Electronic Supplementary Material (ESI) for JAAS.

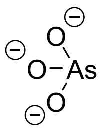
Arsenic speciation analysis of environmental samples

Francisco Ardini, Greta Dan, Marco Grotti

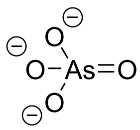
Supplementary information

Investigated arsenic species and abbreviations

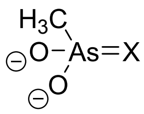
(compounds are drawn in their most deprotonated form)



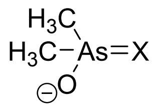
1. [iAs(III)]



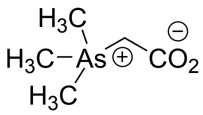
2. [iAs(V)]



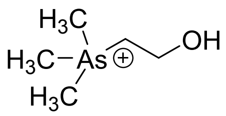
3. X = O [MA]
T3. X = S [Thio-MA]



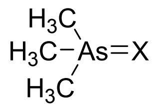
4. X = O [DMA]
T4. X = S [Thio-DMA]



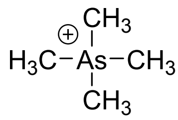
5. [AB]



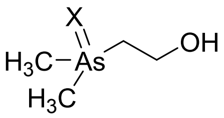
6. [AC]



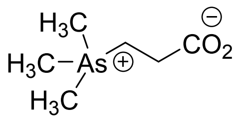
7. X = O [TMAO]
T7. X = S [TMAS]



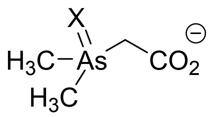
8. [TETRA]



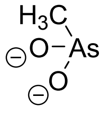
9. X = O [DMAE]
T9. X = S [Thio-DMAE]



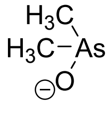
10. [TMAP]



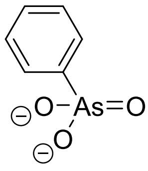
11. X = O [DMAA]
T11. X = S [Thio-DMAA]



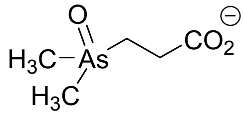
12. [MAs(III)]



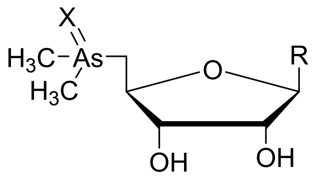
13. [DMAs(III)]

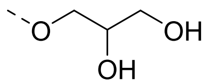
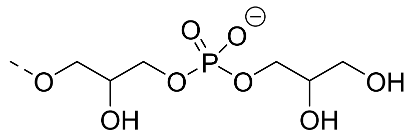


14. [PA]



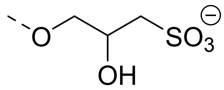
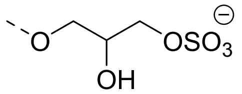
15. [DMAP]



R =  

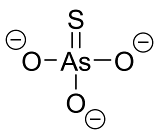
S1. X = O [Arsenosugar-Gly]
TS1. X = S [Thio-arsenosugar-Gly]

S2. X = O [Arsenosugar-PO_4]
TS2. X = S [Thio-arsenosugar-PO_4]

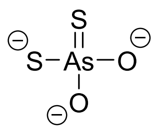
R =  

S3. X = O [Arsenosugar-SO_3]
TS3. X = S [Thio-arsenosugar-SO_3]

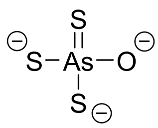
S4. X = O [Arsenosugar-SO_4]
TS4. X = S [Thio-arsenosugar-SO_4]



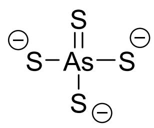
T2. [TAs(V)]



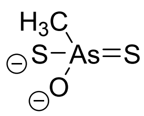
T2b. [DTAs(V)]



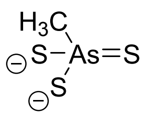
T2c. [TriTAs(V)]



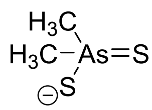
T2d. [TetraTAs(V)]



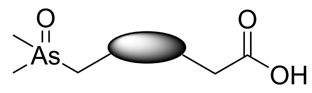
T3b. [Dithio-MA]



