Environ Earth Sci (2010) 59:1601–1606
DOI 10.1007/s12665-009-0369-x

ERRATUM

Erratum to: Prediction of the thermodynamic properties of metal–arsenate and metal–arsenite aqueous complexes to high temperatures and pressures and some geological consequences

Luigi Marini · Marina Accornero

Published online: 11 December 2009

Erratum to: Environ Geol (2007) 52:1343–1363
DOI 10.1007/s00254-006-0578-5

Marini and Accornero (2007) evaluated the standard thermodynamic properties (ΔG°_{f}, ΔH°_{f}, S°, C°_{P}, V°, ω) of several aqueous complexes formed by dissolved metals and dihydrogenarsenate, monohydrogenarsenate, arsenate and dihydrogenarsenite ions at reference pressure, Pr = 1 bar, and reference temperature, Tr = 298.15 K, as well as the pressure- and temperature-independent coefficients of the revised Helgeson–Kirkham–Flowers (HKF) equations of state $a_{1,ML}$, $a_{2,ML}$, $a_{3,ML}$, $a_{4,ML}$, $c_{1,ML}$, and $c_{2,ML}$, where the subscript ML identifies a generic aqueous complex formed by metal M and ligand L.

Unfortunately, we recently realized that there is a wrong sign in the Eq. 37 of Sverjensky et al. (1997), corresponding to Eq. 48 of Marini and Accornero (2007), which was used to calculate the EOS coefficient $c_{1,ML}$. In the correct equation:

$$c_{1,ML} = 0.6087 \cdot C^{\circ}_{P,ML,Pr,Tr} - \omega_{ML,Pr,Tr} \cdot 298.15 \cdot X_{Pr,Tr} + 5.85 \quad (1)$$

the term containing the solvent Born function X must have a negative sign. This is easy inferable by solving the HKF equation of state (see Marini and Accornero 2007 for the explanation of symbols):

$$C^{\circ}_{P,ML,Pr,T} = \omega_{ML} \cdot T \cdot X + 2 \cdot T \cdot Y \left(\frac{\partial \omega_{ML}}{\partial T}\right)_P - T\left(\frac{1}{\varepsilon} - 1\right) \cdot \left(\frac{\partial^2 \omega_{ML}}{\partial T^2}\right)_P + c_{1,ML} + \frac{c_{2,ML}}{(T-\Theta)^2}, \quad (2)$$

for T = Tr and rearranging it as follows:

$$c_{1,ML} = C^{\circ}_{P,ML,Pr,T} - \omega_{ML} \cdot 298.15 \cdot X_{Pr,Tr} - \frac{c_{2,ML}}{(298.15-\Theta)^2}. \quad (3)$$

The wrong values obtained by Marini and Accornero (2007) for the EOS coefficient $c_{1,ML}$ determine increasingly large errors in the thermodynamic properties of the aqueous complexes of interest at temperatures increasingly different from Tr and, consequently, in the log K of their destruction reactions.

To compute the correct values of the EOS coefficient $c_{1,ML}$, Eq. 3 was used, in which the value of $c_{2,ML}$ is given by (Sverjensky et al. 1997):

$$c_{2,ML} = 2037 \cdot C^{\circ}_{P,ML,Pr,Tr} - 30460. \quad (4)$$

The calculated values of the EOS coefficient $c_{1,ML}$ are reported in Table 1, together with all other estimated standard partial molal thermodynamic properties, at Pr, Tr, for the metal–arsenate and metal–arsenite complexes of

The online version of the original article can be found under doi:10.1007/s00254-006-0578-5.

Electronic supplementary material The online version of this article (doi:10.1007/s12665-009-0369-x) contains supplementary material, which is available to authorized users.

L. Marini (✉) · M. Accornero
Laboratory of Geochemistry, Dip. Te. Ris,
University of Genova, Corso Europa 26,
16132 Genova, Italy
e-mail: lmarini@dipteris.unige.it

M. Accornero
e-mail: m.accornero@unige.it

Present Address:
M. Accornero
D'Appolonia SpA, Via San Nazaro, 19, 16145 Genova, Italy
e-mail: marina.accornero@dappolonia.it

interest as well as the equation-of-state parameters for calculating the corresponding properties at high temperatures and pressures. In addition to the new values of the EOS coefficient $c_{1,ML}$, little modifications in the ΔH_f^o and S^o of the complexes $MgAsO_4^-$, $CaAsO_4^-$, $MnAsO_4^-$, $AlAsO_4^o$, and $FeAsO_4^o$ were introduced.

