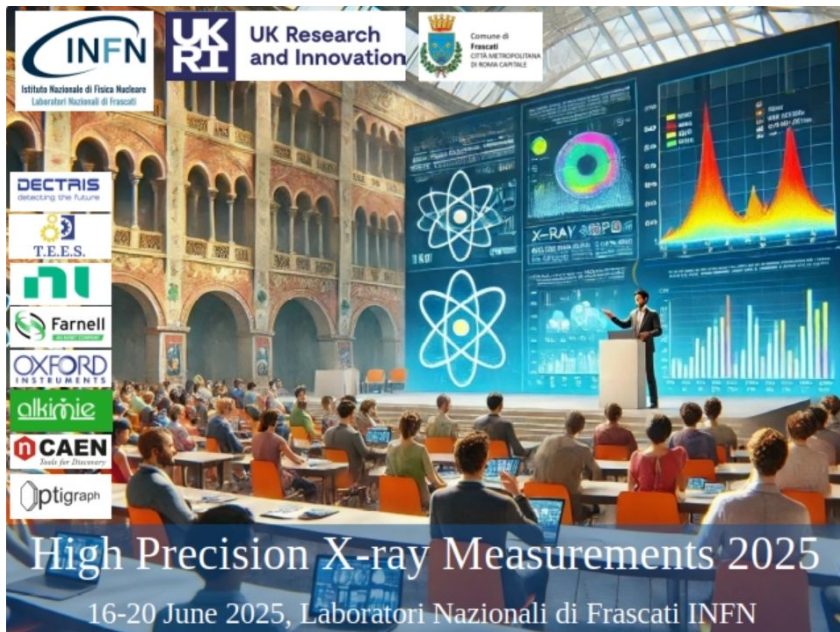


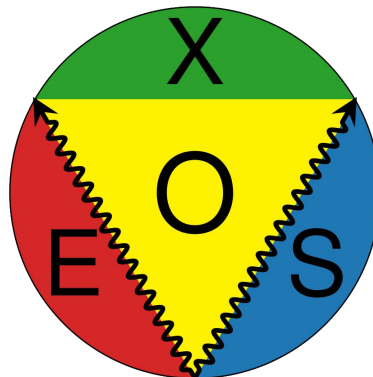


XRF Spectroscopy with VOXES: Techniques, Optimization and Applications

Simone Manti, Alberto Clozza, Gabriel Moskal,
Kristian Piscicchia, Diana Sirghi , Catalina
Curceanu and Alessandro Scordo



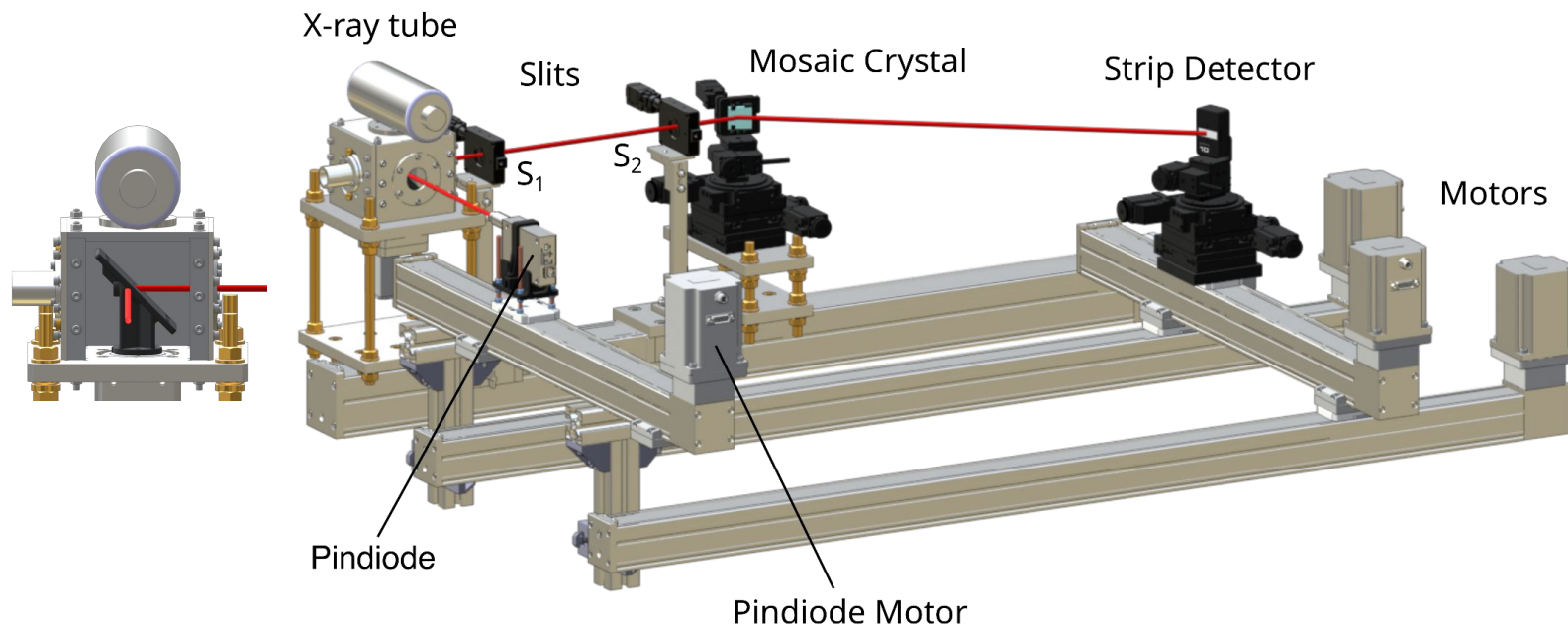
High resolution von-Hamos X-Ray spectrometer using HAPG for Extended Sources in a broad energy range



