Waters
Lab Highlights
An Internal Communication of Applications and Techniques
LAH 0161 4/84
AN/SC/MD/OC

THE USE OF WATERS LC IN THE ANALYSIS OF EXPLOSIVES

Explosives are one of the more difficult classes of organic compounds to analyze at the trace level. Many of them are just not suitable for GC separations, because they are thermally unstable, shock sensitive, and chemically reactive. (After all they are explosives.) TLC is not suitable because of poor resolution of this class of compounds. Also, TLC suffers from inaccuracy in the quantitative aspects of trace analysis. Thus, it seemed in the early 1970's, that LC should offer a sure solution to performing trace explosive analyses. To some extent this "sure solution" has now been realized, but there is much yet to be accomplished.

Beginning in the early 1970's and continuing to date, investigators have demonstrated the significant advantages and capabilities of LC over prior GC and TLC separation-detection methods. LC operates routinely at ambient temperatures, thus making it very easy to work with thermally and shock-sensitive materials. LC also provides a wide variety of approaches to the separation enabling one to separate nonpolar, polar, and highly polar compounds within one run or a combination of two runs. In LC there is a minimum of sample preparation for most applications.

The practical demands of the average forensic laboratory define the ideal instrumentation. The system should be inexpensive to purchase and operate, simple to maintain and repair, easy to automate, and have a high degree of accuracy, precision, and reproducibility in day-to-day operations. Using LC with UV detection offers excellent sensitivity for most explosives over the range of usable wavelengths of 190-254nm (see Fig. 1), but it can also have lack of specificity for a particular compound of interest. Thus, the use of other confirmatory techniques may be required. The standard Waters LC (with gradient) provides an adequate match for many of the explosives commonly encountered in the forensic area (Table I; Figure 1).

TABLE 1. Some of the More Commonly Encountered Explosives in Trace Analysis

Abbreviation Used	Common and Formal Names
TNT	2,4,6-Trinitrotoluene, Tri, Trotyl, Trolit, sym-TNT, α-TNT
TNC	2,4,6-Trinitro-m-cresol
RDX	1,3,5-Trinitro-1,3,5-triazacyclohexane, hexogen, cyclonit, T4, 1,3,5-trinitro-s-triazin, hexahydro-1,3,5-trinitro-s-triazine
HMX	1,3,5,7-Tetranitro-1,3,5,7-tetrazacyclooctane, octogen, homocyclonit
TETR	2,4,6-N-Tetranitro-N-methylaniline, CE, tetryl
EGDN	Ethylene glycol dinitrate, 1,2-ethanediol dinitrate, glycoldinitrate, dinitroglycol
PETN	Pentaerythritol tetranitrate, 2,2-bis(nitroxymethyl)-1,3-propanediol-1,3-dinitrate, pentrit, pentryl, penta, nitropenta
NG	Nitroglycerin, glycerol trinitrate, trinitroglycerin
NGU	1-Nitroguanidine
NC	Nitrocellulose
HNS	Hexanitrostilbene, 2,2',4,4',6,6'-hexanitrostilbene
TNB	Trinitrobenzene, benzit, 1,3,5-trinitrobenzene
DNT	Dinitrotoluene (2,6; 2,5; 2,4; 2,3; 3,5; 3,4)
MNT	Mononitrotoluene (o-, m-, p-)

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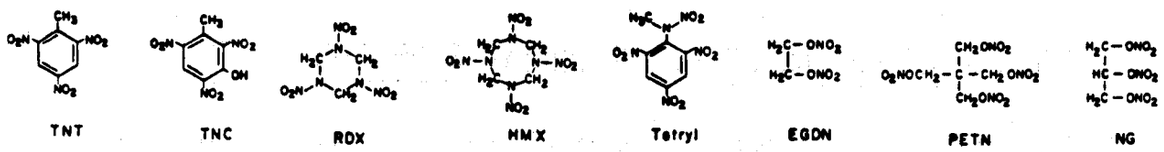
FIGURE 1. Structure of Some Typical Explosives



The series of figures below shows the variety of typical applications which one can expect for Forensic work. Figure 2 shows how the variable wavelength detector can increase sensitivity. Figure 3 shows a typical reverse phase separation using gradient elution. Figure 4 shows a normal phase separation of explosives and Figure 5 demonstrates the use of an amine bonded column.