The SUPCRT-generated logarithms of the thermodynamic constants of the reactions of destruction (consistent with the requirements of the software package EQ3/6) for all the considered aqueous complexes, at 1.013 bar and 0.01, 25, 60, 100°C and at saturation pressure and 150, 200, 250 and 300°C, are listed in Table 2.

All the data reported in Tables 1 and 2 are also given in the electronic supplementary material 1 (which is a patch for supcrt) and electronic supplementary material 2 (which is a patch for eq3/6).

Table 1 Estimated standard partial molal thermodynamic properties of metal–arsenate and metal–arsenite complexes at 25°C, 1 bar and estimated equation-of-state parameters for calculation of the corresponding properties at high temperatures and pressures

Complex	ΔG_f^o (cal mol^{-1})	ΔH_f^o (cal mol^{-1})	S° (cal mol^{-1} K^{-1})	C_P° (cal mol^{-1} K^{-1})	V° (cm^3 mol^{-1})	$a_1 \times 10$ (cal mol^{-1} bar^{-1})	$a_2 \times 10^{-2}$ (cal mol^{-1})	a_3 (cal K mol^{-1} bar^{-1})	$a_4 \times 10^{-4}$ (cal K mol^{-1})	c_1 (cal mol^{-1} K^{-1})	$c_2 \times 10^{-4}$ (cal K mol^{-1})	$\omega \times 10^{-5}$ (cal mol^{-1})
NaH_2AsO_4°	−240179	−272608	41.2	37.8	41.1	7.3772	10.2353	1.1421	−3.2022	27.9202	4.6622	−0.0380
KH_2AsO_4°	−244935	−274352	54.5	21.9	52.4	8.9277	14.0226	−0.4840	−3.3587	18.6125	1.4173	−0.0380
$MgH_2AsO_4^+$	−290910	−332717	−10.4	50.7	18.3	4.5105	3.2335	4.1483	−2.9127	42.2650	7.2899	0.7009
$CaH_2AsO_4^+$	−314170	−348007	18.5	45.8	22.2	4.8949	4.1724	3.7452	−2.9515	35.3597	6.2862	0.2639
$SrH_2AsO_4^+$	−315896	−347841	27.3	40.1	22.9	4.9488	4.3041	3.6887	−2.9570	30.8142	5.1312	0.1301
$MnH_2AsO_4^+$	−236482	−270828	14.5	53.5	23.3	5.0617	4.5799	3.5702	−2.9684	40.4264	7.8583	0.3244
$FeH_2AsO_4^+$	−205693	−243719	1.0	44.9	17.6	4.3531	2.8490	4.3134	−2.8968	37.3097	6.1166	0.5283
$CoH_2AsO_4^+$	−193388	−232357	−1.5	45.2	13.9	3.8628	1.6516	4.8275	−2.8473	37.7921	6.1625	0.5664
$NiH_2AsO_4^+$	−193146	−233785	−7.1	36.4	10.0	3.3580	0.4185	5.3569	−2.7963	33.4496	4.3750	0.6516
$CuH_2AsO_4^+$	−166866	−204382	4.1	49.9	14.9	3.9712	1.9164	4.7138	−2.8583	39.7683	7.1249	0.4813
$ZnH_2AsO_4^+$	−215927	−255372	−0.3	50.7	15.3	4.0397	2.0836	4.6420	−2.8652	40.8741	7.2945	0.5485
$PbH_2AsO_4^+$	−187896	−215577	44.7	34.1	25.0	5.1359	4.7611	3.4924	−2.9759	24.9084	3.9167	−0.1328