Applications:

- Nuclear (Kaonic Atoms)
- Elemental mapping
- XRF of trace metals
- Food control
- Medical applications

VOXES Setup for X-ray Fluorescence (XRF) Measurements





Application of VOXES with the MITIQO project

MITIQO

Monitoraggio In situ di Tossicità, Indicazione geografica e Qualità di Olio d'oliva, vino e altri liquidi edibili

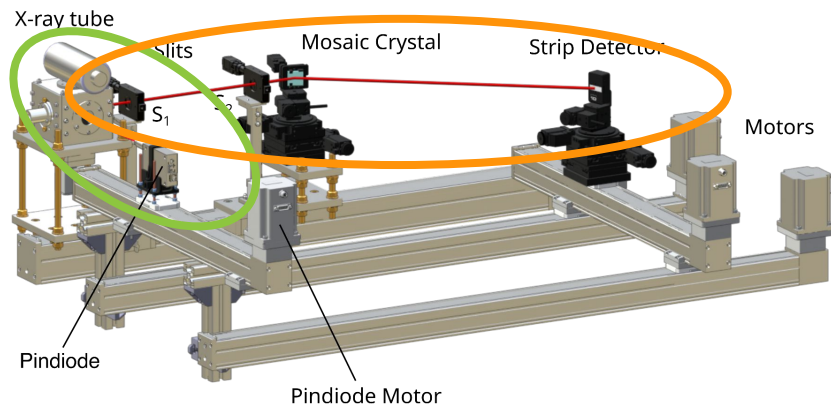
1																	2
H																	He
3	4															10	
Li	Be															Ne	
11	12															18	
Na	Mg															Ar	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

Trade organization or country	Concentration/mg l ⁻¹																		Reference
	Ag	Al	As	B	Br	Cd	Cr	Cu	F	Fe (red)	Fe (rosé)	Fe (white)	Na	Ni	Sb	Sn	Pb	Zn	
OIV	–	–	0.2	80	1	0.01	–	1	–	–	–	–	–	–	–	0.15	5	[7]	
Brazil	–	–	–	–	0.2	–	–	–	–	–	–	–	–	–	–	0.5	–	[29]	
Croatia	0.1	10	0.2	80	1	0.01	0.1	1	1	20	15	10	20	0.1	0.2	10	0.2	5 [80]	
Hungary	–	–	0.05	–	–	0.02	–	1	–	–	–	–	–	–	–	–	0.25	– [27]	
Australia	–	–	0.1	–	–	0.05	–	5	–	–	–	–	–	–	–	–	0.2	5 [53]	
Germany	–	8	0.1	–	–	0.01	–	5	–	–	–	–	–	–	–	–	0.3	5 [53]	
Italy	–	–	–	–	–	–	–	10	–	–	–	–	–	–	–	–	0.3	5 [53]	

- **XRF measurements** in Edible Liquids
- Applications for **Wine** and **Olive Oils**
- **Metals' Concentrations** for:
 - **Quality**
 - **Geographical Origin**

MITIQO applications for the different lines of VOXES

MITIQO



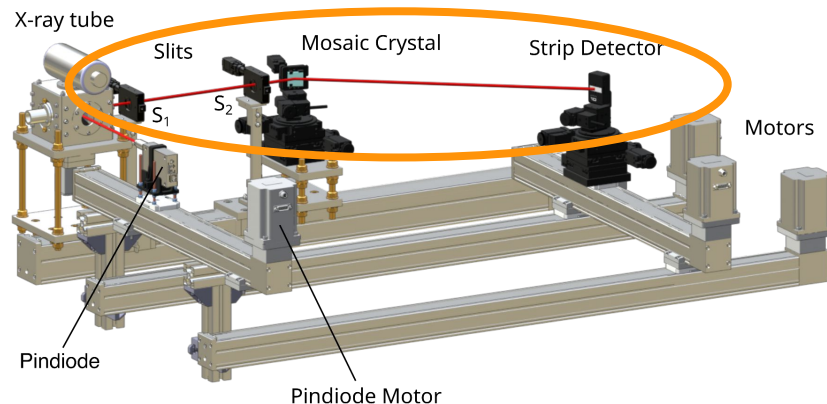
Wavelength Dispersive (WD-XRF)

- Dynamic Range of 0.5 keV
- Resolution $\sim 1-10$ eV at 7 keV
- Metal's Spin and Oxidation state
- Limit of Detection ~ 100 ppm

Energy Dispersive (ED-XRF)

- Fixed Range of 2-20 keV
- Resolution ~ 150 eV at 7 keV
- Metal Concentrations
- Limit of Detection ~ 1 ppm

