

# The analysis of poly aromatic compounds: a never-ending story?

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For close to 30 years the analysis of environmental pollutants has attracted some of the best minds in science. Chemists have sought to improve the accuracy and precision of the analytical process whilst biologists and biochemists have studied the mechanisms of both bio-availability and toxicity. For the most part the molecules under examination have retreated from the environment, as a full understanding of their toxicity led to their production and use being prohibited. But for one group, as rapidly as knowledge has developed so has the ubiquity of their presence. I refer, of course, to the group known as poly aromatic hydrocarbons, or PAHs.

There are many hundreds of organic molecules which can be described as PAHs, most have been known since the 1960s. Table 1 lists those, identified by the USA, of concern. The CAS Numbers are provided for reference.

In addition, in Table 2 are the PAH listed by the EPA as priority chemicals.

These two listings cover 28 PAHs that are of such concern that they should not be used for any purpose: the result is that much has been written about them and their analysis and that research into them continues at quite a high level: why is this?

Over the years it has become clear that hydrocarbons are the main source of PAH pollution. So why are they not only commonly found in the environment but are still known to be entering the environment and food chain? The answer is that PAHs are in many ways unique as environmental pollutants! They are produced continuously, not only by the activities of the society that is concerned by their toxicity, but also by the environment: for example, forest fires, tar sands and coal outcrops are all signifi-

cant sources of PAHs. Human activity remains the main source: burning fossil fuels generates PAHs.

It might be reasonably assumed that humans would seek to minimise exposure to PAHs: in most cases this is so, but when the subject is BBQ food, logic flies out of the window. Why? Because many of the key components of the smoky, carbonised flavours that characterise BBQ'd food are PAHs. So to eliminate them would fundamentally change the nature of human food!

As mentioned, the study of PAHs attracts much scientific research and regulatory oversight: indeed the US EPA recently revised their generic description of molecules including PAHs to "Polycyclic Organic Matter" (<http://www3.epa.gov/airtoxics/hlthef/polycycl.html>).

Table 1		CAS Number
1)	Benzo(a)anthracene	56-55-3
2)	Benzo(a)phenanthrene (chrysene)	218-01-9
3)	Benzo(a)pyrene	50-32-8
4)	Benzo(b)fluoranthene	205-99-2
5)	Benzo(j)fluoranthene	205-82-3
6)	Benzo(k)fluoranthene	207-08-9
7)	Benzo(j,k)fluorene (fluoranthene)	206-44-0
8)	Benzo(r,s,t)pentaphene	189-55-9
9)	Dibenz(a,h)acridine	226-36-8
10)	Dibenz(a,j)acridine	224-42-0
11)	Dibenzo(a,h)anthracene	53-70-3
12)	Dibenzo(a,e)fluoranthene	5385-75-1
13)	Dibenzo(a,e)pyrene	192-65-4
14)	Dibenzo(a,h)pyrene	189-64-0

15)	Dibenzo(a,1)pyrene	191-30-0
16)	7H-Dibenzo(c,g)carbazole	194-59-2
17)	7,12-Dimethylbenz(a)anthracene	57-97-6
18)	Indeno(1,2,3-cd)pyrene	193-39-5
19)	3-Methylcholanthrene	56-49-5
20)	5-Methylchrysene	3697-24-3
21)	1-Nitropyrene	5522-43-0

  

Table 2		CAS Number
1)	Acenaphthene	83-32-9
2)	Acenaphthylene	208-96-8
3)	Anthracene	120-12-7
4)	Benzo(g,h,i)perylene	191-24-2
5)	Fluorene	86-73-7
6)	Phenanthrene	85-01-8
7)	Pyrene	129-00-0

# QUALITY MATTERS

To catch up on what has been happening in the world of PAH analysis, this September I took part in the 25<sup>th</sup> International Symposium on Poly Aromatic Compounds, or PACs (the term PAC encompasses all PAHs, plus a growing number of modified PAHs).

Held in Bordeaux, France, (<http://ispac2015.ism.u-bordeaux1.fr>) the symposium is the latest in a series that has been running for more than 40 years. This event attracted close to 200 delegates who spent five days reviewing recent developments, including:

- The production and application of certified reference materials for PAH analysis
- Biodegradation and environmental fate of PAHs
- Geno and reproductive toxicity of PACs
- The analysis of PACs
- Microbiological degradation of PAHs
- PACs in air and water and eco-toxicity
- Endogenous and exogenous synthesis of PACs
- The presence of PACs outside the Earth's biosphere
- The role of food in PAC exposure
- The particular impact of polar PACs
- PACs in hydrocarbons

There were 98 oral and 97 poster presentations covering the wide area of topics listed above: all in all a very interesting programme. With two and sometimes three parallel sessions, it was not possible to participate in all the sessions, I focussed on those that matched my particular interests in reference materials, environmental and food analysis. There were a number of really good presentations, but a few that left me wondering about the quality of the data upon which conclusions had been developed.

The production of reference materials is well established: the US National Institute of Standards and Technology (NIST) has been producing pure substance calibrators and matrix CRMs for many years and Dr Stephen Wise reviewed recent matrix CRMs certified for PAH content in urine, tea and weathered oil. Certification was achieved using a range of analytical procedures from which a certified value was developed.

Alan Nichols, from Sigma Aldrich described how high performance quantitative proton NMR (HP-QNMR) could

be used to directly measure the amount of substance and so allow the rapid and direct development of certified values. Of late Sigma Aldrich has published regularly on the use of HP-QNMR for the certification of organic materials. It is, without doubt, a powerful tool, but the very high capital and running cost of the necessary 600 MHz NMR instruments makes it unlikely that this technique will become widely adopted.

Turning to environmental aspects, I listened to a number of fascinating presentations that detailed how PAHs find their way into the environment from a range of activities, including coal mining and harvesting sugar cane. In the latter case the cause is stubble burning. In all the presentations there was only one, by Robert McCrindle from Tshwane University in South Africa, where specific reference was made to the use of CRMs for method validation. But in no other paper, or poster, was the use of a CRM in method development or as a calibration material mentioned.

Over the last 15 years the use of CRMs, or RMs, in commercial testing laboratories has become virtually universal as accreditation to ISO 17025 has become normal. But it seems that in academic and government research laboratories analytical quality control is 20 years behind. Why is this?

Talking to young researchers from many countries I have formed the opinion that the fundamentals of good analytical metrology are not taught at undergraduate level. Further, that there is a worrying lack of understanding that without instrument qualification, method validation and some form of analytical quality control, data can neither be compared nor entirely trusted. Perhaps it is too much to expect these labs to be accredited to ISO/IEC 17025, but I do believe that there needs to be an acceptance that Quality Matters and it is not good enough to go on relying on data that is not underpinned by good analytical quality assurance.

Why does it matter so much? Because data from the academic and research community often acts as a stimulus for government concern and the data may ultimately result in legislation. It concerns me that legislation may be driven by bad data.



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