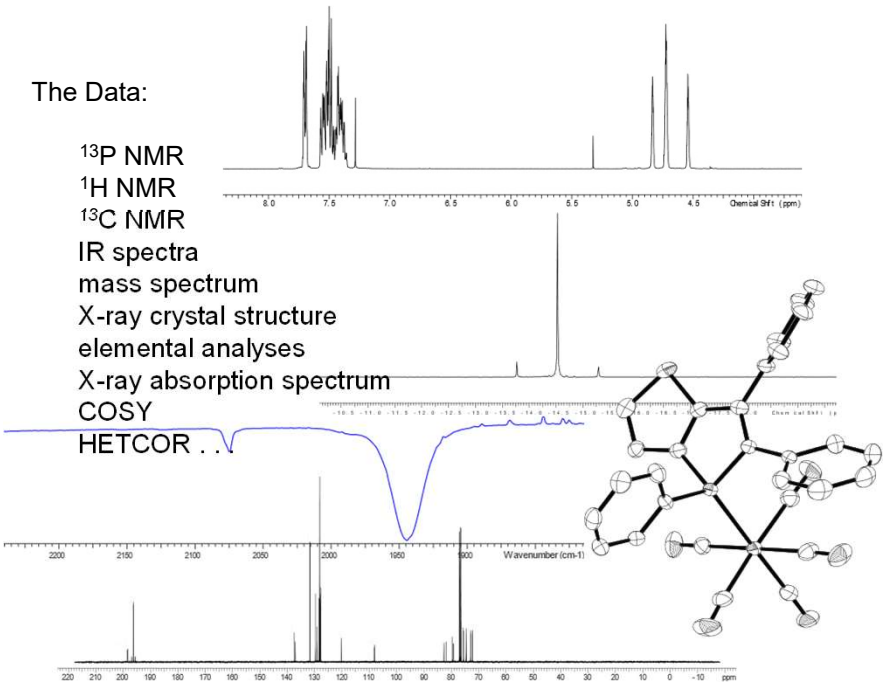
Research Data Management in a Synthetic Chemistry Lab

1

The Data:

- ^{13}P NMR
- ^{1}H NMR
- ^{13}C NMR
- IR spectra
- mass spectrum
- X-ray crystal structure
- elemental analyses
- X-ray absorption spectrum
- COSY
- HETCOR . . .



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The easy part:

Synthetic chemistry has an inherent organization into synthesized compound

The hard part:

It requires a lot of exploratory work, method optimization to reach the point where you have a targeted compound. Large volumes of spectral data are accumulated in this process.

3

Taming large volumes of research data:

one key tool – a consistent file naming convention

BTS20250127Plb2p34 P(O)PPh3

field one: researcher initials

field two: date in year:month:day format

field three: experiment type

P – ^{31}P NMR	C – ^{13}C NMR	IR
H – ^{1}H NMR etc.	COSY	MS

field four: page reference to lab notebook

field five: notes for quick reference

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Data transfer of large volume of data, for example from the NMR instrument computer:

Sort by file name results sorts first by researcher initial – allows files to be easily moved in blocks to research (and therefore project) specific folders.

Within researcher specific folders, the files then sort by experiment date, allowing rapid access to experiments conducted by date (for example, but referencing date in lab notebook).

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Once an effective synthesis of a targeted compound has been achieved, an alternate organization system is needed:

Documents > papers > Phosphenium ions with P-H bonds >Spectroscopic data

- Compound 5
- Compound 6
- Compound 7
- Compound 8
- Compound 9
- Compound 10
- Compound 11 . . .

6

Since the total data volume is relatively small by modern computing standards, appropriate spectra folders are copied into the new organization system rather than moved.

Data analyses never modifies original data, meaning that the original data stays the same in both locations.

This also allows me and students to work independently on data analysis

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Software

- Spectrus Processor (ACDLabs)
  - Handles NMR, IR, Mass Spec, UV-visible
- OLEX-2
  - X-ray crystallography

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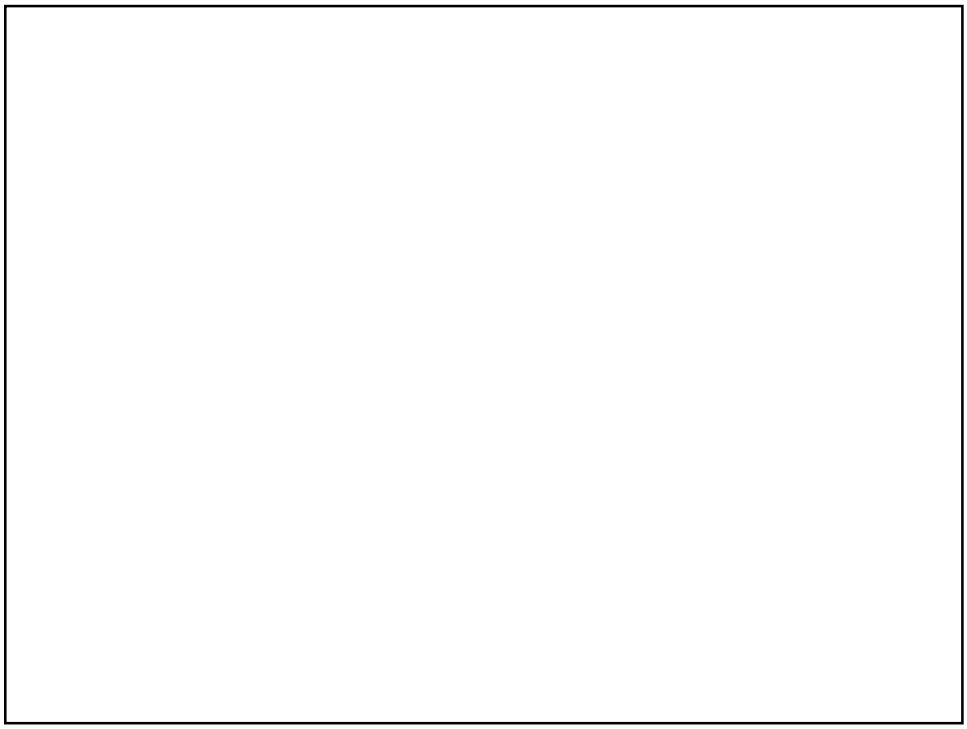

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