

Identification of Polymers

DART can be used to analyze polymers, cements, resins, and glues by increasing the gas temperature to 450-550° C to induce pyrolysis. This has been applied to a variety of polymers including Nylons, polypropylene and polyethylene, polyethylene terephthalate (PET), polyesters, poly(methyl methacrylate) (PMMA), polycarbonate, phenoxy resin, polystyrene, and cellulose. Examples are shown here for standard samples of Nylon, polystyrene, and cellulose.

The DART source was operated with helium in positive-ion mode. The gas heater was set to 475° C. Resins were cured in an oven for several hours before analysis; some resin samples had been cured for longer periods of time (months or years). Exact masses and accurate isotopic abundances were used to assign elemental compositions for peaks in the mass spectra. Nominal-mass spectra were exported into a library database in NIST format to facilitate identification of unknowns.

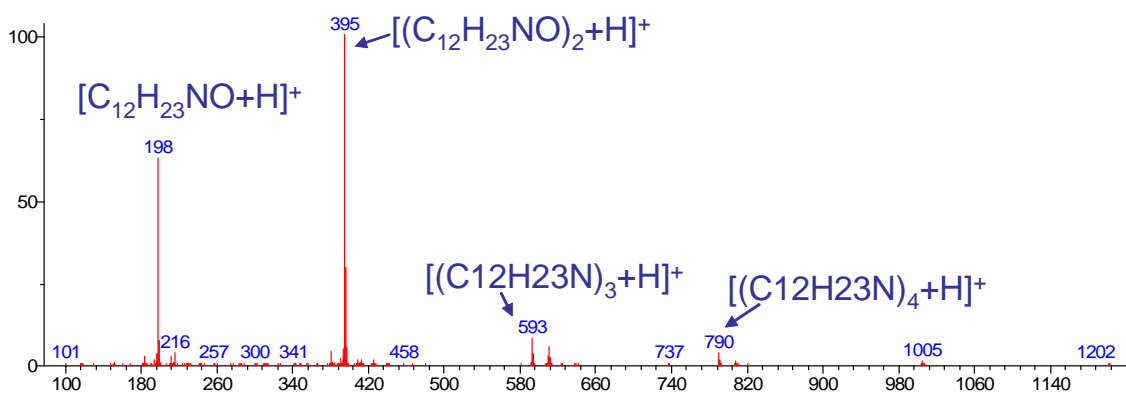


Figure 1. Nylon 12: Poly(lauryl lactam).

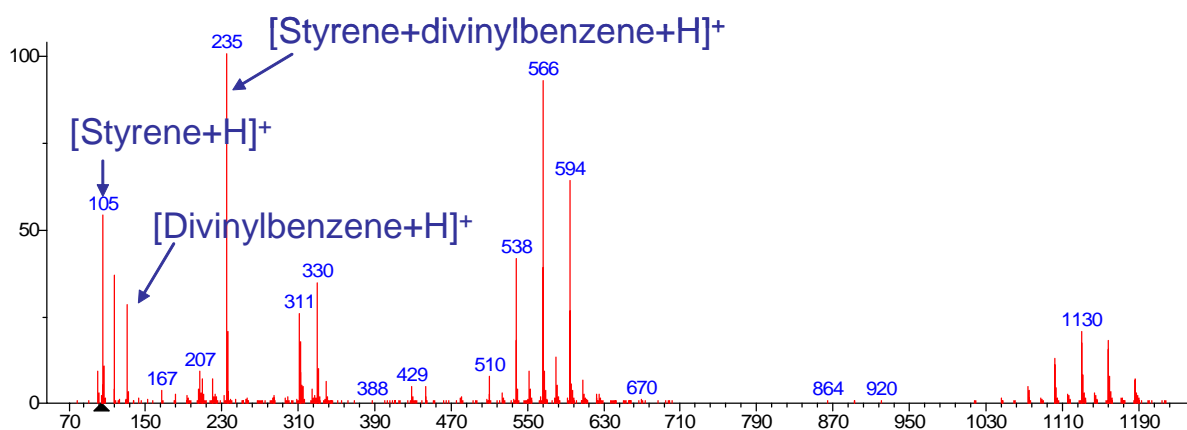


Figure 2. Polystyrene bead, average molecular weight ~ 240,000

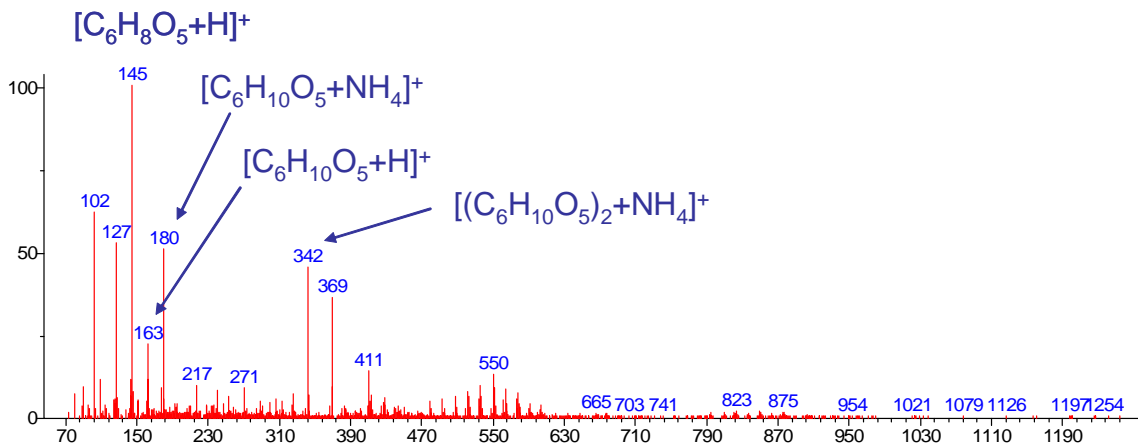


Figure 3. Cotton fibers showing peaks characteristic of cellulose $(C_6H_{10}O_5)_n$. Dilute ammonium hydroxide vapor enhanced $[M+NH_4]^+$ formation.

It should be noted that mass spectra of commercial polymers may be dominated by plasticizers and other additives which can complicate the analysis. Nevertheless, it was possible to identify polyethylene in a milk bottle, poly(ethylene terephthalate) in a soda bottle, and polystyrene in a CD case and a mass spectrometer filament box.

Conclusion

Polymers can be analyzed by DART. Fingerprint mass spectra are produced, and common formulation components can often be identified and confirmed by exact mass measurements.