$AlH_2AsO_4^{2+}$	−299978	−350717	−57.0	34.9	−7.1	1.4490	−4.2440	7.3587	−2.6036	44.5413	4.0694	1.9507
$FeH_2AsO_4^{2+}$	−189949	−235535	−39.9	66.2	1.1	2.4901	−1.7013	6.2670	−2.7087	60.4374	10.4402	1.6926
$NaHAsO_4^-$	−234026	−272938	19.4	11.0	16.4	4.4640	3.1200	4.1970	−2.9080	24.8601	−0.7900	1.3274
$KHAsO_4^-$	−238754	−275247	30.7	3.9	26.1	5.7282	6.2078	2.8713	−3.0357	19.1455	−2.2322	1.1561
$MgHAsO_4$°	−282655	−326456	−17.1	−3.4	−0.5	1.6885	−3.6591	7.1076	−2.6278	3.8675	−3.7233	−0.0380
$CaHAsO_4$°	−306038	−344341	3.5	−5.6	2.0	2.0228	−2.8426	6.7570	−2.6615	2.5879	−4.1694	−0.0380
$SrHAsO_4$°	−307750	−344917	9.8	−8.1	2.4	2.0851	−2.6905	6.6917	−2.6678	1.1155	−4.6827	−0.0380
$MnHAsO_4$°	−229564	−268033	0.7	−2.1	2.7	2.1148	−2.6180	6.6606	−2.6708	4.5920	−3.4707	−0.0380
$FeHAsO_4$°	−196961	−237958	−8.9	−5.9	−0.9	1.6263	−3.8112	7.1729	−2.6215	2.3717	−4.2448	−0.0380
$CoHAsO_4$°	−187516	−229240	−10.7	−5.8	−3.2	1.3102	−4.5832	7.5044	−2.5896	2.4302	−4.2244	−0.0380
$NiHAsO_4$°	−185083	−227995	−14.7	−9.7	−5.7	0.9749	−5.4021	7.8559	−2.5557	0.1514	−5.0188	−0.0380
$CuHAsO_4$°	−160044	−200797	−6.7	−3.7	−2.6	1.3964	−4.3727	7.4140	−2.5983	3.6572	−3.7966	−0.0380
$ZnHAsO_4$°	−209827	−252128	−9.9	−3.4	−2.4	1.4251	−4.3025	7.3838	−2.6012	3.8733	−3.7213	−0.0380
$PbHAsO_4$°	−180119	−214509	22.2	−10.7	3.7	2.2585	−2.2670	6.5099	−2.6853	−0.4328	−5.2225	−0.0380
$AlHAsO_4^+$	−295884	−343378	−46.1	−37.3	−8.2	1.0572	−5.2011	7.7696	−2.5640	−4.1613	−10.6336	1.2420
$FeHAsO_4^+$	−188188	−232211	−34.7	−23.405	−4.91	1.4545	−4.2306	7.3530	−2.6042	2.3700	−7.8022	1.0694
$NaAsO_4^{2-}$	−223700	−253943	48.5	−38.4	−17.0	0.2824	−7.0935	8.5822	−2.4858	6.8433	−10.8648	2.5085
$KAsO_4^{2-}$	−228428	−249049	84.0	−45.5	−9.6	1.1121	−5.0669	7.7120	−2.5696	−2.2416	−12.3070	1.9714
$MgAsO_4^-$	−271474	−307316	9.64	−55.0	−26.0	−1.2915	−10.9377	10.2326	−2.3269	−12.3300	−14.2311	1.4754
$CaAsO_4^-$	−294913	−323114	37.4	−57.2	−25.5	−1.3678	−11.1242	10.3127	−2.3192	−17.4821	−14.6772	1.0550
$SrAsO_4^-$	−296243	−323239	43.9	−59.7	−25.4	−1.3889	−11.1758	10.3349	−2.3170	−19.8655	−15.1905	0.9562
$MnAsO_4^-$	−218289	−247805	30.7	−53.7	−25.4	−1.3158	−10.9970	10.2581	−2.3244	−14.5434	−13.9785	1.1565
$FeAsO_4^-$	−186668	−218541	21.7	−57.5	−26.1	−1.3653	−11.1181	10.3101	−2.3194	−15.5040	−14.7525	1.2932