MITIQU applications for the different lines of VOXES: WD-XRF

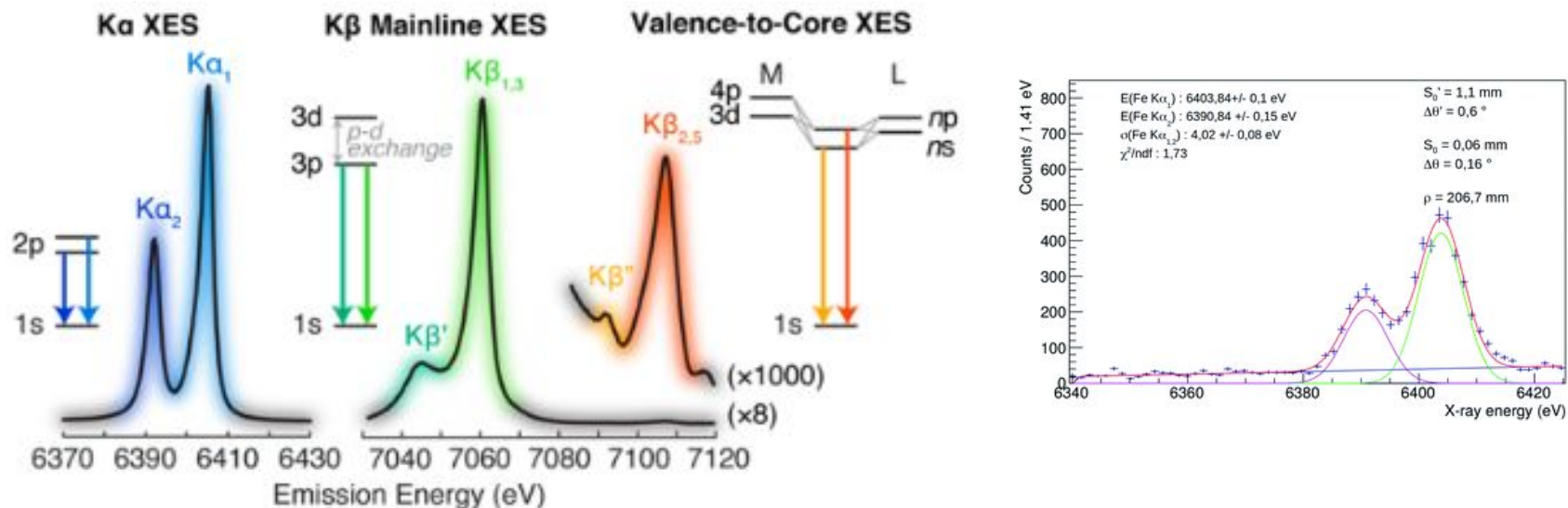


Wavelength Dispersive (WD-XRF)

- Dynamic Range of 0.5 keV
- Resolution ~1-10 eV at 7 keV
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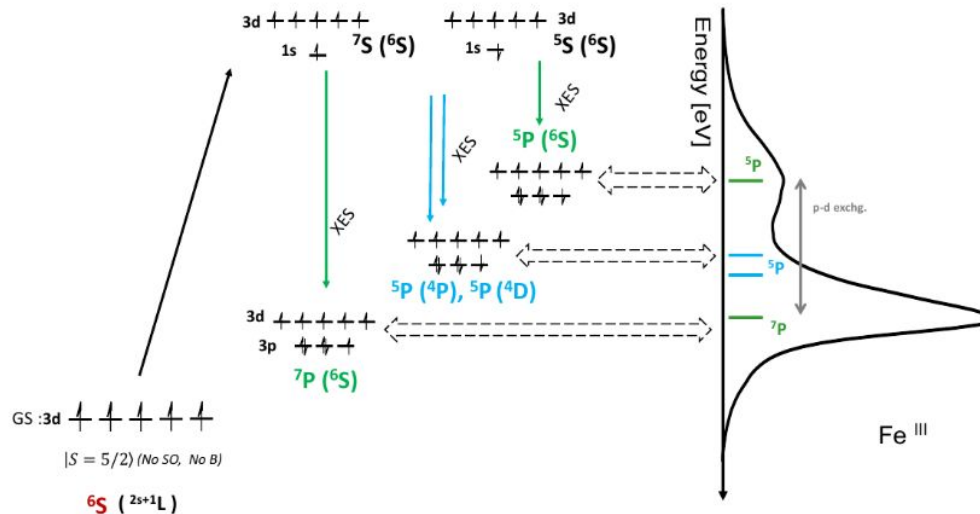
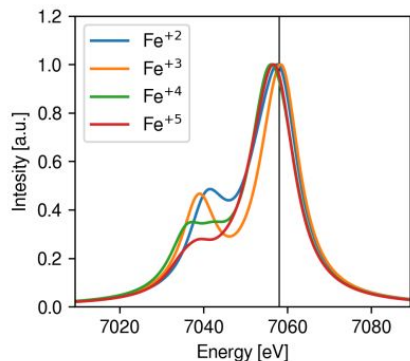
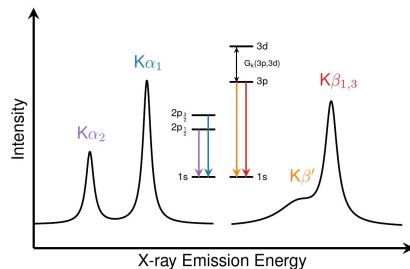
Different Information from Different Emission Lines



Nicole Lee, Taras Petrenko, Uwe Bergmann, Frank Neese, and Serena DeBeer, Journal of the American Chemical Society 2010 132 (28), 9715-9727 DOI: 10.1021/ja101281e



