Appendix C

Arsenic Thermodynamic Data

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C.1 Introduction

Italicized terms in the text of this appendix or words derived from the italicized terms are defined in the glossary of Appendix B.

Table C.1 lists published *thermodynamic data* for arsenic, including: the more common elemental forms, selected compounds, and some aqueous and gaseous species. The table contains *Gibbs free energy* (ΔG_f), *enthalpy* (ΔH_f), *entropy* (S), and *heat capacity* (Cp) values at 1 bar pressure and mostly at 298.15 K (25 °C). For thermodynamic data of chemical species not containing arsenic, extensive tables occur in geochemistry textbooks and other references, including: (Barin, 1995; Robie, Hemingway and Fisher, 1979; Wagman *et al*., 1982; Drever, 1997; Eby, 2004; Faure, 1998; Lide, 2007; Krauskopf and Bird, 1995). Thermodynamic data are important in examining the behavior of arsenic in mineral–water interactions, studying water quality issues, investigating the formation of ore deposits, developing and interpreting *Eh-pH* diagrams, and designing environmental *remediation* projects (Nordstrom and Archer, 2003, 1–2).

Not all published and widely accepted thermodynamic values are reliable. Nordstrom and Archer (2003) provide a detailed review of the controversies, uncertainties, and problems related to thermodynamic data for arsenic and its compounds and aqueous species. Many of the data are contradictory and the methods that produce the data are sometimes questionable or have not been thoroughly documented. Too often, data in the literature have been passed from reference to reference without critical evaluations. Some of the data have high measurement errors, were produced under undefined or poorly defined laboratory conditions, and involved unrepresentative sampling (Matschullat 2000, 298; Nordstrom and Archer, 2003). Furthermore, other questionable data originate from obscure documents or are written in languages that many individuals cannot read and properly interpret. Therefore, thermodynamic results must be accepted with a certain amount of caution. The table in this appendix includes thermodynamic data from various sources, which provide users with some idea of their variability. Although sometimes unavoidable, users

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are cautioned to avoid mixing data from different literature sources when performing calculations for a reaction. Using data from multiple sources may introduce serious errors (Wagman *et al.*, 1982; Eby, 2004, 474).

C.2 Modeling applications with thermodynamic data

Once high-quality laboratory data are available, they may be used in geochemical computer models, such as MINTEQA2 (Allison, Brown and Novo-Gradac, 1991) and PHREEQC (Parkhurst and Appelo, 1999). Langmuir (1997, 558–561) provides a brief review of the different types of geochemical models and their advantages and limitations. Geochemical models allow users to avoid tedious calculations. When properly utilized, they may: (1) derive *adsorption* models, (2) identify probable aqueous species and estimate their *activities*, (3) model the effects of pH, *reduction/oxidation* (*redox* conditions), temperature, *ionic strength*, and other factors on arsenic chemistry, and/or (4) identify possible *precipitates*. However, as discussed in Chapter 2, geochemical models are often incapable of accurately representing and predicting the complex behavior of arsenic in natural environments. Specifically, the models typically fail to predict the presence of *metastable* species, sluggish chemical reactions, and the effects of biological organisms.