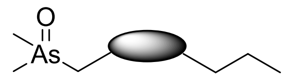
T3c. [Trithio-MA]



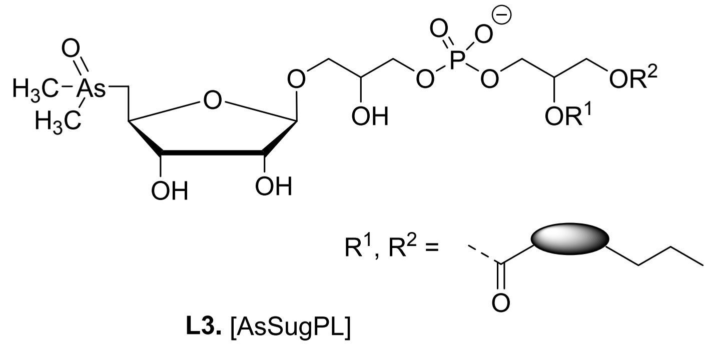
T4b. [Dithio-DMA]



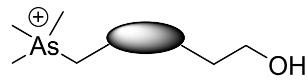
L1. [AsFA]



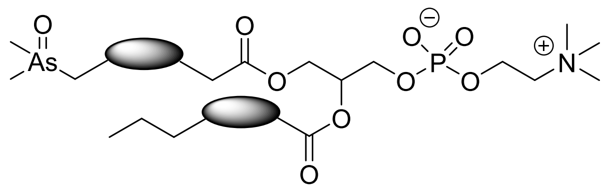
L2. [AsHC]



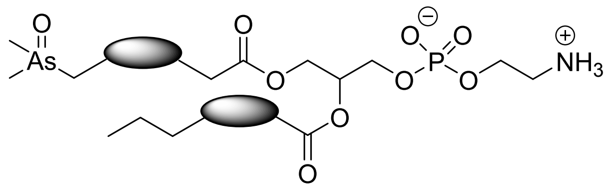
L3. [AsSugPL]



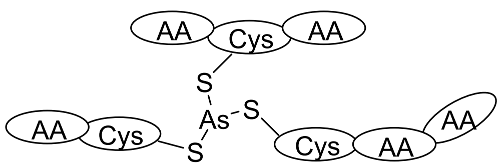
L4. [AsFOH]



L5. [AsPC]



L6. [AsPE]



ASPCC. [As(III)PC-complexes]

Table S1. Environmental CRMs with reference values for As species.

Producer	Name	Matrix	As species ‡	References
EU Joint Research Centre	BCR-279	Sea lettuce	iAs(V), MA, DMA, S1	[1]
EU Joint Research Centre	BCR-320	River sediment	iAs(III), iAs(V)	[2]
EU Joint Research Centre	BCR-414	Plankton	iAs(III), iAs(V)	[3]
EU Joint Research Centre	BCR-627 §	Tuna fish tissue	TETRA, TMAP, AC, S2	[4,5]
EU Joint Research Centre	BCR-278R	Mussel tissue	AB, TMAO, TETRA, DMA, S1, S2	[4]
National Research Council of Canada	TMDA-54.4	Lake water	iAs(III), iAs(V)	[6]
National Research Council of Canada	DORM-1	Dogfish muscle	AB, DMA	[7]
National Research Council of Canada	DORM-2 §	Dogfish muscle	iAs(III), iAs(V), TMAP, DMA, MA, TMAO, S2, AC	[1,4,5,8–12]
National Research Council of Canada	DORM-3	Fish protein	AB, MA, DMA, iAs(III), iAs(V)	[13]
National Research Council of Canada	HISS-1	Marine sediment	iAs(III), iAs(V), MA	[2]
National Research Council of Canada	TORT-1	Lobster hepatopancreas	AB, MA	[7]
National Research Council of Canada	TORT-2	Lobster hepatopancreas	iAs(V), AB, S1, TMAP, AC, TETRA, DMA, S2, MA	[1,13–15]
National Research Center for Certified Reference Materials, China	GBW 07405	Soil	iAs(V)	[16,17]
International Atomic Energy Agency	IAEA-140	Seaweed	S1, S2, S3, S4, iAs(V), DMA	[18]
International Atomic Energy Agency	IAEA-405	Estuarine sediment	iAs(III), iAs(V)	[2]
National Institute of Standards & Technology, USA	NIST 1566a	Oyster tissue	AB, DMA, iAs(V), S2	[9]
National Institute of Standards & Technology, USA	NIST 1566b	Oyster tissue	AB, TMAO, S1, S2, AC, DMA	[4]
Istituto Superiore di Sanità, Italy	MURST-ISS-A2	Antarctic krill	DMA, AB, TMAP, iAs(V), AC, S1, S2, S3, S4, TS1	[19,20]
National Institute for Environmental Studies, Japan	NIES 9	Seaweed	DMA, iAs(V), S1, S2, S3, S4	[21,22]
Resource Technology Corporation, USA	CRM025-050	Soil	iAs(III), iAs(V)	[16,17]