K β Emission Line is sensible to the Metal's (Spin~Oxidation) State

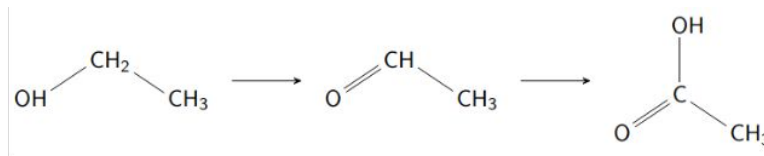


Nicole Lee, Taras Petrenko, Uwe Bergmann, Frank Neese, and Serena DeBeer, Journal of the American Chemical Society 2010 132 (28), 9715-9727 DOI: 10.1021/ja101281e

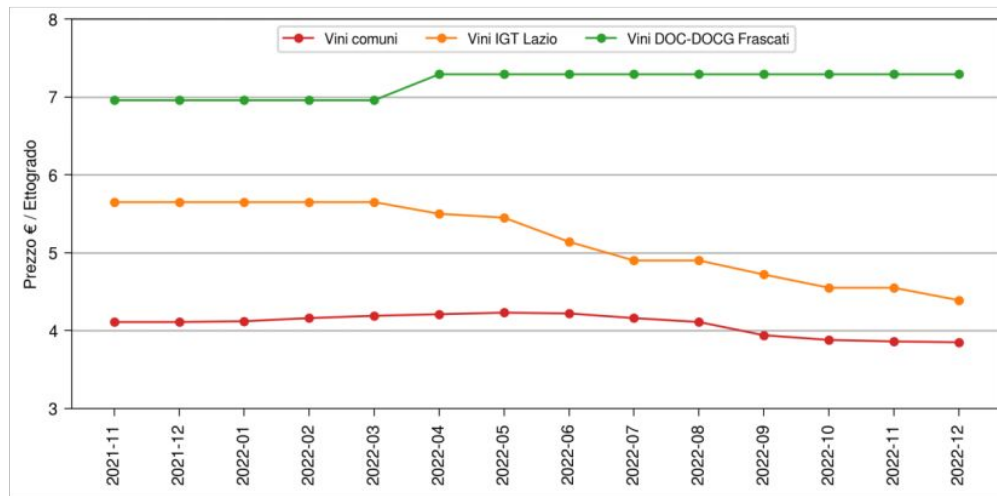


Metal's State (Oxidation) reduces the Quality and it is driven by Metals

e.g. $\text{Fe}^{+2}, \text{Fe}^{+3}$



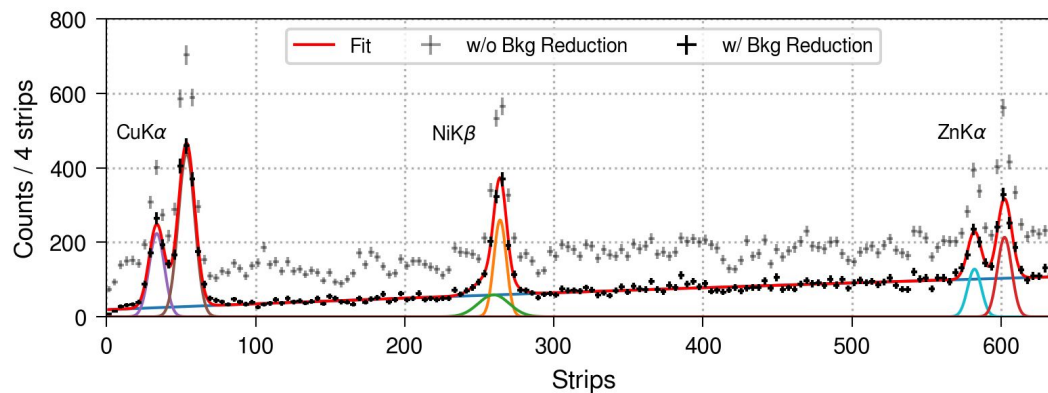
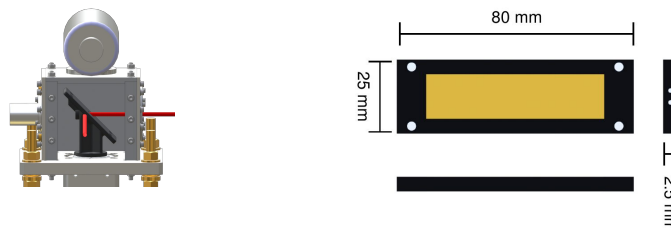
<https://winefolly.com/tips/how-to-tell-if-wine-has-gone-bad/>



[https://www.ismeamercati.it/flex/cm/pages/ServeBLOB.php/L/IT/IDPagina/\[962,2603,2604\]](https://www.ismeamercati.it/flex/cm/pages/ServeBLOB.php/L/IT/IDPagina/[962,2603,2604])



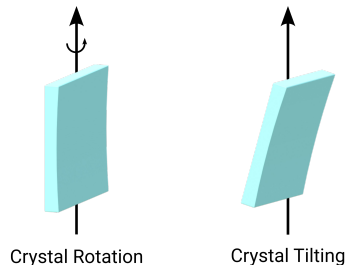
Optimization of VOXES Setup for Metal's State Analysis in Liquid