Table 1 continued

Complex	ΔG_f^o (cal mol^{-1})	ΔH_f^o (cal mol^{-1})	S° (cal mol^{-1} K^{-1})	C_P° (cal mol^{-1} K^{-1})	V° (cm^3 mol^{-1})	$a_1 \times 10$ (cal mol^{-1} bar^{-1})	$a_2 \times 10^{-2}$ (cal mol^{-1})	a_3 (cal K mol^{-1} bar^{-1})	$a_4 \times 10^{-4}$ (cal K mol^{-1})	c_1 (cal mol^{-1} K^{-1})	$c_2 \times 10^{-4}$ (cal K mol^{-1})	$\omega \times 10^{-5}$ (cal mol^{-1})
$CoAsO_4^-$	−177190	−210481	17.6	−57.4	−26.5	−1.4073	−11.2205	10.3541	−2.3152	−14.8722	−14.7322	1.3555
$NiAsO_4^-$	−176304	−211320	11.8	−61.3	−27.0	−1.4432	−11.3083	10.3918	−2.3116	−16.3404	−15.5266	1.4434
$CuAsO_4^-$	−151743	−183607	23.1	−55.3	−26.4	−1.4178	−11.2463	10.3651	−2.3141	−14.4180	−14.3044	1.2716
$ZnAsO_4^-$	−200121	−233853	18.9	−55.0	−26.36	−1.3907	−11.1799	10.3366	−2.3169	−13.6104	−14.2290	1.3358
$PbAsO_4^-$	−169793	−194437	54.9	−62.3	−25.16	−1.4108	−11.2291	10.3577	−2.3148	−22.9414	−15.7303	0.7904
$AlAsO_4$°	−285558	−330011	−35.9	−60.2	−9.75	0.4180	−6.7624	8.4400	−2.4995	−29.3427	−15.3014	−0.0380
$FeAsO_4$°	−177862	−218546	−23.5	−84.8	−13.09	−0.0391	−7.8787	8.9193	−2.4533	−43.7161	−20.3124	−0.0380
NaH_2AsO_3°	−203270	−228832	39.7	28.4	32.7	6.2236	7.4178	2.3518	−3.0857	22.4338	2.7495	−0.0380
AgH_2AsO_3°	−123526	−147071	44.3	25.8	33.0	6.2709	7.5332	2.3022	−3.0905	20.9088	2.2178	−0.0380
$MgH_2AsO_3^+$	−251410	−286183	−11.3	41.3	9.9	3.3617	0.4276	5.3530	−2.7967	36.9078	5.3772	0.7149
$CaH_2AsO_3^+$	−274922	−301872	17.1	36.4	13.8	3.7486	1.3726	4.9473	−2.8358	30.0706	4.3735	0.2853
$SrH_2AsO_3^+$	−275601	−300702	25.8	30.7	14.5	3.8032	1.5060	4.8900	−2.8413	25.5459	3.2185	0.1538
$BaH_2AsO_3^+$	−276315	−297936	40.1	25.6	19.9	4.4634	3.1185	4.1977	−2.9080	20.5926	2.1872	−0.0628
$CuH_2AsO_3^+$	−134368	−164924	3.0	40.5	6.5	2.8237	−0.8865	5.9172	−2.7424	34.4453	5.2122	0.4990
$PbH_2AsO_3^+$	−153138	−174063	42.8	24.7	16.5	3.9918	1.9667	4.6922	−2.8603	19.6811	2.0039	−0.1047
$AlH_2AsO_3^{2+}$	−266611	−309612	−55.5	25.5	−15.6	0.2881	−7.0796	8.5762	−2.4864	38.8545	2.1567	1.9289
$FeH_2AsO_3^{2+}$	−154392	−192413	−39.1	56.8	−7.3	1.3321	−4.5296	7.4814	−2.5918	54.8314	8.5274	1.6796

Table 2 Logarithms of thermodynamic constants of the reactions of destruction (as required by the software package EQ3/6) of the aqueous complexes containing arsenate and arsenite ions at 1.013 bar and 0.01, 25, 60, 100°C and at saturation pressure and 150, 200, 250 and 300°C

