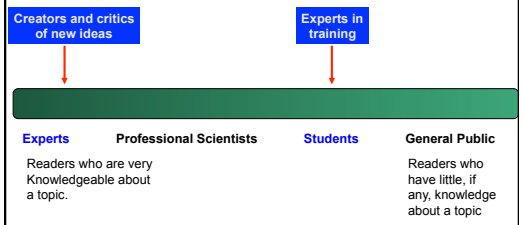
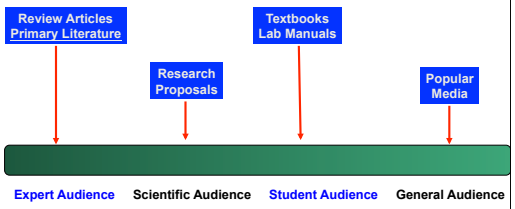
Critical Reading of the Literature

Writing for Chemists
CHEM 360
Krishna L. Foster
Wednesday April 8, 2009

Types of Readers



Types of Scientific Literature



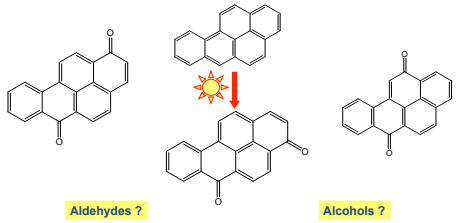
Student Reader → ? ? ? → **Expert Reader**

Learn to read critically!

Day One Outline

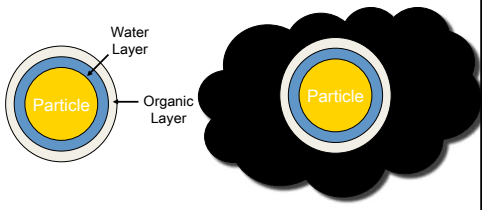
- Polycyclic aromatic hydrocarbon photodegradation background
- Dissection of a primary article
- Target reading techniques
- Application of target reading techniques to Bernstein, *Science*, 1999.
- Introduction to critical reading

PAH Photooxidation Products



- **Chemistry has implications for earth science and biogenisis.**

Particulate Matter in Solutions



Impact of solvents on PAH degradation → 1st step for understanding chemistry on particles

The Big Question

What is the role of solvent on the types and yields of PAH derivatives?

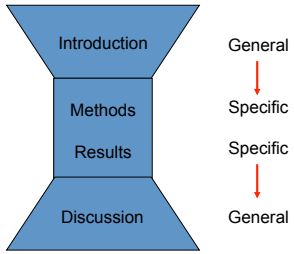
Where Can We Learn More?

- Textbooks: Simplified statements of facts written to introduce general concepts to a student audience.
- Review Articles: Reflection on the current state-of-affairs in a specific sub-topic of chemistry (many citations).
- Primary Literature (peer-reviewed articles): new experiments, the results, and discussion of these results written for an expert audience.

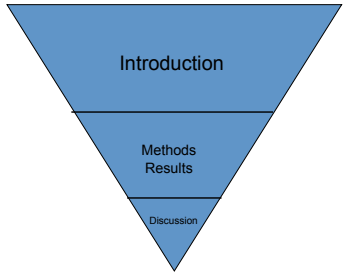
Primary Literature Case Study

- Bernstein, M.P., S.A. Sandford, L.J. Allamandola, J.S. Gillette, S.J. Clemett, R.N. Zare (1999). "UV Irradiation of Polycyclic Aromatic Hydrocarbons in Ices: Production of Alcohols, Quinones, and Ethers." Science 283: 1135-1138.

Hourglass IMRD Format



How not to read!



The Results and Discussion

- **Results:** summarizes quantitative and qualitative data collected during the study.
- **Discussion:** author's interpretation of their data and presentation of the larger implications or applications of their results.

Heart of the critical reading process!!

Exercise

- **Number the paragraphs in the Bernstein paper. Which paragraphs form the introduction, methods, results, and discussion section? Read the topic sentences of each paragraph to identify these sections.**

Introduction: P1- 2 (12%) Results: P6- 12 (41%)
Methods: P3- 5 (18%) Discussion: P13- 17 (29%)

Targeted Reading

- Screening procedure used by busy people (*not* critical reading)!
- Target a given section to look for specific information before reading the article.
- Quickly answer three important questions:
  - 1. What is the study about?
  - 2. What methods were used?
  - 3. What conclusions were drawn?

How to Target Read

- Read the title, abstract (synopsis), and key words
- Read the conclusions or last paragraph
- Quickly study figures
- Read subtitles or topic sentences

EXERCISE

- With only a cursory glance at the title, abstract, key words, and the IMRD sections of the Bernstein article, determine the topic of research, the methods used, and summarize the conclusions. (Note: You should be able to identify the topic and methods, even if you do not understand them.)