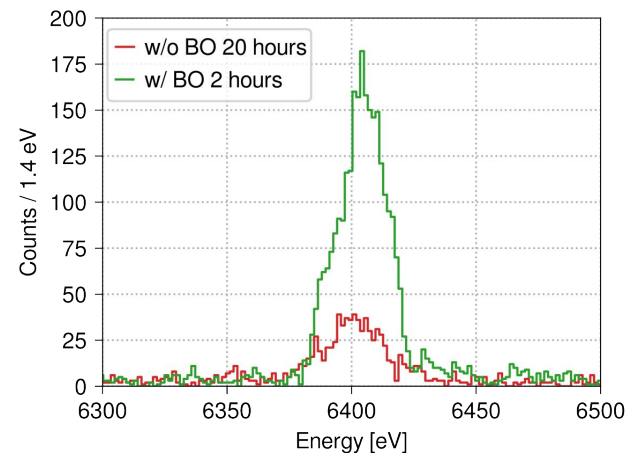
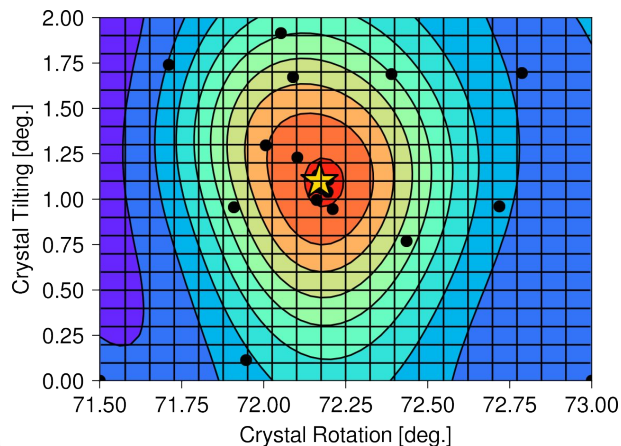
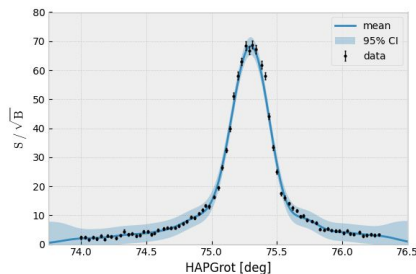
Manti, Simone, et al. "Enhancing Performances of the VOXES Bragg Spectrometer for XES Investigations." *Condensed Matter* 9.1 (2024): 19.



Bayesian Optimization Reduces Operation Time

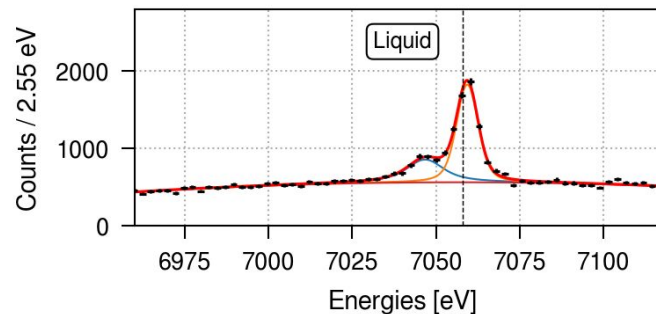
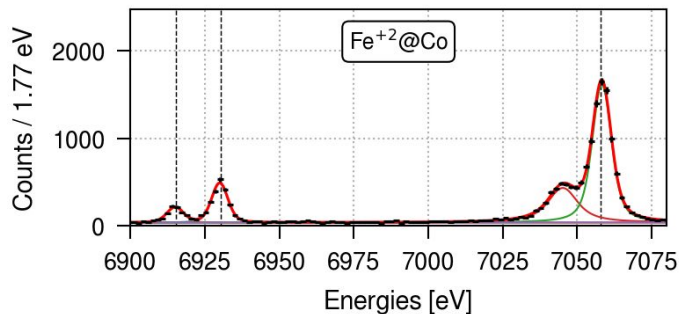
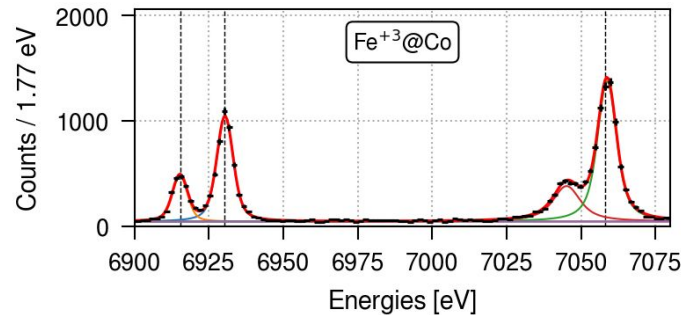
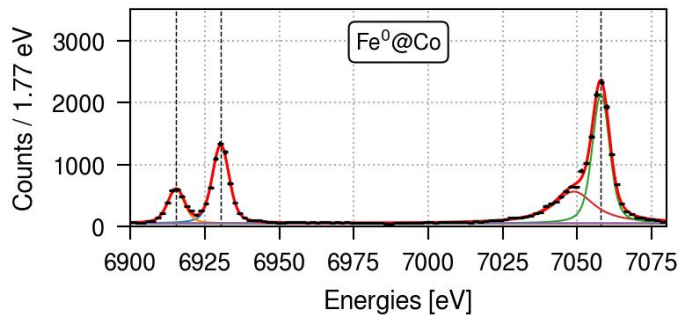


