

Supplementary Materials

Binding of Arsenic by common functional groups: an experimental and quantum-mechanical study

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Table S1. As(III) hydrolysis and ligand protonation constants at $I = 0.15 \text{ mol L}^{-1}$ (NaCl) and $T = 298.15 \text{ K}$.

	$\log K^a$	$\log K_1^{H\ b)}$	$\log \beta_2^{H\ b)}$	$\log \beta_3^{H\ b)}$	$\log \beta_4^{H\ b)}$	$\log \beta_5^{H\ b)}$	$\log \beta_6^{H\ b)}$	Ref. ^{c)}
As(III)	-9.096							1
mal		5.22	7.99					2
tca		5.819	10.331	13.729				3
btc		6.21	11.31	15.39	18.55			4
mlt		6.39	11.623	15.743	18.500	20.176	20.898	5
gly		9.571	11.933					6
asp		9.63	13.09	15.04				6
lys		11.06	20.26	22.21				6
cys		10.46	18.78	21.04				7
etan		10.66±0.03 ^{c)}						8
en		9.94	17.04					9
dien		9.84	18.84	23.04				9
trien		9.69	18.79	25.38	28.43			10
tetren		9.81	19.05	27.19	31.76	34.45		10
tla		10.02	13.52					11
tma		10.227	14.997	18.507				11
dmsa		11.01	20.32	23.87	26.39			12

^{a)} It refers to the reaction: $\text{As}(\text{OH})_3 + \text{H}_2\text{O} = \text{As}(\text{OH})_4^- + \text{H}^+$; ^{b)} β_i refers to the reaction $i\text{H} + \text{L} = \text{H}_i\text{L}$ (charges omitted for simplicity); ^{c)} 1. G. Cassone G., D. Chillè, V. Mollica Nardo, O. Giuffrè, R.C. Ponterio, J. Sponer, S. Trusso, F. Saija, C. Foti, *Dalton Trans.*, 2020, 49, 6302-6311; 2. A. De Robertis, C. De Stefano, C. Foti, *J. Chem. Eng. Data*, 1999, 44, 262-270; 3. C. De Stefano, C. Foti, A. Gianguzza, *Talanta* 1994, 41, (10), 1715-1722.; 4. A. De Robertis, C. Foti, A. Gianguzza, *Ann. Chim. (Rome)* 1993, 83, 485-497; 5. A. De Robertis, C. De Stefano, C. Foti, *Ann. Chim. (Rome)*, 1996, 86, 155-166; 6. C. De Stefano, C. Foti, A. Gianguzza, C. Rigano, S. Sammartano, *Chem. Spec. Bioavail.*, 1995, 7(1), 1-8; 7. V.K. Sharma, F. Casteran, F.J. Millero, C. De Stefano, *J. Solution Chem.*, 2002, 31, 783-792. 8. Unpublished data; 9. A. De Robertis, C. Foti, O. Giuffrè, S. Sammartano, *J. Chem. Eng. Data*, 2001, 46, 1425-1435; 10. A. De Robertis, C. De Stefano, G. Patanè, S. Sammartano, *J. Sol. Chem.*, 1993, 22; 11. C. Bretti, C. De Stefano, C. Foti, O. Giuffrè, S. Sammartano, *J. Solution Chem.*, 2009, 38(10), 1225-1245; 12. Chillè, D.; Cassone, G.; Giacobello, F.; Giuffrè, O.; Mollica Nardo, V.; R.C., P.; Saija, F.; Sponer, J.; Trusso, S.; Foti, C., *Chem. Res. Toxicol.* **2020**, 33, 967-974.