Critical Reading of the Literature

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Friday April 10, 2009

EXERCISE

- With only a cursory glance at the title, abstract, key words, and the IMRD sections of the Bernstein article, determine the topic of research, the methods used, and summarize the conclusions. (Note: You should be able to identify the topic and methods, even if you do not understand them.)

TOPIC:	Formation of PAH derivatives by UV irradiation in water ice.
METHODS:	UV irradiated ices analyzed with Fourier transform infrared spectroscopy and microprobe laser desorption, laser ionization mass spectrometry.
CONCLUSIONS:	**(1)** UV irradiation → peripheral carbon oxidation → oxidized PAH alcohols, ketones and esters, **AND** UV irradiation → reduced partially hydrogenated aromatic hydrocarbons. Implications for biogenesis. **(2)** H and D exchange rapidly between PAHs and ice. May explain D enrichment in meteorites.

The BIG EXECRISE: Critical Reading

Do the experiments support the conclusions stated in the article?

Dissect the methods and results to critique the article.

Guide for Analysis of Tables and Figures

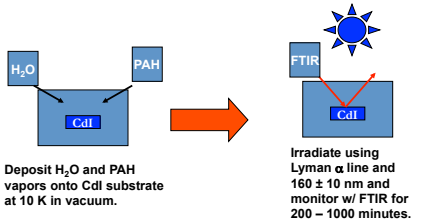
- What is the question being asked in the experiment?
- What experiment is being done to answer the question? What techniques are being used to carry out the experiment?
  - Do the techniques makes sense given the question being asked?
- What are the results of the experiment?
  - – and what should we be looking for in the figure?
- What conclusions does your group draw from the data?
  - Do your conclusions support the authors' claims?
- Additional questions or comments regarding the experimental design.

Bernstein et al., 1999

Table 1. IR spectral features observed at 300 K and functional group assignments.

IR spectral feature	Implied functional group (3,9)
3350 cm^{-1} (very broad: 3600 to 2950 cm^{-1})	O–H stretching (alcohol, H_2O)
2930 and 2850 cm^{-1}	C–H stretch of aliphatic $-CH_2-$ (methylene)
1665 cm^{-1}	C=O stretch of C=C–C=O (conjugated ketone)
1440 cm^{-1}	$=CH_2-$ bending of $=CH_2$–C=O or H_2-PAH
1325 cm^{-1} (broad: 1475 to 1175 cm^{-1})	$-CH_2-$ bending of $-CH_2$–C=O or H_2-PAH
1350 cm^{-1}	C–H or OH in-plane bend (aromatic alcohol)
1240 and 1090 cm^{-1}	C–O–R stretches (aromatic)
~965 and 810 cm^{-1}	C–H out-of-plane bend (aromatic)

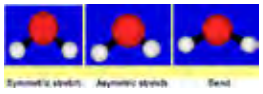
- **QUESTION** ⇨ **Functional groups on PAH photoproducts?**
- **EXPERIMENT/ TECHNIQUES**
- **RESULTS:**
- **CONCLUSIONS:**
- **YOUR QUESTION?:**



Deposit H_2O and PAH vapors onto CdI substrate at 10 K in vacuum.

Irradiate using Lyman α line and 160 ± 10 nm and monitor w/ FTIR for 200 – 1000 minutes.

- FTIR examines vibrational molecular motion



- Measures % transmission through sample as a function of wavenumber (cm^{-1})

- Uses spectra to determine structural features of the sample.

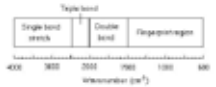


Image Source : http://sis.bris.ac.uk/~sd9319/spec/IR.htm

- **QUESTION** ⇨ **Functional groups on PAH photoproducts?**
- **EXPERIMENT/ TECHNIQUES** ⇨ **Sample vapor deposition in vacuum, UV irradiation, and FTIR spectroscopy analysis.**
- **RESULTS:**
- **CONCLUSIONS:**
- **YOUR QUESTION?:**

Bernstein et al., 1999

Table 1. IR spectral features observed at 300 K and functional group assignments.

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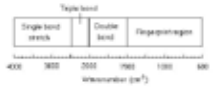


Image Source : http://sis.bris.ac.uk/~sd9319/spec/IR.htm

- **QUESTION** ⇨ **Functional groups on PAH photoproducts?**
- **EXPERIMENT/ TECHNIQUES** ⇨ **Sample vapor deposition in vacuum, UV irradiation, and FTIR spectroscopy analysis.**
- **RESULTS:** ⇨ **Wavenumbers used to identify structural features of photoproducts.**
- **CONCLUSIONS:** ⇨ **Confirmed presence of alcohols and ketones.**
- **YOUR QUESTION?:** ⇨ **How did they insure the surface temperature was the same as the substrate? Are the select wavelengths for irradiation representative of all possible forms of photoexitation? Are the select wavelengths present in interstellar medium?**

EXECRISE

- Analyze Figure 1 in groups, and determine if experiments support the conclusions.