- Improved Alignment
- Faster Convergence
- Enhanced Rate and Efficiency





Effects of the Metal's State on the $K\beta$ Lineshape

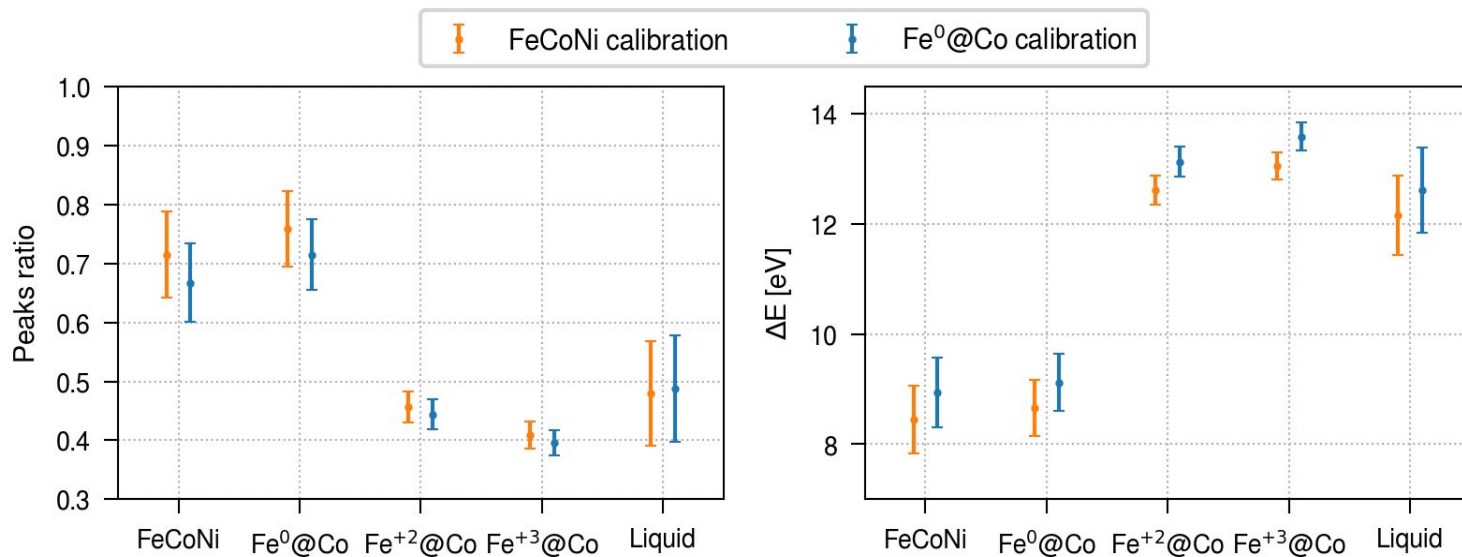




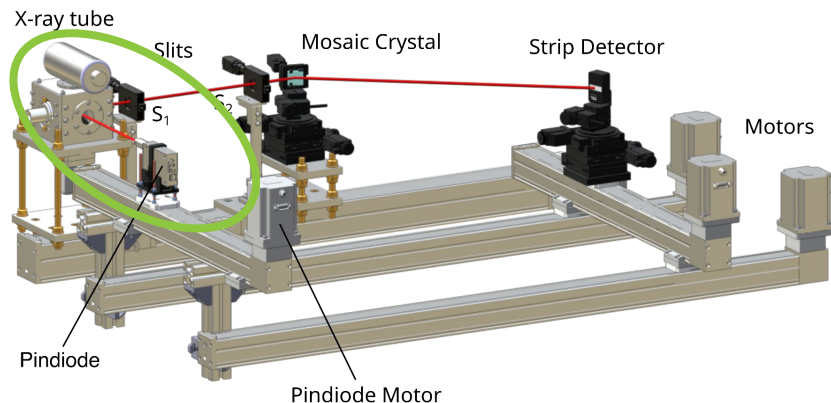
Effects of the Metal's State on the $K\beta$ Lineshape

$$\Delta E = E(FeK\beta_{1,3}) - E(FeK\beta')$$

$$\text{Ratio} = A(FeK\beta') / A(FeK\beta_{1,3})$$



MITIQU applications for the different lines of VOXES: ED-XRF



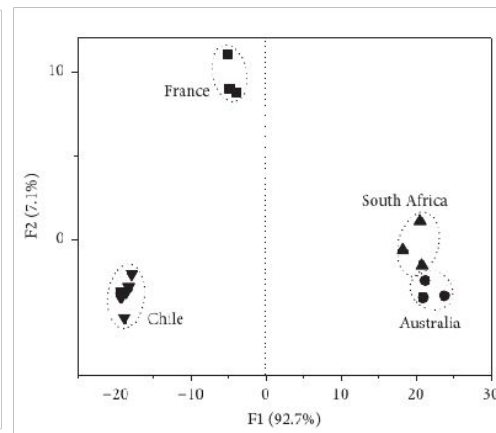
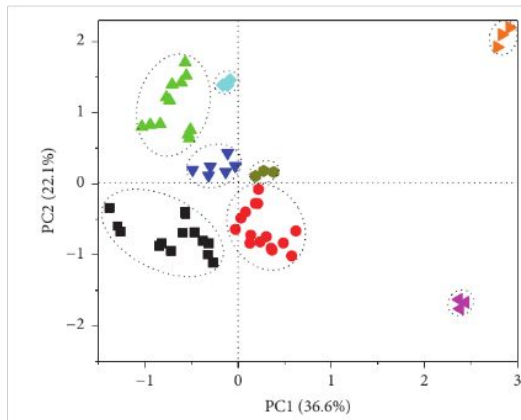
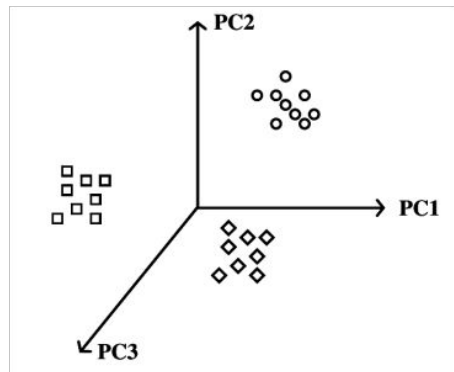
Energy Dispersive (ED-XRF)

