UDC 535.34:621.373

EMISSION SPECTRA FOR ANALYSING ELEMENTS IN CLUES USING OPTICAL METHOD

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The following research was dedicated to the investigation of emission spectra of different elements and their use in the analysis of clues. The used equipment was a spectrometer, the "Red Tide USB-650", and an application called "Overture". The spectrometer has a spectral range from 350 nm to 1000 nm. It's a very lightweight and portable device, not taking up much space and weighting only 190 g. The sensitivity of the device is 75 photons at a wavelength of 400 nm. The optical resolution of the spectrometer is 2 nm, while the program can display accurate graphs with a resolution of up to 0.1 nm. The spectrometer's integration time ranges from 3 ms to up to 65 seconds, but typically it doesn't exceed 15 seconds. For very precise data recording the spectrometer can also use the optic fibres. The used program has a library of emission spectra of different elements. The experiment is performed by making the substance to emit photons by exciting it. The light from this substance is received by the spectroscope and the data are transmitted to the computer. The program generates an "Intensity-Wavelength" graph right away. But to analyse and to detect elements in clues a graph is not the only required thing. Luckily, we have access to the emission spectra library built into the program. Those can be enabled and disabled to detect if the given element is present in the earlier analysed substance. Such a method can be used to detect elements in clues using spectral analisys at remarkable speeds and accuracies.

Keywords: emission spectra, clue, resolution, sensivity, photon.

Cercetări de faţă sunt dedicate studiului spectrelor de emisie a diferitor elemente şi utilizarea lor în analiza probelor în criminalistică. Echipamentul folosit era spectrometrul „Red Tide USB-650" şi aplicaţia „Overture". Spectrometrul are diapazonul spectral de la 350 nm pînă la 1000 nm. Este un dispozitiv foarte uşor şi portativ, nu ocupă mult spaţiu şi cîntăreşte numai 190 g. Sensibilitatea dispozitivului este 75 fotoni la lungime de undă de 400 nm. Rezoliţia optică a spectrometrului este 2 nm, pe cînd programul poate afişa grafice precise cu rezoluţia de pînă la 0,1 nm. Timpul de integrare a spectrometrului variază de la 3 ms pînă la 65 s, dar de obicei nu depăşeşte 15 s. Pentru înregistrarea datelor cu precizie foarte înaltă spectrometrul de asemenea poate folosi fibre optice. Programul utilizat are o bibliotecă de spectre de emisie a diferitor elemente. Experimentul se realizează prin emiterea de substanţă la excitarea ei a fotonilor. Lumina de la aceasta substanţă este primită de spectroscopul şi datele se transmit la calculator. Programul imediat generează dependenţa „Intensitate-Lungime de undă". Dar pentru a analiza şi a detecta elementele din probe graficul nu este suficient. Din fericire, avem acces la biblioteca de spectre de emisie încorporat în program. Acestea pot fi activate şi dezactivate pentru a detecta dacă elementul dat este prezent în substanţă analizată anterior. Aşa metodă poate fi folosită pentru detectarea elementelor din probe în criminalistică utilizînd analiza spectrală cu viteză şi precizie remarcabilă.

Cuvinte-cheie: spectrul de emisie, dovadă, rezoluţie, sensibilitate, foton.

INTRODUCTION

The following article explains how the elements found in clues can be analysed using spectral methods by a spectrometer and software. By measuring the emission spectra of excited substances it was possible to detect elements in the sample.

Every known single element has a different emission spectrum. It can be compared with a type passport for every known substance. But to understand this concept of emission spectra, it's necessary to know the concept of emission of photons from substances.

To explain this concept Bohr's atom model will be used. Niels Bohr first proposed that electrons can only gain and lose energy by jumping from one allowed orbit to another, absorbing or emitting electromagnetic radiation with a frequency ν determined by the energy difference of the levels according to the Planck relation:

$$\Delta E = E_2 - E_1 = h\nu \qquad (1)$$

Bohr stated that photons are produced when electrons move from a lower energy state to a lower one, giving off that energy in the form of an electromagnetic wave – a photon (fig. 1). The wavelength of the photon can either be derived from the Planck relation, where $v = \frac{1}{T}$, or using the Rydberg formula:

$$\frac{1}{\lambda_{if}} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad (2)$$

where R is the Rydberg constant, which is different for various elements.

