

IN THIS ISSUE

ISSN 0267-9477 CODEN JASPE2 38(9) 1723–1896 (2023)



Cover

See Alexander Meshik *et al.*, pp. 1785–1797. Image reproduced by permission of JAXA (Japan Aerospace Exploration Agency) from *J. Anal. At. Spectrom.*, 2023, **38**, 1785.

ATOMIC SPECTROMETRY UPDATES

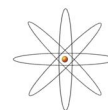
1730

2023 atomic spectrometry update – a review of advances in X-ray fluorescence spectrometry and its special applications

Christine Vanhoof, Jeffrey R. Bacon, Ursula E. A. Fittschen and Laszlo Vincze



Atomic
Spectrometry
Updates

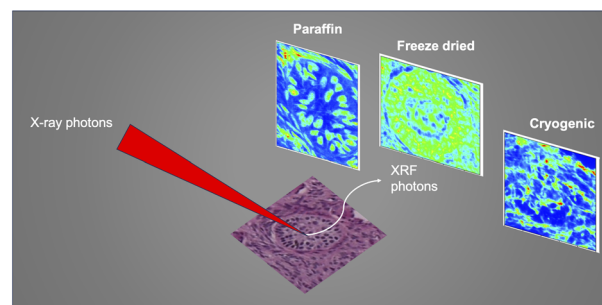


COMMUNICATION

1744

Difficulties and artefacts in cryo-fixation of ovarian tissues for X-ray fluorescence analyses

Alessandra Gianoncelli,* Katarina Vogel- Mikuš, Murielle Salomé, Ernesto Pascotto, Giuseppe Ricci and Lorella Pascolo



Editorial Staff

Executive Editor

Philippa Ross

Deputy Editor

Alice Smallwood

Editorial Production Manager

Jason Woolford

Development Editor

Celeste Brady

Publishing Editors

Gabriel Clarke, Derya Kara-Fisher,
Emma Stephen, Ziva Whitelock

Publishing Assistant

Andrea Whiteside

Editorial Assistant

Leo Curtis

Publisher

Jeanne Andres

For queries about submitted articles please contact Jason Woolford, Editorial production manager, in the first instance. E-mail jaas@rsc.org

For pre-submission queries please contact Philippa Ross, Executive editor. E-mail jaas-rsc@rsc.org

Journal of Analytical Atomic Spectrometry (JAAS) (electronic: ISSN 1364-5544) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail orders@rsc.org

2023 Annual (electronic) subscription price: £2531; US\$3447. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

JAAS

Journal of Analytical Atomic Spectrometry

rsc.li/jaas

Innovative research on the fundamental theory and application of spectrometric techniques.

