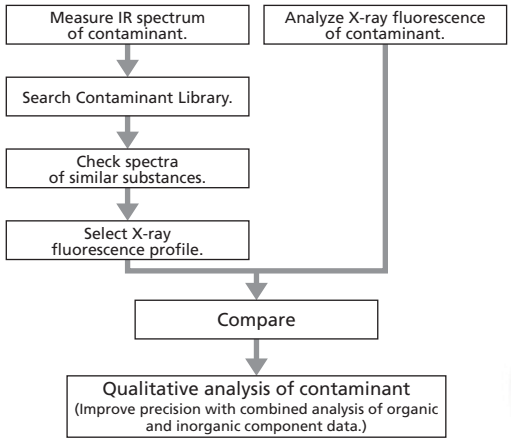
SHIMADZU
Excellence in Science

FTIR/EDX Contaminant Analysis System

for LabSolutions IR

Inquiries regarding contaminant reflect a wide range of issues, including musty odor, chlorinous odor or other abnormal odors and tastes; and the inclusion of contaminants such as various rubber, metal packings and sealing materials. The major cause of contaminants revolves around the aging of the infrastructure and equipment as well as operator's body and clothing surface. While eliminating these causes is difficult, identifying the contaminants as quickly as possible helps to ease the concerns of users.
Infrared spectrometry and X-ray fluorescence spectrometry provide an effective way to identify contaminants.
FTIR/EDX contaminant analysis system is a comprehensive search system that incorporates both techniques.

Procedure for Qualitative Analysis of Contaminants



Features

- Shimadzu's proprietary contaminant library was prepared with cooperation from organizations in the public water supply industry and food manufactures.
- Includes information from actual contaminant samples.
- Includes both an infrared spectral library and X-ray fluorescence profiles (in PDF file format), which significantly improves precision of contaminant searches.

Applicable Fields

- Food, beverage
- Petroleum, chemical and material
- Electrical, electronic
- Machine, transportation
- Contract research organizations, etc.


IRAffinity-1S

Contents

Infrared Spectral Library

Instrument used : Shimadzu Fourier Transform Infrared Spectrophotometer
Measurement method : Single-reflection ATR (prism: Ge or diamond/ZnSe)
Number of spectra : 485 spectra
Information included : Material names, colors, shapes, hardness, etc.
Prism selection criteria : Ge - Enables measurement of samples with high refractive indices (such as black rubber).
Absorption peak is smaller than diamond/ZnSe.
Diamond/ZnSe - Less prone to scratching and provides larger absorption peaks than Ge. Cannot measure samples with high refractive indices (such as black rubber).


EDX-7000/8000/8100

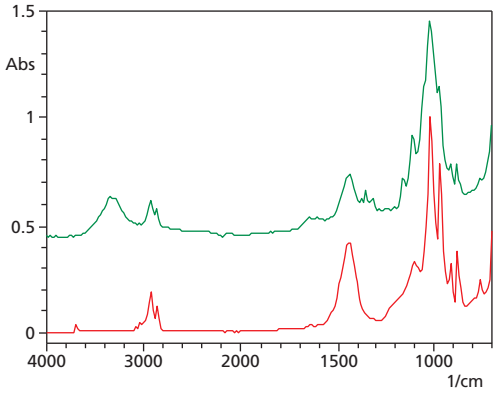
X-Ray Fluorescence Profile Library

Instrument used : Shimadzu Energy Dispersive X-Ray Fluorescence Spectrometer
* The number of available data differs depending on the detection limit of the instruments.
Profile count : 485 profiles
Information included : Qualitative results and FP method quantitative results
(Uses FTIR qualitative results for principal components.)

Example of Infrared Spectral Search Results and Corresponding X-Ray Fluorescence Profile for a Contaminant

The following shows an example of infrared spectral search results and qualitative/quantitative EDX information for matching substances in search results. The contaminant was discovered in a public water system. The Contaminant Library was utilized to determine the contaminant and corresponding profile.