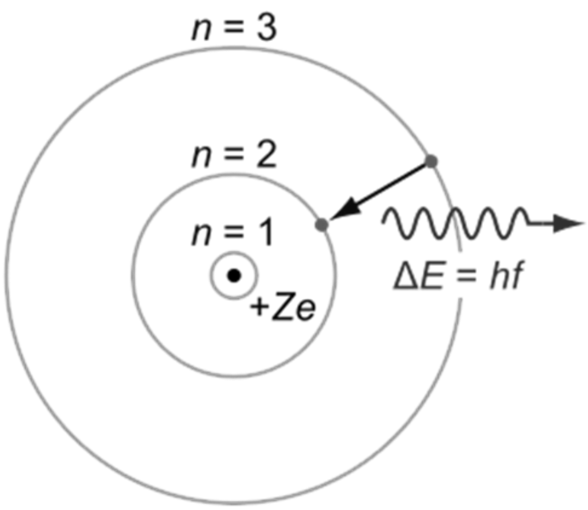

Fig. 1. A hydrogen atom according to Bohr's model, emitting a photon at a wavelength of 656 nm, which would be a red visible light

For every atom there are multiple different emission spectra. They have their own intensities and wavelengths. For example, hydrogen has 4 spectra in the visible range. This series of spectra is called the Balmer series. Photons of this series are emitted when electrons transition from a higher orbit to the second orbit (fig. 2).

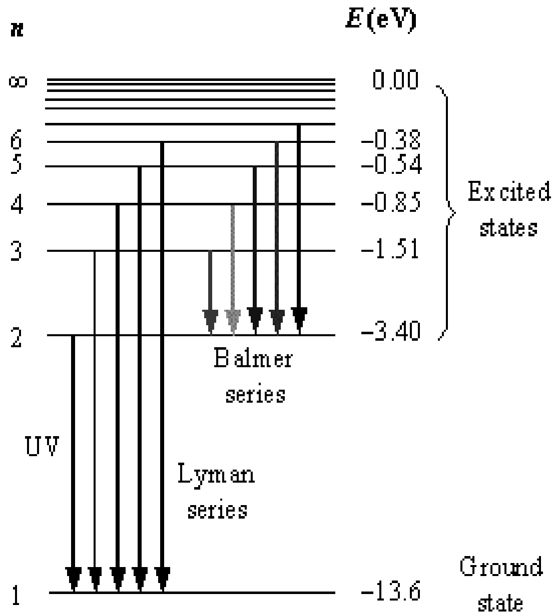

Fig. 2. Electron transitions from different energy states

There are other series for the hydrogen atom, like the Lyman (Ultraviolet) and Paschen, Brackett, Pfund, Humphreys (Infrared) (fig. 3).

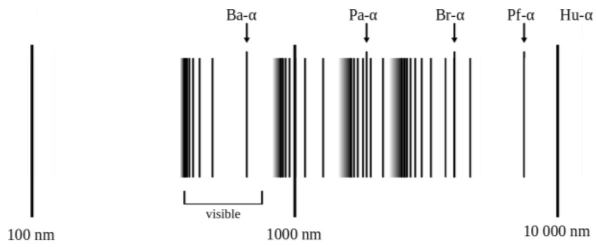

Fig. 3. The emission spectra of the hydrogen

There is also another way of demonstrating the different electron transitions occurring in a hydrogen atom and the photon energies according to the Rydberg equation.

Such a representation helps to visualise the energy of the photons emitted from different electron transitions.

Again, we see that emitted photons have different energies depending on the exact electron transitions that occur inside the atoms. Along with that the energies vary depending on the atom emitting the photon, so this again proves that the emission spectra of all atoms are different.

But they vary not only from atom to atom. The emission spectra vary from isotope to isotope as well. Although the nucleus charge of isotopes is the same, the mass is different. This affects the emission spectra by a slight amount. To explore this phenomenon hydrogen and its isotope deuterium will be used as examples.

Deuterium has an additional neutron in its core, which changes the mass of the nucleus. By expanding the Rydberg equation we get the following formula:

$$E_i - E_f = \frac{\mu_x Z^2 e^4}{(4\pi\varepsilon_0)^2 2h^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad (3)$$

where μ_x is the reduced mass of the atom X. Since the equation depends on this mass, isotopes have slightly different emission spectra.

Looking at the image (fig. 4) we can see that both emission spectra of deuterium have a slightly shorter wavelength than the hydrogen spectra, but only by a very slight amount.

