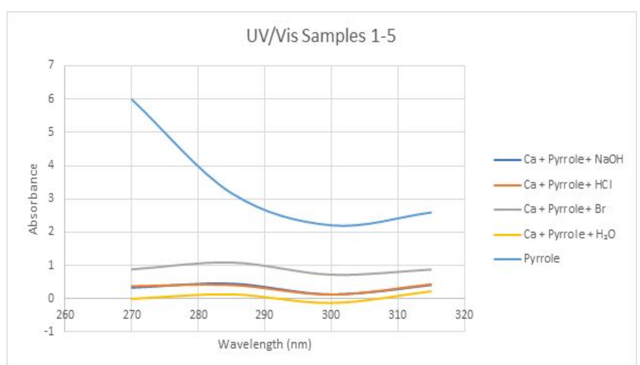
Ca (s) + $H_2O$ (l) → $Ca(OH)_2$ (aq) + $H_2$ (g) E°= -2.76 V

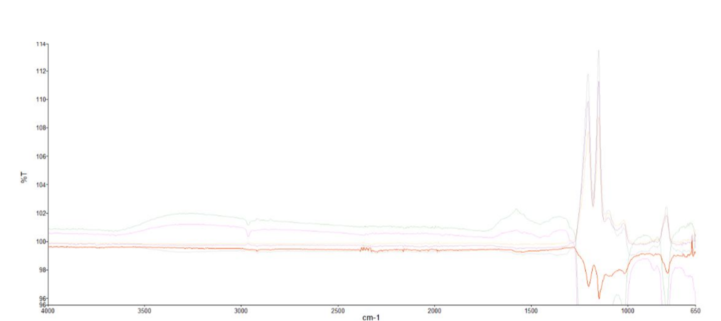
$Br_2$ (aq) + 2e⁻ → 2Br⁻ (aq) E°= 1.0873 V

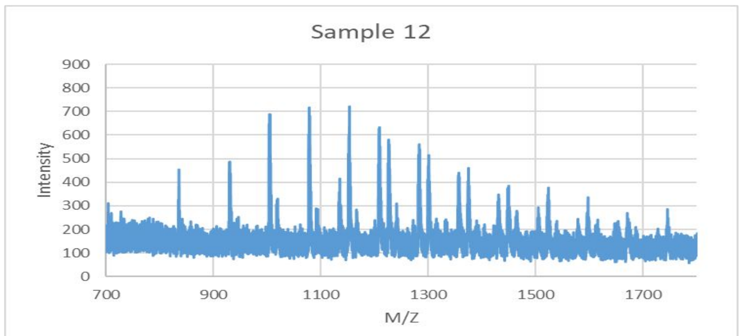
Ca (s) + $Br_2$ (l) → $CaBr_2$ (s) E°= -1.69 V

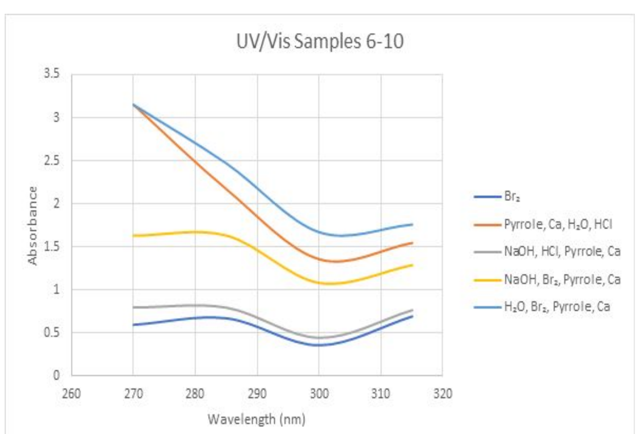
Ca (s) + 2HCl (aq) → $CaCl_2$ (aq) + $H_2$ (g) E°= -2.76 V

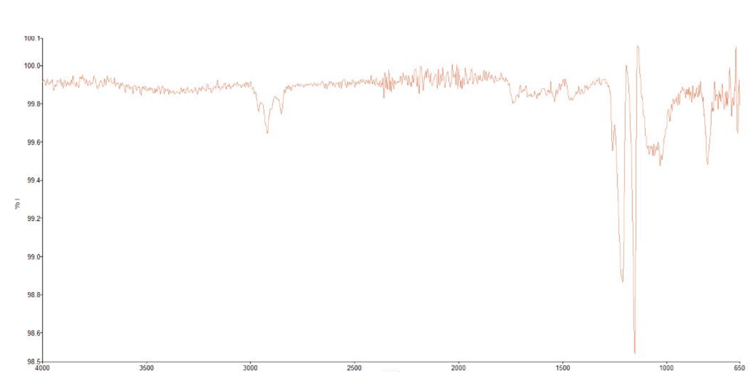
$Ca^{2+}$ (aq) + 2e⁻ → Ca (s) E°= -2.84 V