- Fixed Range of 2-20 keV
- Resolution ~150 eV at 7 keV
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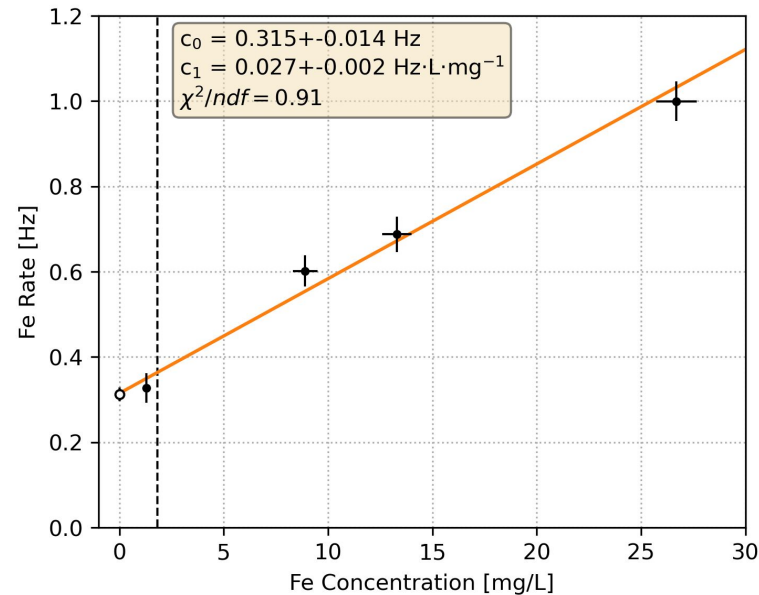
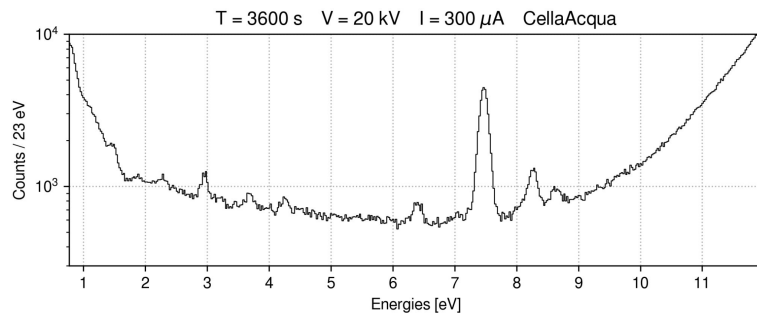
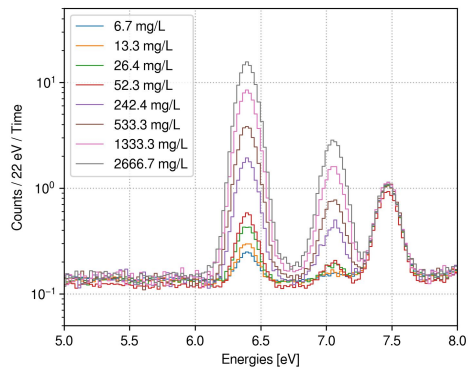
Metals Concentrations as a Fingerprint for Geographical Origin

	1	2	3	...	N
Al	$C_{Al,1}$	$C_{Al,2}$	$C_{Al,3}$		$C_{Al,N}$
Ba	$C_{Ba,1}$	$C_{Ba,2}$	$C_{Ba,3}$		$C_{Ba,N}$
Ca	$C_{Ca,1}$	$C_{Ca,2}$	$C_{Ca,3}$		$C_{Ca,N}$
...					
M	$C_{M,1}$	$C_{M,2}$	$C_{M,3}$		$C_{M,N}$

