APPLICATION NOTE

No. AN41129

Explosives in forensic science using benchtop ARL EQUINOX 100 X-ray Diffractometer

Author: Dr. Simon Welzmiller, Application Specialist, Dr. Henry Pilliere, Research Manager

Introduction

The analysis of explosives is an important part of forensic science. Due to the ever-present threat of attacks by terrorist organizations and criminals, it is crucial to improve explosive detection and analysis techniques, even if case numbers are quite low compared to other forensic applications like drug analysis. Outside of forensic work within law enforcement agencies, there is a demand for mobile labs in hot zones from military bodies and contractors due to the extensive thread of IEDs (improvised explosive devices). Approximately 60% of forensic cases involve intact explosive devices like IEDs, grenades, or illegal fireworks. An important part of forensic explosives investigations is rooting the origin of the explosive as well as clustering similar samples. Explosive materials often contain side phase due to synthesis, storage, or mixing of the material. Additionally, investigations on remains from explosions, like parts of casings, allow drawing conclusions about the type of explosive device.

X-ray diffraction (XRD) is a powerful method in analyzing crystalline materials and mixtures to identify explosive materials. The Thermo Scientific™ ARL™ EQUINOX 100 benchtop XRD instrument is a transportable and versatile tool which perfectly fits the requirements in forensic science.

Instrument

The ARL EQUINOX Series represents a portfolio of XRD instruments from simple, easy-to-use bench-top systems for routine analysis to more advanced floor-standing, research-grade systems.

Figure 1: ARL EQUINOX 100 diffraction system

The ARL EQUINOX 100 employs a custom-designed 50 W (Cu or Mo) or 15 W Co high-brilliance micro-focus tube with mirror optics which does not require an external water chiller. The unit can be transported between laboratories or into the field without requiring any special infrastructure and operated using batteries or other low-grade power sources due to its low power consumption (100 W).

The ARL EQUINOX 100 (c.f. Figure 1) provides very fast data collection compared to other diffractometers due to its unique curved position sensitive detector (CPS) that measures all diffraction peaks simultaneously and in real-time.

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Experimental

Powdered explosive samples were provided by law enforcement authorities and measured as is in reflection using an ARL EQUINOX 100 with Cu Kα radiation (5 min). Data evaluation (qualitative and quantitative) was performed using MDI JADE 2010 and ICDD pdf4 Organic database. Quantification (crystalline and amorphous part) was carried out using WPF Rietveld refinements.

Results

Many explosive-related compounds are mixtures of amorphous (e.g. binders) and crystalline parts. The mixtures could contain several components like reductants and oxidants or different explosives which are mixed for better performance. Sometimes it is possible to find contaminants from storing or synthesis, especially in improvised explosives.

Ammonium Nitrate is vastly available because it is a widely used fertilizer. Figure 2 shows a sample of Ammonium Nitrate containing traces of Polymorph 2 and TATB (triaminotrinitrobenzene) but mostly Polymorph 4.

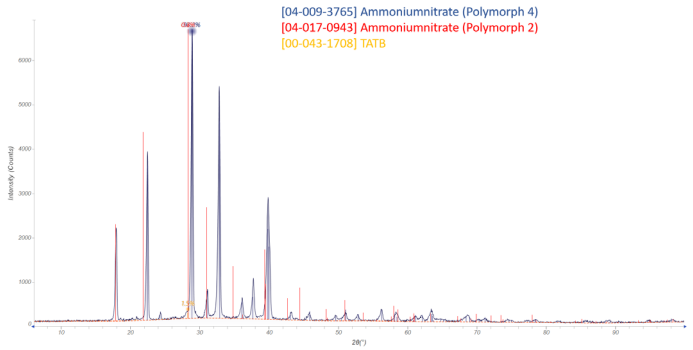

Figure 2: Ammonium nitrate (10 min measurement time)

Sodium Chlorate is another example of a commonly available material which can easily be used as an explosive. Figure 3 shows a mixture of Sodium Chlorate with PEG (polyethylene glycol) and traces of Cobalt Hydroxide. About 80% of the sample are amorphous which is most likely part of the PEG.

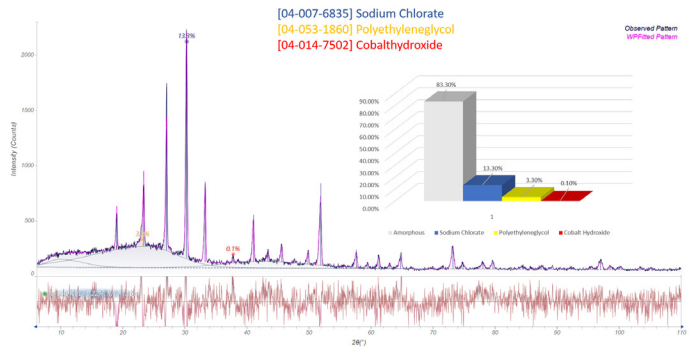

Figure 3: Sodium Chlorate mixture (10 min measurement time)

TNT (trinitrotoluene) is one of the most used explosives in military applications. Plenty of mixtures with other explosives are currently in use. Figure 4 shows a TNT sample with traces of Triethylaminium Picrate and Octogen.

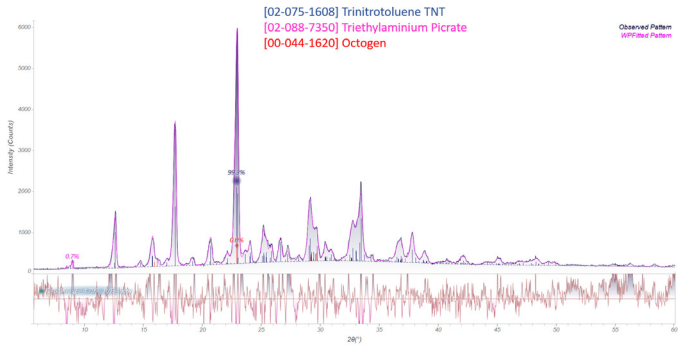

Figure 4: Trinitrotoluene TNT (10 min measurement time)

Conclusion

The ARL EQUINOX 100 XRD can collect data of explosives within 5 min measurement time. The combination of MDI JADE 2010 and ICDD pdf 4 Organics database allows qualitative and quantitative phase analysis (WPF Rietveld refinement) of the samples. The results clearly show the type of explosive material as well as trace phases. Due to the low footprint and energy demand as well as the rugged design of the ARL EQUINOX 100, it is perfectly suited for a mobile lab in a rough environment.

Find out more at **thermofisher.com/xrd**

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