Bernstein et al., 1999

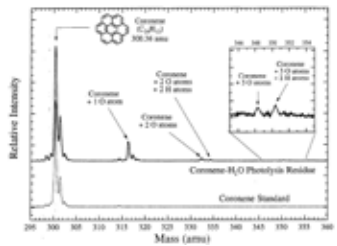


Fig. 1 (left). The μL²MS spectrum of coronene ($C_{24}H_{12}$) compared with that of a residue from a photolyzed coronene-H_2O ice (H_2O/PAH > 800). The peaks at 316, 332, and 348 amu correspond to the addition of one to three O atoms, respectively, likely in the form of ketones or hydroxyl side groups (or both). Elevated peaks at 334 and 350 amu (**inset**) indicate the addition of two H atoms to the doubly and triply oxygenated species. **Fig. 2 (right).** The μL²MS

- **QUESTION** ⇨ **Structural information of OH and O groups proposed in IR experiments?**
- **EXPERIMENT/ TECHNIQUES** ⇨ **Search "mass spectrometry" for information on microprobe laser desorption laser ionization mass spectrometry (μL² MS)**
- **RESULTS:** ⇨ ***m/z* representative of coronene, and coronene plus 1-3 oxygens.**
- **CONCLUSIONS:** ⇨ **Hydroxyl and oxygen functional groups possible on coronene.**
- **YOUR QUESTION?:** ⇨ **More oxygens observed with higher instrument sensitivity? Are the oxygens MS artifacts (soft ionization or space charge effects) or real? Other possible assignments for these masses?**

Bernstein et al., 1999

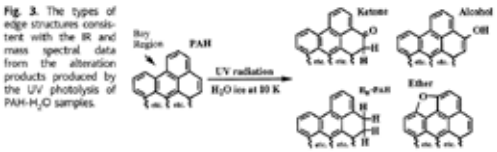
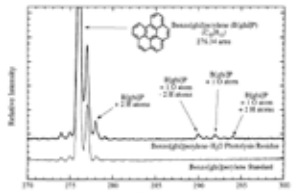


Fig. 3. The types of edge structures consistent with the IR and mass spectral data from the alteration products produced by the UV photolysis of PAH-H_2O samples.

Author's interpretation → Discussion

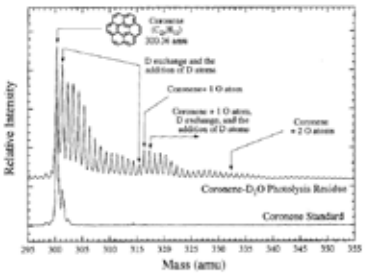
Bernstein et al., 1999



doubly and triply oxygenated species. **Fig. 2 (right).** The μL²MS spectrum of benzo[ghi]perylene ($C_{22}H_{12}$) compared with that of a residue from a photolyzed benzo[ghi]perylene-H_2O ice (H_2O/PAH > 800). The increase in the peak at 278 amu indicates the addition of two H atoms. The peak at 290 amu corresponds to the addition of an O atom with loss of two H atoms, consistent with an ether bridging the molecule's "bay" region. The peak at 292 amu corresponds to the addition of one O atom (as a ketone or hydroxyl group), and the peak at 294 amu corresponds to the addition of one O and two H atoms.

Bernstein et al., 1999

Fig. 4. The μL²MS spectrum of coronene ($C_{24}H_{12}$) compared with that of a residue from a photolyzed coronene-D_2O ice (D_2O/PAH > 800). In addition to the unreacted parent coronene (mass peak at 300 amu) and oxidized coronene (masses of 316 amu and possibly 332 and 348 amu), strong peaks are seen in the 301 to 315, 317 to 331, 333 to 347, and 349+ amu ranges, corresponding to deuterium exchange and addition to the original coronene and its oxidation products.



- **QUESTION** ⇨ **Frequency of hydrogen/ deuterium exchange?**
- **EXPERIMENT/ TECHNIQUES** ⇨ **Microprobe laser desorption laser ionization mass spectrometry (μL² MS)**
- **RESULTS:** ⇨ ***m/z* representative of coronene, and coronene plus 1-3 oxygens and their deuterated forms.**
- **CONCLUSIONS:** ⇨ **Deuterium exchange and addition to the original coronene and its oxidation products.**
- **YOUR QUESTION?:** ⇨ **Is hydrogen more labile in oxygenated PAHs?**