Complex T(°C)	0.01	25	60	100	150	200	250	300
$NaH_2AsO_4^\circ$	1.8911	1.7753	1.5746	1.3381	1.0408	0.7263	0.3609	−0.1285
$KH_2AsO_4^\circ$	2.0939	1.8948	1.6188	1.3247	0.9791	0.6336	0.2515	−0.2405
$MgH_2AsO_4^+$	−2.0823	−1.7555	−1.5109	−1.3987	−1.4183	−1.5750	−1.8676	−2.3445
$CaH_2AsO_4^+$	−1.6054	−1.4953	−1.4931	−1.6081	−1.8662	−2.2289	−2.7076	−3.3615
$SrH_2AsO_4^+$	−0.8157	−0.8254	−0.9536	−1.1756	−1.5231	−1.9423	−2.4564	−3.1350
$MnH_2AsO_4^+$	−1.1024	−1.0057	−1.0288	−1.1704	−1.4554	−1.8397	−2.3362	−3.0039
$FeH_2AsO_4^+$	−3.1387	−2.7950	−2.5235	−2.3856	−2.3830	−2.5271	−2.8156	−3.2959
$CoH_2AsO_4^+$	−0.4066	−0.2771	−0.2519	−0.3392	−0.5585	−0.8781	−1.3089	−1.9068
$NiH_2AsO_4^+$	−1.9243	−1.6390	−1.4238	−1.3272	−1.3545	−1.5123	−1.8031	−2.2769
$CuH_2AsO_4^+$	−2.0928	−1.8552	−1.7041	−1.6723	−1.7697	−1.9895	−2.3379	−2.8673
$ZnH_2AsO_4^+$	−0.6738	−0.5256	−0.4867	−0.5648	−0.7764	−1.0900	−1.5155	−2.1087
$PbH_2AsO_4^+$	−1.5392	−1.5950	−1.7688	−2.0265	−2.4056	−2.8506	−3.3929	−4.1134
$AlH_2AsO_4^{2+}$	−3.6996	−3.1952	−2.7692	−2.5203	−2.4408	−2.5506	−2.8307	−3.3191
$FeH_2AsO_4^{2+}$	−4.7729	−4.2654	−3.8790	−3.7014	−3.7268	−3.9484	−4.3419	−4.9412
$NaHAsO_4^-$	6.4042	6.2855	6.1432	6.0208	5.9138	5.8400	5.7834	5.7293
$KHAsO_4^-$	6.5807	6.4255	6.2413	6.0729	5.9074	5.7738	5.6561	5.5387
$MgHAsO_4^\circ$	4.4413	4.2954	4.1210	3.9578	3.7683	3.5483	3.2417	2.7585
$CaHAsO_4^\circ$	4.6511	4.4655	4.2456	4.0314	3.7781	3.4977	3.1370	2.6054
$SrHAsO_4^\circ$	5.3989	5.1457	4.8481	4.5692	4.2636	3.9546	3.5832	3.0543
$MnHAsO_4^\circ$	4.2110	4.0653	3.8910	3.7235	3.5233	3.2902	2.9703	2.4738
$FeHAsO_4^\circ$	3.6994	3.6057	3.4911	3.3780	3.2308	3.0385	2.7505	2.2795
$CoHAsO_4^\circ$	4.1574	4.0271	3.8706	3.7190	3.5332	3.3093	2.9942	2.4994
$NiHAsO_4^\circ$	4.4199	4.2712	4.0936	3.9226	3.7174	3.4776	3.1491	2.6430
$CuHAsO_4^\circ$	3.2018	3.1453	3.0815	3.0242	2.9430	2.8122	2.5811	2.1629
$ZnHAsO_4^\circ$	4.0677	3.9458	3.7982	3.6578	3.4885	3.2835	2.9889	2.5154
$PbHAsO_4^\circ$	4.2770	4.1056	3.9019	3.7089	3.4889	3.2490	2.9358	2.4578
$AlHAsO_4^+$	−0.1355	−0.1942	−0.2499	−0.2963	−0.3667	−0.4902	−0.7164	−1.1323
$FeHAsO_4^+$	−3.1723	−2.9745	−2.7389	−2.5187	−2.3236	−2.2341	−2.2842	−2.5488