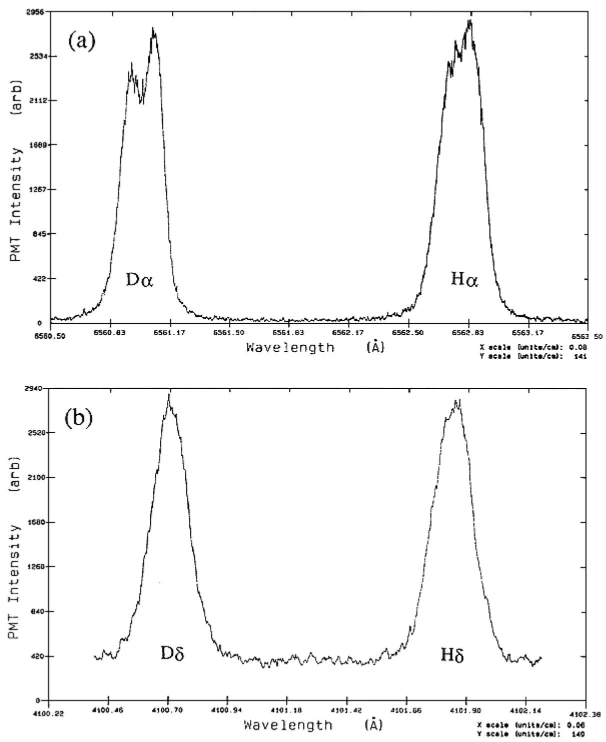

Fig. 4. Comparison of the slightly different (by only about 0.2 nm) emission spectra of hydrogen and deuterium:
a) Emission spectra of D_α and H_α
b) Emission spectra of D_δ and H_δ

But since they vary, it's possible to distinguish deuterium and hydrogen in the experimental studies. This relates to all the elements and isotopes, since the same thing applies to them.

ATOMIC EMISSION SPECTROSCOPY

All of the previously introduced concepts are the basis of atomic emission spectroscopy (AES). It's a method of chemical analysis used to determine the amount of an element in a certain substance or sample.

It is a very precise method of doing this kind of analysis, due to the fact that some spectrometers have a very high sensitivity, and allow measurements with great precision.

Optical methods also allow distinguishing atoms from its isomers if they are present in the sample being analysed, since the emission lines of isomers slightly differ.

It is performed by exciting the atoms of a substance sample using various methods. The data is collected with a spectroscope and is sent to a computer. Then, according to the emission spectra of different elements, the resultant spectrum is matched with the emission spectra. If there is a match it means that the substance, the emission spectrum of which was used, is present in the sample.

There are various methods of performing this analysis. The atoms can be excited by a flame, which gives the atoms thermal energy or, for analysing metallic elements in substances, spark and arc emission spectroscopy can be used. A spark with high voltage excites the atoms and they emit photons.

EQUIPMENT

To perform AES, a spectrometer and computer are required. The used spectrometer was the "Red Tide USB-650", and the program was "Overture".

Red Tide USB-650 spectrometer (fig. 5) [1-3]:

- Dimensions: 89.1×63.3×34.4 mm
- Weight: 190 g;
- Range: 350-1000 nm;
- Sensitivity: 75 photons at 400 nm;
- Integration time: 3 ms to 60 s (usually up to 15 s);
- Optical resolution: ~2 nm;
- Able to work both with and without optical wire.

Fig. 5. Red Tide USB-650 spectrometer

Overture software (fig. 6):

- Contains a library of sample emission spectra of different elements which can be activated and disabled;
- Able to take screenshots of multiple spectra for comparison;

– Allows to work with emission, absorption and transmission spectra;
– Able to save spectra and export data for building graphs and further research.

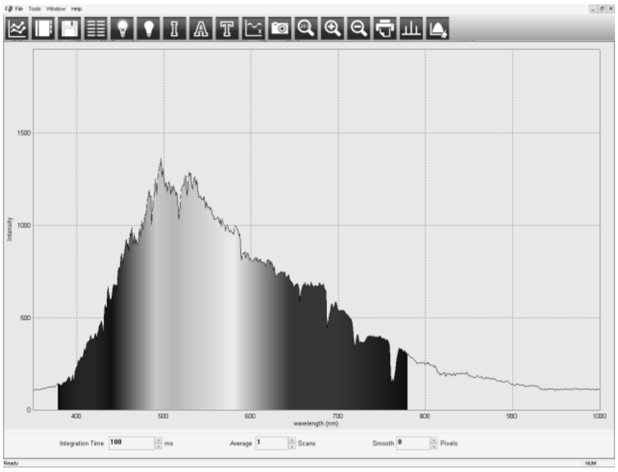

Fig. 6. Overture software interface

EXPERIMENT

After setting up the experimental equipment we decided to try and detect the elements in a simple light source – a lamp installed on the ceiling of the room. By precisely pointing the spectrometer at the light source (fig. 7) we were able to get a good image of the emitted spectrum. (Note the minor error on the bottom - it's the background noise of the spectrometer. It can be cancelled in the program).