C.3 Thermodynamic data

Table C.1 *Thermodynamic data for arsenic, its compounds, and its aqueous and gaseous species at 1 bar pressure. Note that the units of G_i and H_i are 1000 times larger than S_i and Cp_i. 1 kcal = 4.184 kJ. °C = K −273.15. (See Appendix A for other unit conversions). Phases include: amorphous (am), aqueous species (aq), gas, liquid (liq), and crystalline solids (xls).*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
Elemental							
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	298.15	0	0	35.63	24.43	Nordstrom and Archer (2003)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	298.15	0	0	35.1	—	Wagman *et al*. (1982)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	298.15	0	0	35.69	24.65	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	298.15	0	0	35.6	—	Naumov, Ryzhenko and Khodakovsky (1974)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	298.15	0	0	35.706	24.652	Barin (1995)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	400	0	0	43.04	25.38	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	400	0	0	43.065	25.388	Barin (1995)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	500	0	0	48.77	25.96	Robie, Hemingway, and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	500	0	0	48.790	25.945	Barin (1995)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	600	0	0	53.55	26.51	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	600	0	0	53.569	26.501	Barin (1995)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	700	0	0	57.68	27.05	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	700	0	0	57.696	27.054	Barin (1995)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	800	0	0	61.33	27.60	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	800	0	0	61.344	27.580	Barin (1995)
As(0) (elemental arsenic, rhombohedral or 'gray')	xls	875	0	0	63.82	28.03	Robie, Hemingway and Fisher (1979)
As(0) (elemental arsenic, amorphous or 'black')	am	298.15	—	4.2	—	—	Wagman *et al*. (1982)
As(0) (elemental arsenic, amorphous or 'black')	am	298.15	—	13.6	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
As^+	gas	298.15	—	1255.6	—	—	Wagman *et al*. (1982)
As^{2+}	gas	298.15	—	3059.8	—	—	Wagman *et al*. (1982)
As^{3+}	gas	298.15	—	5801.1	—	—	Wagman *et al*. (1982)
As^{4+}	gas	298.15	—	10644	—	—	Wagman *et al*. (1982)
As^{5+}	gas	298.15	—	16694	—	—	Wagman *et al*. (1982)
As^{6+}	gas	298.15	—	29045	—	—	Wagman *et al*. (1982)
As_2	gas	298.15	171.9	222.2	239.4	35.003	Wagman *et al*. (1982)
As_2	gas	298.15	143	194	242.2	—	Naumov, Ryzhenko and Khodakovsky (1974)
As_4	gas	298.15	92.4	143.9	314	—	Wagman *et al*. (1982)
As_4	gas	298.15	87.9	144	330	—	Naumov, Ryzhenko and Khodakovsky (1974)
As_4	gas	298.15	98.261	153.30	327.43	77.208	Barin (1995)
Gases and aqueous species of arsenic compounds							