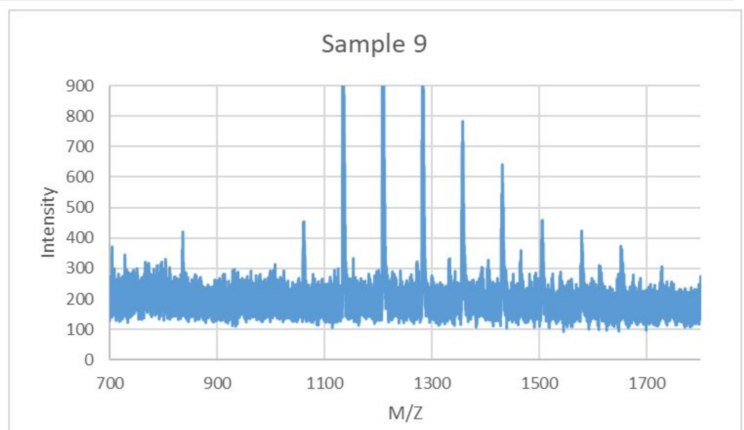


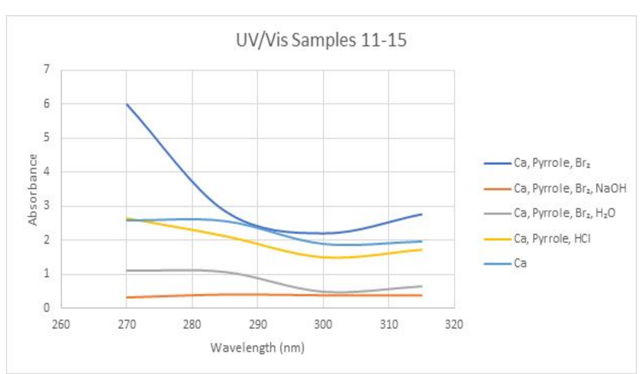



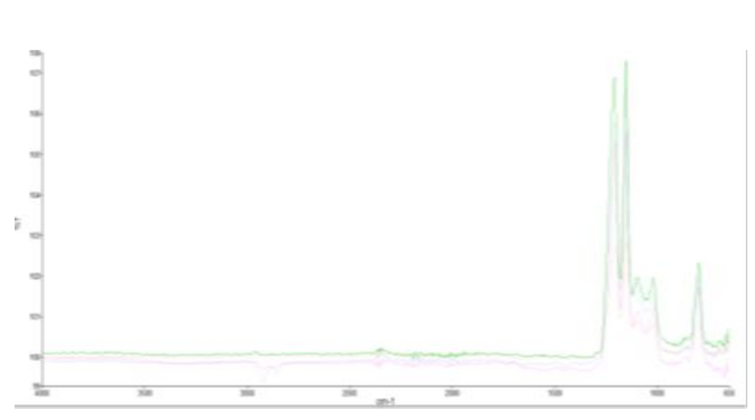


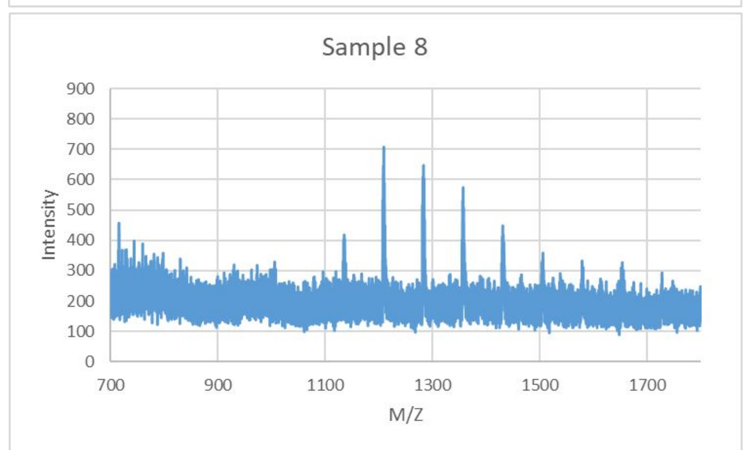








| Number of Pyrroles | Empirical Formula | Molecular Weight (amu) | PSA ($A^2$) |
|---|---|---|---|
| 1 pyrrole | $C_4H_5N$ | 67 | 13.89 |
| 2 pyrrole | $C_8H_8N_2$ | 132.166 | 27.78 |
| 3 pyrrole | $C_{12}H_{11}N_3$ | 201 | 33.877 |
| 4 pyrrole | $C_{16}H_{14}N_4$ | 262.316 | 50.785 |
| 5 pyrrole | $C_{20}H_{17}N_5$ | 327.391 | 69.459 |
| 6 pyrrole | $C_{24}H_{20}N_6$ | 392.466 | 66.674 |
| 7 pyrrole | $C_{28}H_{23}N_7$ | 457.541 | 87.9 |
| 8 pyrrole | $C_{32}H_{26}N_8$ | 522.616 | 88.649 |
| 9 pyrrole | $C_{36}H_{29}N_9$ | 587.691 | 104.378 |
| 10 pyrrole | $C_{40}H_{32}N_{10}$ | 652.766 | 110.415 |
| 11 pyrrole | $C_{44}H_{35}N_{11}$ | 717.841 | 128.356 |
| 12 pyrrole | $C_{48}H_{38}N_{12}$ | 752.906 | 145.429 |
| 13 pyrrole | $C_{52}H_{41}N_{13}$ | 847.991 | 143.358 |
| 14 pyrrole | $C_{56}H_{44}N_{14}$ | 913.066 | 154.418 |
| 15 pyrrole | $C_{60}H_{47}N_{15}$ | 978.141 | 165.731 |
| 16 pyrrole | $C_{64}H_{50}N_{16}$ | 1043.216 | 176.667 |
| 17 pyrrole | $C_{68}H_{53}N_{17}$ | 1108.291 | 187.905 |
| 18 pyrrole | $C_{72}H_{56}N_{18}$ | 1173.366 | 198.279 |
| 19 pyrrole | $C_{76}H_{59}N_{19}$ | 1238.441 | 209.281 |
| 20 pyrrole | $C_{80}H_{62}N_{20}$ | 1303.5 | 227.835 |