

MS38-P7 XRD analysis as a complementary tool of phase analysis in a forensic fieldMarek Kotrly^{1,2}

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Analyses of materials from an extremely wide spectrum are performed in a forensic field, but a number of which can be potentially dangerous - biological substances, explosives, poisons, etc. It is also often necessary to analyze materials that include organic and inorganic components and here is the role of XRD phase analysis irreplaceable.

In a forensic field, a broad range of analytical methods, such as optical microscopy, SEM/EDS/WDS, XRF, ion chromatography, Raman spectroscopy, FTIR, ICP MS, GC-MS, MS/MS, MSn, NMR, etc., are used for identification of unknown materials and by phase analysis. A needed synergic effect arises by combination of these methods and XRD techniques, which leads to a successful acquisition of evidence material applicable at trial.

XRD techniques are currently used for soil analysis, mineralogical and petrological objects, precious stones and other gemmological objects, pigment phases in the broadest sense, postblast residues, components of explosives and pyrotechnic compositions (inorganic and organic phases), plastics and polymers, pharmaceutical and cosmetic products (including narcotics), building materials, alloys and metals, fillers and additives (polymers, paper products, etc.), fillers of safes, "unknown" samples (in the broadest sense). X-ray powder diffraction in reflection and transmission mode and microdiffraction are usually applied. Gandolfi chamber is used in special cases and monocrystal methods are employed exceptionally.

So called "Legal Highs" - new synthetic drugs, which began appearing on the world market, currently pose a significant problem. These are structural variations of known substances with psychotomimetic effects, which have not been yet registered on the list of state controlled substances and are synthesized to evade the law. Many of the substances are temporarily sold legally. Analysis, identification and quantification of these substances are rather complex because they are not entered to identification databases. The methods of X-ray diffraction are a very convenient complementary technique to common methods of sophisticated organic analysis. The occurrence of Legal Highs on the market can be also considered very dangerous, since the toxicity in most of these substances has not been yet known.

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Keywords: forensic science, X-ray powder diffraction, microdiffraction, electron microscopy

MS38-P8 High-resolution crystallographic investigations of organometallic compoundsDarina Storozhuk¹, Dirk Raiser², Simone Teichert^{1,2,3}

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Our motivation is to shed more light into the ultrafast dynamics of some organometallic molecules and study the mechanism underlying, drawing the complete picture of the system under investigation. But since the important electronic changes due to optical excitation take place on very short ps- and sub-ps timescales it gives rise to the necessity of faster time-resolved measurements than those, which are currently possible at third generation synchrotrons. We performed high-resolution crystallographic measurements at various temperatures and study the dynamics of the system as the function of temperature and will be presented.

Keywords: organometallic molecules, time-resolved measurements, high-resolution