Editorial Board

Chair

Heidi Goenaga-Infante, LGC, Middlesex

Members

Márcia Foster Mesko, Universidade Federal de

Pelotas, Brazil

Gerardo Gamez, Texas Tech University, USA

Steve Hill, University of Plymouth, UK

Xiandeng Hou, Sichuan University, China

Bin Hu, Wuhan University, China

Pelotas, Brazil

Björn Meermann, BAM, Germany

José Luís Todolí, University of Alicante, Spain

Frank Vanhaecke, University of Ghent,

Belgium

Vassilia Zorba, Lawrence Berkeley National

Laboratory, USA

Advisory Board

Marco Aurelio Zezzi Arruda, UNICAMP, Brazil

Ramon M. Barnes, University Research

Institute for Analytical Chemistry, USA

Mathieu Baudelet, University of Central

Florida, USA

Annie Bogaerts, University of Antwerp,

Belgium

José Broekaert, University of Hamburg,

Germany

Marta Costas-Rodríguez, Ghent University,

Belgium

George Donati, Wake Forest University, USA

Carsten Engelhard, University of Siegen,

Germany

Joerg Feldmann, University of Graz, Austria

Alexander Gundlach-Graham, Iowa State

University, USA

Detlef Günther, ETH Zürich, Switzerland

Wei Hang, Xiamen University, China

Gary M. Hieftje, Indiana University, USA

Takafumi Hirata, University of Tokyo, Japan

Zhaochu Hu, China University of Geosciences,

China

Norbert Jakubowski, Federal Institute for

Materials Research and Testing, Germany

Gunda Köllensperger, University of Vienna,

Austria

David W. Koppenaal, Pacific Northwest

National Laboratory, USA

Kerstin Leopold, University of Ulm, Germany

Kelvin Leung, Hong Kong Baptist University,

Hong Kong, China

Lara Lobo, University of Oviedo, Spain

Yi Lv, Sichuan University, China

R. Kenneth Marcus, Clemson University, USA

Érico Marlon Moraes Flores, Universidade

Vincent Motto-Ros, Claude Bernard University

Lyon 1, France

Sohail Mushtaq, University of Bristol, UK

John W Olesik, Ohio State University, USA

Christophe Pécheyan, University of Pau and

Pays de l'Adour, France

Spiros Pergantis, University of Crete, Greece

Jorge Pisonero, University of Oviedo, Spain

Steven Ray, State University of New York at

Buffalo, USA

Mark Rehkemper, Imperial College London,

UK

Martín Resano, University of Zaragoza, Spain

Jacob Shelley, Rensselaer Polytechnic Institute,

USA

Patricia Smichowski, National Atomic Energy

Commission, Argentina

Ralph E. Sturgeon, National Research Council

of Canada, Canada

Joanna Szpunar, CNRS EP 132, France

Johannes van Elteren, National Institute of

Chemistry, Slovenia

Lu Yang, National Research Council Canada,

Canada

Atomic Spectrometry Updates Editorial Board

J R Bacon, University of Strathclyde, UK

N Barlow, Sandwell General Hospital, UK

S Branch, Herbalife, UK

O Butler, Health & Safety Laboratory Buxton,

UK

W R I Cairns, Institute for the Dynamics

of Environmental Processes of the Italian

CNR, Italy

S Carter, INEOS, UK

M R Cave, British Geological Survey, UK

O Cavoura, University of West Attica, Greece

R Clough, University of Plymouth, UK

J M Cook, British Geological Survey, UK

A Cross, Reading Scientific Service Limited

(RSSI), UK

C M Davidson, University of Strathclyde, UK

L Ebdon, UK

H Evans, University of Plymouth, UK

A Fisher, University of Plymouth, UK

U Fittschen, Technical University of Clausthal,

Germany

M Foulkes, University of Plymouth, UK

B Gibson, Intertek Sunbury, UK

C Harrington, SAS Trace Element Laboratory,

Surrey Pathology Services, UK

S Hill, LGC, UK

S J Hill, University of Plymouth, UK

Y Madrid, Universidad Complutense de

Madrid, Spain

R Mertz-Kraus, Johannes Gutenberg-

Universität Mainz, Germany

M Patriarca, Istituto Superiore di Sanita, Italy

J Pisonero, University of Oviedo, Spain

A Robson, Manchester University NHS

Foundation Trust, UK

B Russell, National Physical Laboratory, UK

M Sargent, LGC, UK

C M M Smith, St Ambrose High School, UK

A Taylor, Royal Surrey County Hospital, UK

R Taylor, University of Southampton, UK

J F Tyson, University of Massachusetts, USA

C Vanhoof, Flemish Institute for Technological

Research (VITO), Belgium

L Vincez, Ghent University, Belgium

M White, Health & Safety Laboratory, UK

*Members of the ASU Executive Committee

Information for Authors

Full details on how to submit material for publication in JAAS are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/jaas

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

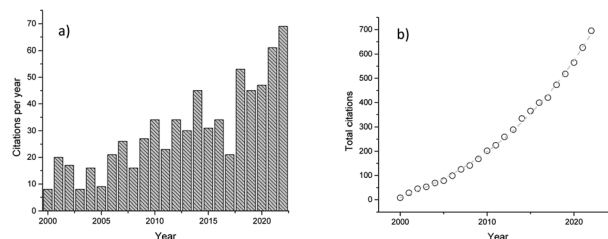


CRITICAL REVIEW

1751

Catching up on calibration-free LIBS

Francesco Poggialini, Beatrice Campanella, Bruno Cocciaro, Giulia Lorenzetti, Vincenzo Palleschi* and Stefano Legnaioli

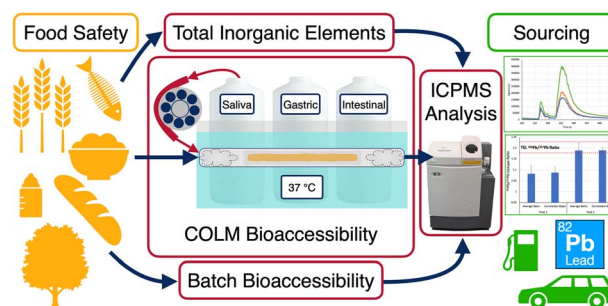


TUTORIAL REVIEW

1772

The continuous on-line leaching method coupled to inductively coupled plasma mass spectrometry for risk assessment of food safety and for sourcing of elements: a tutorial review