Notes: ‡ See Table 1. § Additional As speciation data besides the certified species.

References

1 S. Foster, W. Maher, F. Krikowa and S. Apte, *Talanta*, 2007, **71**, 537–549.
2 L. Orero Iserte, A. Roig-Navarro and F. Hernandez, *Anal. Chim. Acta*, 2004, **527**, 97–104.
3 E. L. Lehmann, A. H. Fostier and M. A. Z. Arruda, *Talanta*, 2013, **104**, 187–192.
4 V. Nischwitz and S. A. Pergantis, *Anal. Chem.*, 2005, **77**, 5551–5563.
5 M. J. Ruiz-Chancho, T. Pichler and R. E. Price, *Chem. Geol.*, 2013, **348**, 56–64.
6 X. Gao, Y. Wang and Q. Hu, *Environ. Geochem. Health*, 2012, **34**, 113–122.
7 S. Rattanachongkiat, G. E. Millward and M. E. Foulkes, *J. Environ. Monit.*, 2004, **6**, 254–261.
8 S. Karthikeyan and S. Hirata, *Appl. Organomet. Chem.*, 2004, **18**, 323–330.
9 C.-F. Yeh and S.-J. Jiang, *Electrophoresis*, 2005, **26**, 1615–1621.
10 U. Kristan, T. Kanduč, A. Osterc, Z. Šlejkovec, A. Ramšak and V. Stibilj, *Mar. Pollut. Bull.*, 2014, **89**, 455–463.
11 J. Kirby, W. Maher, M. Ellwood and F. Krikowa, *Aust. J. Chem.*, 2004, **57**, 957–966.
12 T. Agusa, K. Takagi, R. Kubota, Y. Anan, H. Iwata and S. Tanabe, *Environ. Pollut. Barking Essex 1987*, 2008, **153**, 127–136.
13 S. Hong, H.-O. Kwon, S.-D. Choi, J.-S. Lee and J. S. Khim, *Mar. Pollut. Bull.*, 2016, **108**, 155–162.
14 G. Rodríguez-Moro, T. García-Barrera, C. Trombini, J. Blasco and J. L. Gómez-Ariza, *Electrophoresis*, 2018, **39**, 635–644.
15 A. M. Orani, A. Barats, W. Zitte, C. Morrow and O. P. Thomas, *Chemosphere*, 2018, **201**, 826–839.
16 M. J. Ruiz-Chancho, R. Sabé, J. F. López-Sánchez, R. Rubio and P. Thomas, *Microchim. Acta*, 2005, **151**, 241–248.
17 M. J. Ruiz-Chancho, J. F. López-Sánchez and R. Rubio, *Anal. Bioanal. Chem.*, 2007, **387**, 627–635.
18 Z. Šlejkovec, E. Kápolna, I. Ipolyi and J. T. van Elteren, *Chemosphere*, 2006, **63**, 1098–1105.
19 A. Terol, F. Ardini, M. Grotti and J. L. Todolí, *J. Chromatogr. A*, 2012, **1262**, 70–76.
20 M. Grotti, F. Soggia, W. Goessler, S. Findenig and K. A. Francesconi, *Talanta*, 2010, **80**, 1441–1444.
21 T. Llorente-Mirandes, M. J. Ruiz-Chancho, M. Barbero, R. Rubio and J. F. López-Sánchez, *Chemosphere*, 2010, **81**, 867–875.
22 T. Llorente-Mirandes, M. J. Ruiz-Chancho, M. Barbero, R. Rubio and J. F. López-Sánchez, *J. Agric. Food Chem.*, 2011, **59**, 12963–12968.