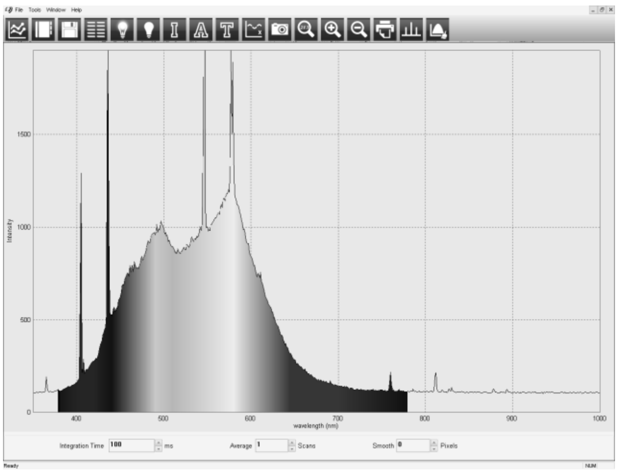

Fig. 7. Spectrum received from the device while pointing at the source

The software used in the experiment had a database of emission spectra of different elements integrated into it (fig. 8).

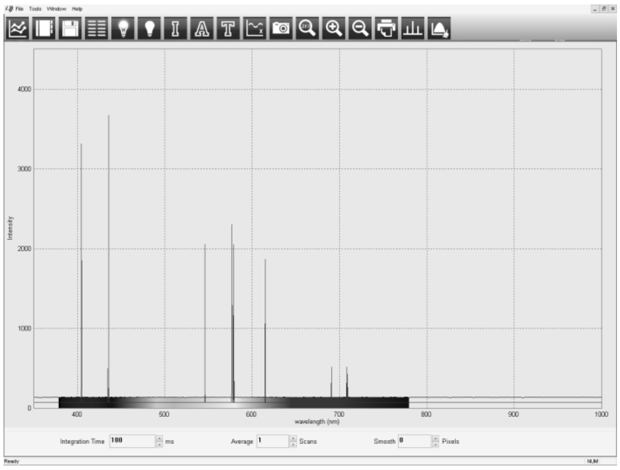

Fig. 8. Mercury emission spectrum, taken from the integrated database

The process of matching sample spectra with the spectrum of the light source was easy. It was done by simply disabling and enabling different emission spectra in the database, and matching them with the emission lines of the spectrum (fig. 9).

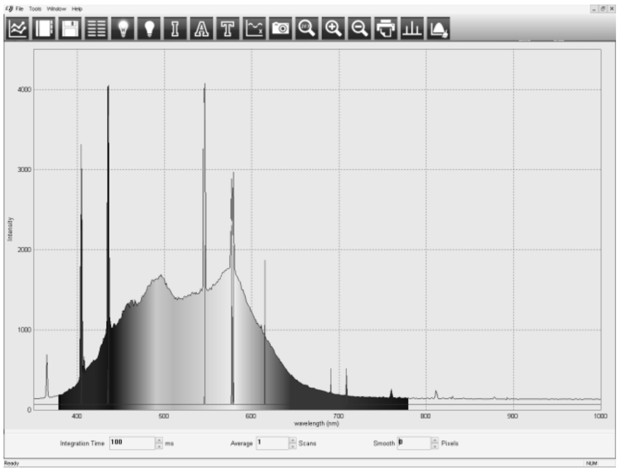

Fig. 9. The mercury emission spectrum matched with the received spectrum

After turning on the mercury emission spectrum in the software it matched the emission lines peaking from the continuous spectrum. This meant that the source contained mercury, and proved the fact that the lamp emitting the photons was a mercury lamp.

Due to the limited resolution of the spectrometer it would be very hard to precisely detect the amount of substance emitting the light, but using latest laboratory technologies it is possible to do this job with great precision.

APPLICATIONS IN CRIMINOLOGY

This method of analysis has a vast variety of applications, one of which is the analysis of elements in clues in criminology. Performing this analysis using optical methods has a lot of advantages compared to other methods.

Firstly, it's very fast. In chemical analysis for example in some cases it could take a lot of time to detect the elements making up a certain substance. Optical methods are much faster compared to some other methods. In criminology, this time could be crucial.

Secondly, optical methods are very accurate. Since the intensity depends on the quantity of a certain element, it's possible to detect the amounts very precisely.

Optical methods allow very precise and rapid detection of elements in clues.

CONCLUSIONS

The analysis of elements in clues using optical methods is a very large part of criminology. Due to the fact that atoms have their fixed emission spectra, it is possible to use them as passports in the detection of elements. Using the latest technologies it is possible to work with substances with astonishing precision. But even using standard equipment it is possible to detect certain elements in substance samples using optical methods.

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Prezentat la redacţie la 12.09.2015