Ag_3AsO_4	xls	298.15	−545.39	−634.29	275.83	173.86	Barin (1995)
AlAs	xls	298.15	—	−116.3	—	—	Wagman *et al*. (1982)
AlAs	xls	298.15	−115.20	−116.32	60.25	45.80	Barin (1995)
$AlAsO_4$	xls	298.15	−1333.1	−1431.1	145.60	118.34	Barin (1995)
$AlAsO_4$	xls	298.15	−1280.8	—	—	—	Ryu *et al*. (2002)
$AlAsO_4 \cdot 2H_2O$ (mansfieldite)	xls	298.15	−1709	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$AsBr_3$	gas	298.15	−161.67	−132.1	363.8	—	Pankratov and Uchaeva (2000)
$AsBr_3$	gas	298.15	−159	−130	363.87	79.16	Wagman *et al*. (1982)
$AsBr_3$	gas	298.15	−159.80	−130.00	363.99	78.992	Barin (1995)
$AsCl_3$	gas	298.15	−258.05	−270.3	328.8	—	Pankratov and Uchaeva (2000)
$AsCl_3$	gas	298.15	−248.9	−261.5	327.17	75.73	Wagman *et al*. (1982)
$AsCl_3$	gas	298.15	−248.66	−261.50	327.30	75.395	Barin (1995)
$AsCl_3$	liq	298.15	−259.4	−305.0	216.3	—	Wagman *et al*. (1982)
$AsCl_3$	liq	298.15	−259.08	−305.01	216.31	133.47	Barin (1995)
AsF_3	gas	298.15	−905.67	−785.8	289.0	—	Pankratov and Uchaeva (2000)
AsF_3	gas	298.15	−770.76	−785.76	298.10	65.61	Wagman *et al*. (1982)
AsF_3	gas	298.15	−770.65	−785.76	289.22	64.684	Barin (1995)
AsF_3	liq	298.15	−774.16	−821.3	181.21	126.57	Wagman *et al*. (1982)
AsF_3	liq	298.15	−774.01	−821.32	181.21	126.55	Barin (1995)
AsF_5	gas	298.15	−1172.5	−1236.7	—	—	Pankratov and Uchaeva (2000)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
AsF_5	gas	298.15	−1169.0	−1234.2	—	87.84	O'Hare (1993)
AsF_5	gas	298.15	−1169.6	−1236.8	317.26	97.541	Barin (1995)
AsH_3 (arsine)	gas	298.15	68.91	66.40	223.0	—	Pankratov and Uchaeva (2000)
AsH_3 (arsine)	gas	298.15	68.93	66.44	222.78	38.07	Wagman *et al*. (1982)
AsH_3 (arsine)	gas	298.15	68.83	66.4	223	—	Naumov, Ryzhenko and Khodakovsky (1974)
AsH_3 (arsine)	gas	298.15	69.109	66.442	222.78	38.072	Barin (1995)
AsI_3	xls	298.15	−59.4	−58.2	213.05	105.77	Wagman *et al*. (1982)
AsI_3	xls	298.15	−59.091	−58.158	213.05	105.77	Barin (1995)
AsI_3	gas	298.15	—	—	388.34	80.63	Wagman *et al*. (1982)
AsI_3	gas	298.15	−15.321	38.911	391.82	80.960	Barin (1995)
AsN	gas	298.15	167.97	196.27	225.6	30.42	Wagman *et al*. (1982)
AsO	gas	298.15	−84.715	−57.287	230.27	32.342	Barin (1995)
As_2O_3 (arsenolite, cubic)	xls	298.15	−576.34	−657.27	107.38	96.88	Nordstrom and Archer (2003)
As_2O_3 (arsenolite, cubic)	xls	298.15	−576	−657	107.4	—	Robie, Hemingway and Fisher (1979)
As_2O_3 (arsenolite, cubic)	xls	298.15	−588.3	−666.1	117	—	Naumov, Ryzhenko and Khodakovsky (1974)
As_2O_3 (arsenolite, cubic)	xls	298.15	−576.41	—	—	—	Davis *et al*. (1996)
As_2O_3 (arsenolite, cubic)	xls	298.15	−575.96	−656.97	107.41	96.878	Barin (1995)
As_2O_3 (claudetite, monoclinic)	xls	298.15	−576.53	−655.67	113.37	96.98	Nordstrom and Archer (2003)
As_2O_3 (claudetite, monoclinic)	xls	298.15	−576	−655	113.3	—	Robie, Hemingway and Fisher (1979)
As_2O_3 (claudetite, monoclinic)	xls	298.15	−589.1	−664.0	127	—	Naumov, Ryzhenko and Khodakovsky (1974)