$NaAsO_4^{2-}$	15.2959	13.8545	12.3070	11.0077	9.8650	9.0982	8.6152	8.3961
$KAsO_4^{2-}$	15.9563	13.9946	11.8493	9.9950	8.2866	7.0479	6.1503	5.5400
$MgAsO_4^-$	13.9719	12.4912	10.9025	9.5600	8.3426	7.4506	6.7551	6.1685
$CaAsO_4^-$	14.2801	12.6202	10.8258	9.2842	7.8502	6.7640	5.8852	5.1099
$SrAsO_4^-$	15.3375	13.5804	11.6743	10.0363	8.5174	7.3736	6.4551	5.6483
$MnAsO_4^-$	13.8821	12.3299	10.6592	9.2359	7.9273	6.9486	6.1646	5.4783
$FeAsO_4^-$	12.5967	11.1505	9.6014	8.2896	7.0926	6.2054	5.5017	4.8926
$CoAsO_4^-$	13.0352	11.5962	10.0553	8.7512	7.5622	6.6823	5.9861	5.3868
$NiAsO_4^-$	12.0239	10.7063	9.3049	8.1283	7.0660	6.2882	5.6784	5.1566
$CuAsO_4^-$	10.4895	9.2300	7.9034	6.8041	5.8271	5.1223	4.5724	4.0949
$ZnAsO_4^-$	12.4594	11.0603	9.5648	8.3049	7.1645	6.3281	5.6713	5.1075
$PbAsO_4^-$	13.2428	11.6746	9.9854	8.5451	7.2187	6.2228	5.4162	4.6855
$AlAsO_4^\circ$	8.3525	7.3748	6.3161	5.3948	4.4910	3.7140	2.9406	2.0425
$FeAsO_4^\circ$	5.3733	4.5945	3.8490	3.2941	2.8374	2.4877	2.1196	1.6021
$NaH_2AsO_3^\circ$	−0.3201	−0.2502	−0.2380	−0.2707	−0.3540	−0.4891	−0.7051	−1.0748
$AgH_2AsO_3^\circ$	−1.3155	−1.1840	−1.0977	−1.0644	−1.0864	−1.1757	−1.3543	−1.6893
$MgH_2AsO_3^+$	−2.2085	−1.8818	−1.6375	−1.5163	−1.5133	−1.6411	−1.9056	−2.3626
$CaH_2AsO_3^+$	−1.9433	−1.8063	−1.7736	−1.8513	−2.0588	−2.3705	−2.8024	−3.4201
$SrH_2AsO_3^+$	−0.3179	−0.3689	−0.5449	−0.8012	−1.1685	−1.5919	−2.1040	−2.7826
$BaH_2AsO_3^+$	−1.3798	−1.4274	−1.5929	−1.8400	−2.2036	−2.6319	−3.1584	−3.8662

Table 2 continued

Complex T(°C)	0.01	25	60	100	150	200	250	300
$CuH_2AsO_3^+$	−7.8251	−7.1140	−6.4194	−5.8821	−5.4680	−5.2734	−5.2815	−5.5329
$PbH_2AsO_3^+$	−5.4793	−5.1972	−4.9832	−4.8774	−4.8847	−5.0251	−5.3150	−5.8279
$AlH_2AsO_3^{2+}$	−8.6846	−7.8170	−6.9742	−6.3355	−5.8591	−5.6460	−5.6612	−5.9349
$FeH_2AsO_3^{2+}$	−8.0194	−7.2819	−6.6317	−6.2040	−5.9700	−5.9767	−6.1925	−6.6491

The reactions of destruction of the aqueous complexes are as follows:

$MH_2AsO_4^{(n-1)+} = M^{n+} + H_2AsO_4^-$

$MHAsO_4^{(n-2)+} + H^+ = M^{n+} + H_2AsO_4^-$

$MAsO_4^{(n-3)+} + 2H^+ = M^{n+} + H_2AsO_4^-$

$MH_2AsO_3^{(n-1)+} = M^{n+} + H_2AsO_3^-$