Alastair Kierulf and Diane Beauchemin*

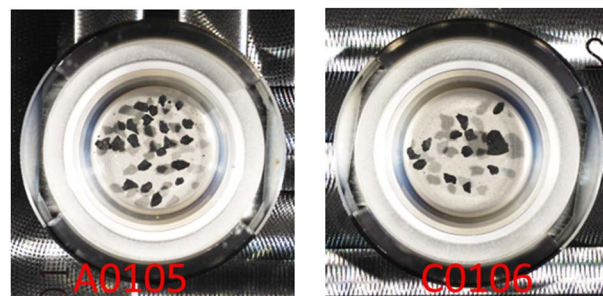


PAPERS

1785

Noble gas mass-spectrometry for extraterrestrial micro-samples: analyses of asteroid matter returned by Hayabusa2 JAXA mission

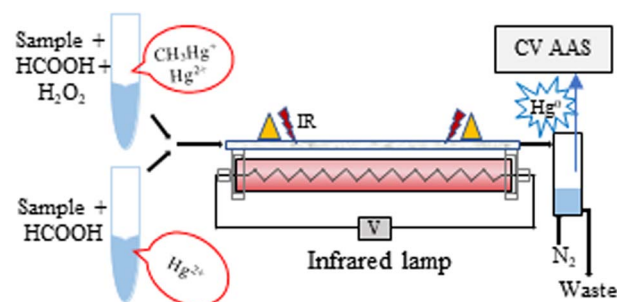
Alexander Meshik,* Olga Pravdivtseva, Ryuji Okazaki, Kasumi Yogata, Toru Yada, Fumio Kitajima, Hisayoshi Yurimoto, Tomoki Nakamura, Takaaki Noguchi, Hikaru Yabuta, Hiroshi Naraoka, Kanako Sakamoto, Shogo Tachibana, Masahiro Nishimura, Aiko Nakato, Akiko Miyazaki, Masanao Abe, Tatsuaki Okada, Tomohiro Usui, Makoto Yoshikawa, Takanao Sakai, Satoshi Tanaka, Fuyuto Terui, Satoru Nakazawa, Seiichiro Watanabe, Yuichi Tsuda and Hayabusa2 Initial Analysis Volatile Team



1798

Infrared radiation-assisted thermochemical vapor generation for mercury speciation by atomic absorption spectrometry

Victor Marques Campos, Jane Kelly Sousa Brito, Wladiana Oliveira Matos, Livia Paulia D. Ribeiro and Gisele Simone Lopes*



1808

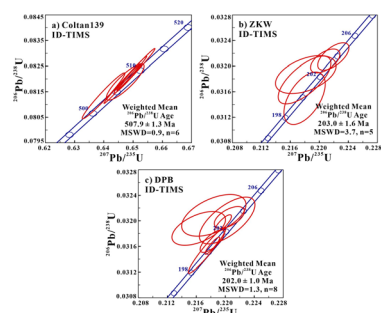
Time min	RD ^a	Sample RD*DF ^b	RSD	Sample + spike		Recovery	
	$\mu\text{g kg}^{-1}$	$\mu\text{g kg}^{-1}$		$\mu\text{g kg}^{-1}$	RSD	%	RSD
0	1.09	109	1.3	11.01	1.3	99.2	2.9
30	0.95	95	6.1	10.30	6.1	93.5	0.5
60	0.97	97	5.4	10.65	5.4	96.7	1.9
90	1.03	103	5.2	10.61	5.2	95.8	3.7
120	0.91	91	5.6	9.94	5.6	90.4	1.9
150	1.00	100	3.3	10.13	3.3	91.2	1.1
180	1.06	106	0.5	10.95	0.5	98.9	1.2

^a Raw data, ^b dilution factor

Determination of chlorine in Hf precursors by high-resolution inductively coupled plasma mass spectrometry

Hanul Lee, Seongkyong Joo and Dongchul Suh*

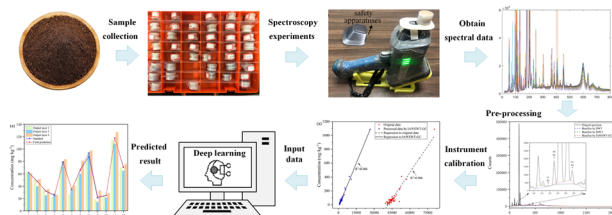
1816



Characterization of reference materials for *in situ* U–Pb dating of columbite group minerals by LA-ICP-MS