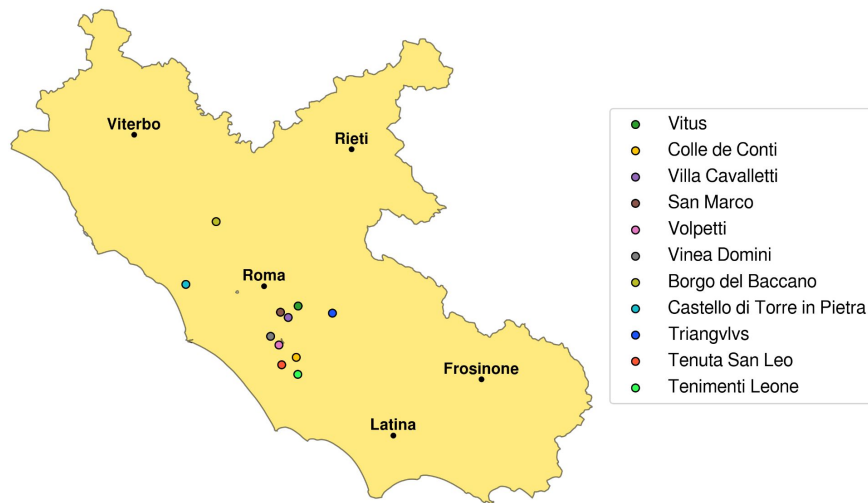




Limit of Detection for ED-XRF

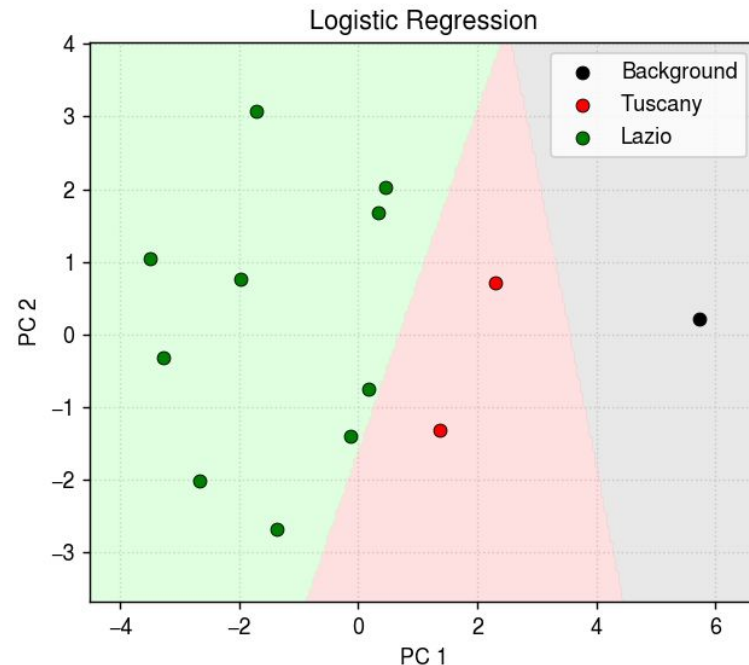
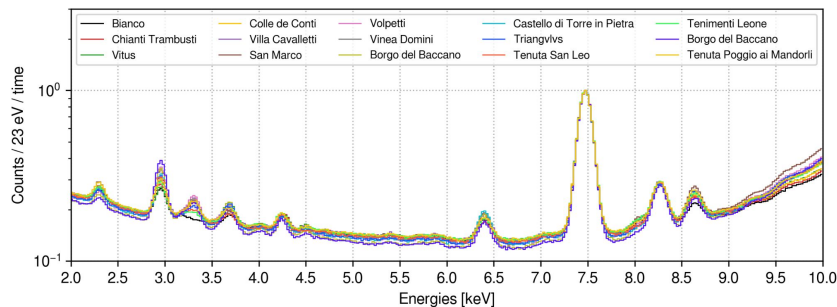
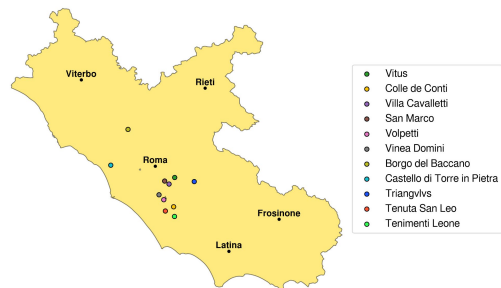


Test Case: Wines by a Consortium from Lazio Region



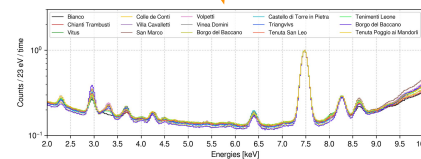
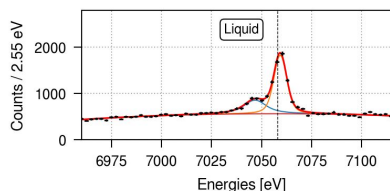
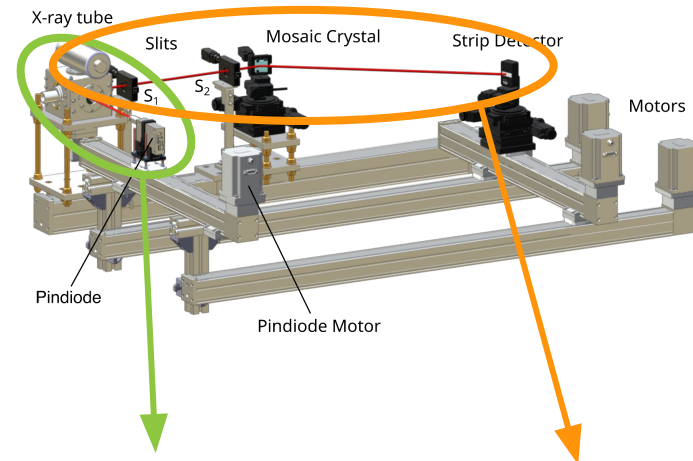


Test Case: Wines by a Consortium from Lazio Region



Conclusion

- **VOXES** Spectrometer for combined XRF measurements (ED-XRF + WD-XRF)
- **Applications** with MITIQO in Edible Liquids:
 - **WD-XRF** Metal state for **Quality**
 - **ED-XRF** Concentration for **Origin**



Thanks for the Attention!