Infrared Spectral Search Results



Detailed information:

Green (measured IR spectrum):

Infrared spectrum from contaminant detected in public drinking water

Red (Contaminant Library):

Interior residue (gray) on fitting seal for 32 mm diameter water drain pipe

Material : Styrene butadiene styrene (SBS), calcium carbonate ($CaCO_3$), and magnesium silicate (talc, $Mg_3Si_4O_{10}(OH)_2$)

Major element: Cl, Ca, Si, Mg, S, Zn, Ti

Color : Gray

Shape : Plastic, ring

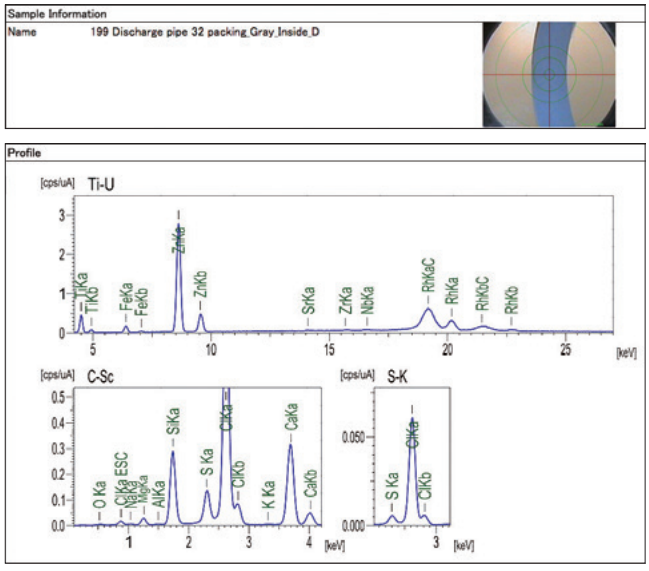
Hardness : Pliable

Metal shine : None

Measurement method : ATR (Diamond)

Infrared spectral search results indicated the contaminant is identical or similar to the metal fitting seal material from the water drain pipe (principal component: styrene butadiene styrene [SBS]).

X-Ray Fluorescence Profile of Corresponding Substance



Qualitative and quantitative information can be obtained for iron rust, scaling, and other inorganic components, which is difficult to obtain only with infrared spectra.
It also provides an effective means for qualitative analysis or refining results for seals and other substances with the same principal components (organic substances), but different additives.

Measurement Condition

Analyte	Voltage	Current	Filter	Acr.(keV)	Anal.(keV)	Collimator	3mm	Atmosphere	Vac.
						Time	DT%		
Ti-U	50	41-Auto	-----	0 - 40	4.20-37.00	Live- 100	25		
S-K	15	1000-Auto	Al	0 - 20	2.42- 2.82	Live- 300	25		
C-Sc	15	318-Auto	-----	0 - 20	0.10- 4.20	Live- 300	26		

Quantitative Result

Analyte	Result		(Std.Dev.)	Proc.-Calc.	Line	Int.
Cl	9.114	%	(0.020)	Quan-FP	ClKa	0.7206
Ca	5.661	%	(0.009)	Quan-FP	CaKa	4.0402
Si	5.391	%	(0.010)	Quan-FP	SiKa	2.9346
Mg	2.043	%	(0.015)	Quan-FP	MgKa	0.2429
S	1.154	%	(0.003)	Quan-FP	S Ka	1.5087
Zn	1.100	%	(0.003)	Quan-FP	ZnKa	27.2646
Ti	1.054	%	(0.009)	Quan-FP	TiKa	3.2267
Na	0.956	%	(0.025)	Quan-FP	NaKa	0.0398
Fe	0.139	%	(0.002)	Quan-FP	FeKa	1.4017
Al	0.069	%	(0.003)	Quan-FP	AlKa	0.0198
K	0.039	%	(0.002)	Quan-FP	K Ka	0.0202
Sr	0.003	%	(0.000)	Quan-FP	SrKa	0.2143
Nb	0.003	%	(0.000)	Quan-FP	NbKa	0.2288
Zr	0.002	%	(0.000)	Quan-FP	ZrKa	0.1738
C12H14	73.272	%	(-------)	Balance	--------	--------

Note: Quantitative results were calculated based on the principal components (SBS) determined from infrared spectral search results.

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