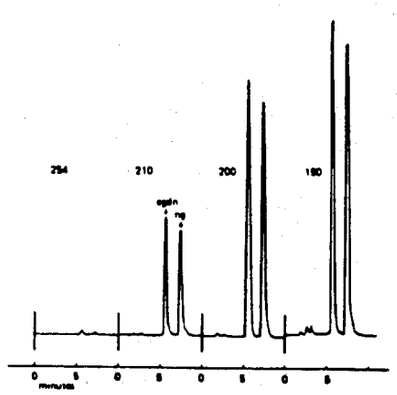


FIG. 2: Variation of response with various UV wavelengths for EDGN and NG. HPLC conditions used isocratic elution with acetonitrile: water (50:50) on a μBONDAPAK™ C_{18} reversed-phase column at 1.0 ml/min. (Ref. 1)

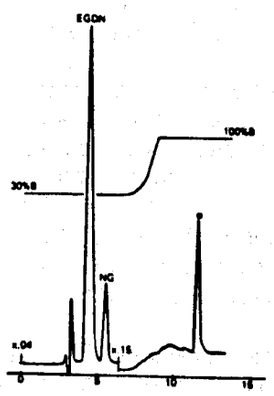


FIG. 3: Separation of EGDN and NG from an extract of dynamite using gradient elution with detection at 254nm. μBONDAPAK™ C_{18} column; initial mobile phase of 30% B and a final eluent of 100% B; 1.0 ml/min; solvent A = methanol:water (50:50), solvent B = methanol. (Ref. 1)

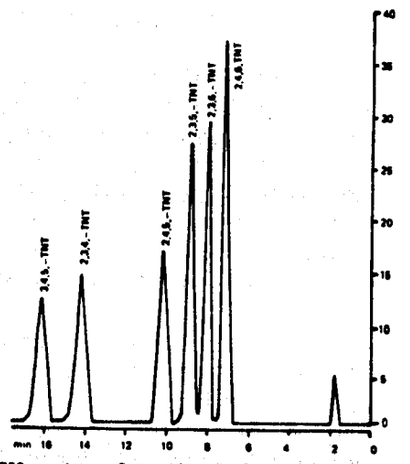


FIG. 4: Separation of trinitrotoluene derivatives. μPORASIL column; mobile phase; n-hexane: methylene chloride (87.5:12.5), 2.0 ml/min flow rate. (Ref. 2)

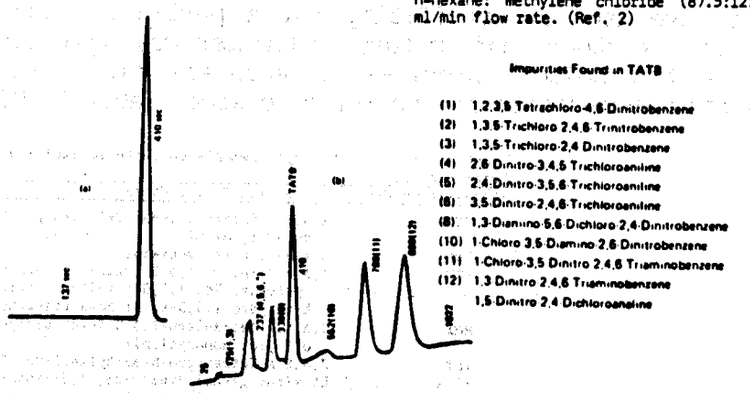


FIG. 5: Separation of TATB from various impurities found in commercial TATB samples. (a) Standard sample of TATB on a μBONDAPAK™ NH_2 column with a mobile phase of DMF:toluene:heptane (1.5:43.5:55.5) at a flow rate of 2.0 ml/min with UV detection at 355 nm. (b) Separation of commercial TATB from its commonly found impurities; conditions as in (a). (From Ref. 3)

For more information concerning forensic analysis using LC consult the references.

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