Ming Yang, Yue-Heng Yang,* Rolf L. Romer, Xu-Dong Che, Ru-Cheng Wang, Fu-Yuan Wu, Guang-Chun Fei, Yun Deng and Tao Wu

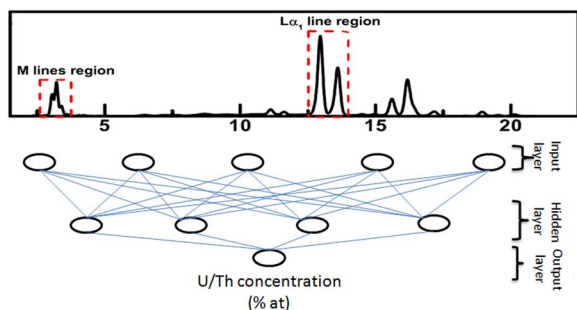
1830



Quantitative analysis of heavy metals in soil via hierarchical deep neural networks with X-ray fluorescence spectroscopy

Wanqi Yang, Fusheng Li,* Shubin Lyu, Qinglun Zhang and Yanchun Zhao

1841



An X-ray fluorescence and machine learning based methodology for the direct non-destructive compositional analysis of $(\text{Th}_{1-x}\text{U}_x)\text{O}_2$ fuel pellets

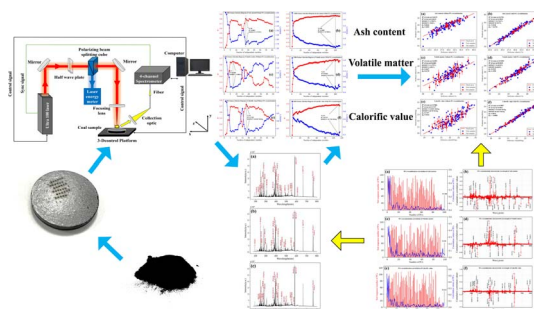
Buddhadev Kanrar,* Kaushik Sanyal, Arnab Sarkar and Rajesh V. Pai



1851

Determination of ash content, volatile matter, and calorific value in coal by OLS combined with laser-induced breakdown spectroscopy based on PC recombination

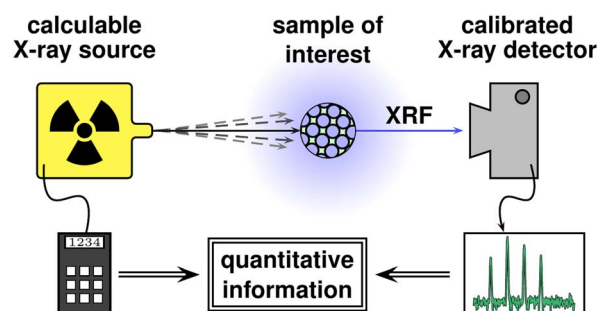
Shengen Zhu, Wenhao Zhang,* Guangdong Song,* Yadong Li, Binxin Hu, Feng Zhu, Hua Zhang, Yubin Wei, Tengfei Sun and Jing Tang



1865

Reference-free X-ray fluorescence analysis using well-known polychromatic synchrotron radiation

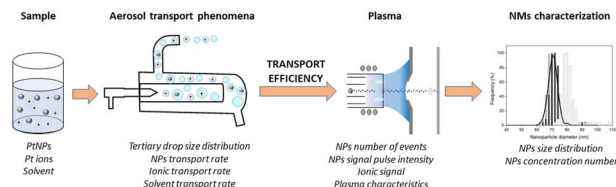
André Wählich,* Malte Wansleben, Rainer Unterumsberger, Yves Kayser and Burkhard Beckhoff



1874

Unraveling the role of aerosol transport on nanomaterial characterization by means single particle inductively coupled plasma mass spectrometry

Daniel Torregrosa, Guillermo Grindlay, Luis Gras and Juan Mora



1885

Titanium and titanium oxides at the K- and L-edges: comparing theoretical calculations to X-ray absorption and X-ray emission measurements

Karina Bzheumikhova,* John Vinson, Rainer Unterumsberger, Malte Wansleben, Claudia Zech, Kai Schüler, Yves Kayser, Philipp Hönicke and Burkhard Beckhoff

