Characterization of 35 organic pigments using multi-functional pyrolysis (Py)-GC/MS and development of a database

[Background] Organic pigments are widely used in paint and ink formulations. The analysis and structure elucidation of organic pigments is challenging because they are not only insoluble in organic solvents but also many of them have similar structures. Py-GC/MS appears to be the most viable analytical technique for the analysis of organic pigments in a complex matrix, like paint. Samples are analyzed directly; no pretreatment such as solvent extraction is necessary. Pyrolyzates are separated on a high resolution capillary column and identified using both spectral(MS) and retention (GC) data. This note describes the Py-GC/MS analysis of relatively large-molecular-weight (MW approx. 1,000) nonvolatile pigments including condensation disazo pigments having similar structures, azo lake pigments, and phthalo-cyanine pigments. The spectral information from the Py-GC/MS analysis is incorporated into a searchable MS library using F-Search. Additional organic pigments can easily be added. Such a “pigment” library can be used to identify pigments in an ‘unknown’ sample.

[Experimental] EGA (evolved gas analysis)-MS: 100→600ºC at 20ºC/min and pyrolysis-GC/MS at 600ºC were performed on 35 organic pigments using a multi-functional 3030D Pyrolyzer (Frontier Laboratories) Py-GC/MS. F-Search was used to create the organic pigment library and process the MS sample data.

[Results] The results obtained by the EGA and Py-GC/MS analysis of Pigment yellow 93 and Pigment yellow 94 are shown below. The molecular structures of these two pigments have similar structures. This data was used to construct a database which can be used to identify unknown pigments which have similar structures. When analyzing samples containing multiple pigments, the Py-GC/MS is extremely useful since the pyrolyzates of each pigment can be separated, identified, and quantitated.

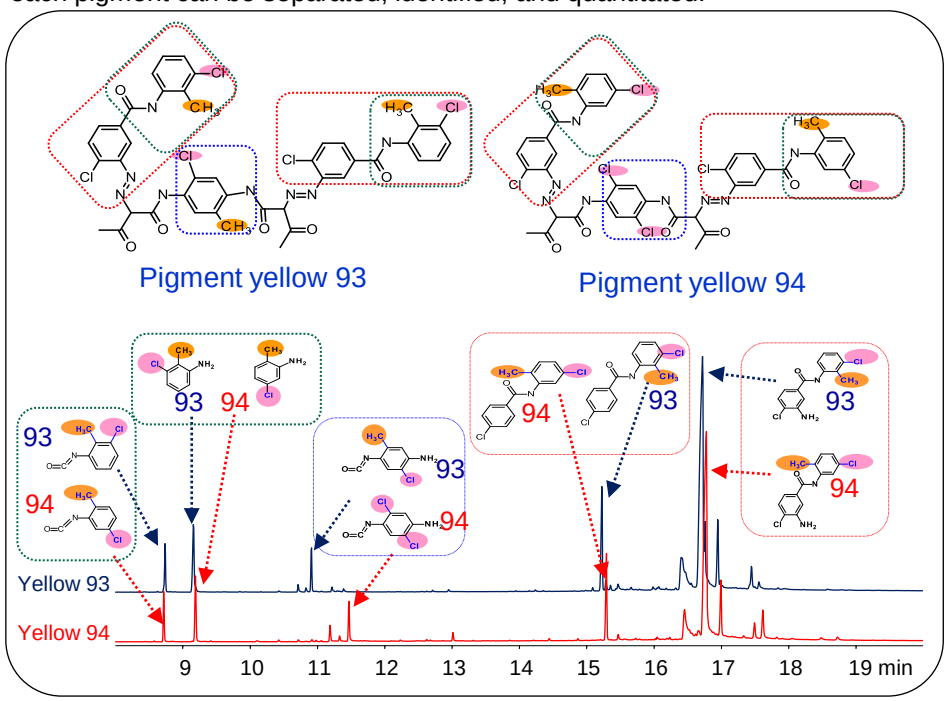

Fig. 1 Structure of Pigment 93 and Pigment 94, pyrograms, and identification of major peaks

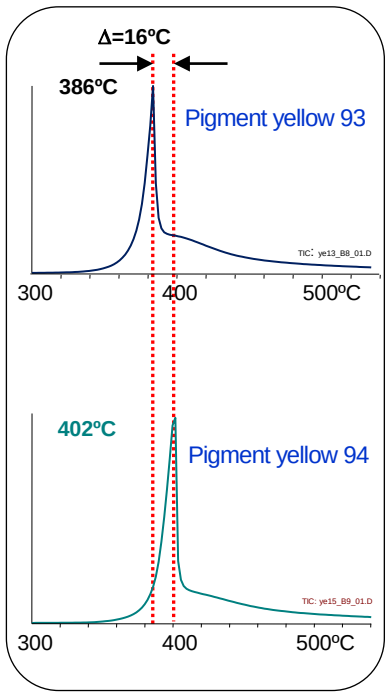

Fig. 2 EGA Thermogram of Pigments 93 and 94

Pyrolysis temperature: 600ºC, GC oven temperature: 40 - 320ºC (20ºC/min)
Separation column: Ultra ALLOY⁺-5 (5% diphenyl 95% dimethylpolysiloxane), L=30 m, i.d.=0.25 mm, df=0.25 µm, split ratio: 1/30, Sample wt.: approx.70 µg

Keywords : Pigment, F-Search, mass spectral library

Products used : Multi-functional pyrolyzer, Vent-free GC/MS adapter, UA+-5, F-Search

Applications : Organic pigment analysis

Related technical notes : PYA1-057E, PYA1-067E, PYA3-012E, PYA3-014E

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