As_2O_3 (claudetite, monoclinic)	xls	298.15	−576.64	−654.80	117.00	96.979	Barin (1995)
$As_2O_3 \cdot SO_3$	xls	298.15	—	−1194.32	—	—	Wagman *et al*. (1982)
As_2O_5	xls	298.15	−774.96	−917.59	105.44	115.9	Nordstrom and Archer (2003)
As_2O_5	xls	298.15	−782.0	−924.7	105	—	Naumov, Ryzhenko and Khodakovsky (1974)
As_2O_5	xls	298.15	−782.78	—	—	—	Davis *et al*. (1996)
As_2O_5	xls	298.15	−782.3	−924.87	105.4	116.52	Wagman *et al*. (1982)
As_2O_5	xls	298.15	−782.09	−924.87	105.40	116.54	Barin (1995)
As_2O_5	xls	400	−733.31	−924.59	142.62	136.54	Barin (1995)
As_2O_5	xls	500	−685.66	−922.93	174.77	151.78	Barin (1995)
$As_2O_5 \cdot 4H_2O$	xls	298.15	—	−2104.6	—	—	Wagman *et al*. (1982)
$As_2O_5 \cdot 4H_2O$	xls	298.15	−1720	—	—	—	Faure (1998)
$(As_2O_5)_3 \cdot 5H_2O$	xls	298.15	—	−4248.4	—	—	Wagman *et al*. (1982)
As_4O_6	gas	298.15	−1092.2	−1196.2	409.35	173.60	Barin (1995)
AsS (α, realgar)	xls	298.15	−31.3	−31.8	62.9	47	Nordstrom and Archer (2003)
AsS (α, realgar)	xls	298.15	−35	−36	63.5	—	Naumov, Ryzhenko and Khodakovsky (1974)
AsS (β)	xls	298.15	−30.9	−31.0	63.5	47	Nordstrom and Archer (2003)
$AsS(OH)(SH)^-$	aq	298.15	−245.11	—	—	—	Helz *et al*. (1995)
As_2S_3	am	298.15	−76.8	−66.9	200	—	Nordstrom and Archer (2003)
As_2S_3 (orpiment)	xls	298.15	−84.9	−85.8	163.8	163	Nordstrom and Archer (2003)
As_2S_3 (orpiment)	xls	298.15	−95.4	−96.2	164	—	Naumov, Ryzhenko and Khodakovsky (1974)
$As_3S_4(SH)_2^-$	aq	298.15	−127.19	—	—	—	Helz *et al*. (1995)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
As_2Se_3	xls	298.15	−88.4	−86.1	7.8	—	O'Hare *et al*. (1990)
As_2Se_3	xls	298.15	—	−81.1	—	—	O'Hare (1993)
As_2Se_3	xls	298.15	−101.43	−102.51	194.56	121.39	Barin (1995)
As_2Se_3	am	298.15	—	−53.1	—	—	O'Hare (1993)
As_2Te_3	xls	298.15	−39.580	−37.656	226.35	127.49	Barin (1995)
$Ba_3(AsO_4)_2$	xls	298.15	−3113.40	—	—	—	Zhu *et al*. (2005)
$Ba_3(AsO_4)_2$	xls	298.15	−3192.2	−3421.7	309.62	257.21	Barin (1995)
$BaHAsO_4·H_2O$	xls	298.15	−1544.47	—	—	—	Zhu *et al*. (2005)
$Be_3(AsO_4)_2$	xls	298.15	−2525.5	−2738.1	207.28	232.52	Barin (1995)
$BiAsO_4$	xls	298.15	−619	—	—	—	Wagman *et al*. (1982)
$BiAsO_4$	xls	298.15	−695.43	−795.21	168.07	121.12	Barin (1995)
$BiAsO_4$ (rooseveltite)	xls	298.15	−613.58	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$(CH_3)_3As$	gas	298.15	—	12	—	—	Pankratov and Uchaeva (2000)
$Ca(H_2AsO_4)_2$	xls	298.15	−2054	—	—	—	Ryu *et al*. (2002)
Ca_2AsO_4OH	xls	298.15	−1988	—	—	—	Ryu *et al*. (2002)
$Ca_3(AsO_4)_2$	xls	298.15	−3061	—	—	—	Ryu *et al*. (2002)
$Ca_3(AsO_4)_2$	xls	298.15	−3063.1	−3298.7	226.00	249.79	Barin (1995)
$Ca_3(AsO_4)_2$	xls	298.15	−3063.0	−3298.7	226	—	Wagman *et al*. (1982)
$Ca_3(AsO_4)_2·2.25H_2O$	xls	298.15	−3611.50	—	—	—	Zhu *et al*. (2006)
$Ca_3(AsO_4)_2·3H_2O$	xls	298.15	−3787.87	—	—	—	Zhu *et al*. (2006)
$Ca_3(AsO_4)_2·3.67H_2O$	xls	296	−3945	—	—	—	Bothe and Brown (1999)
$Ca_3(AsO_4)_2·4H_2O$	xls	298.15	−4019	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$Ca_3(AsO_4)_2·4.25H_2O$	xls	296	−4085	—	—	—	Bothe and Brown (1999)

$Ca_3(AsO_4)_2 \cdot 6H_2O$	xls	298.15	−2732	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$Ca_3(AsO_4)_2 \cdot 8H_2O$	xls	298.15	−3530	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$Ca_4(OH)_2(AsO_4)_2 \cdot 4H_2O$	xls	296	−4941	—	—	—	Bothe and Brown (1999)
$Ca_4(OH)_2(AsO_4)_2 \cdot 4H_2O$	xls	298.15	−4928.86	—	—	—	Zhu *et al*. (2006)
$Ca_5(AsO_4)_3OH$	xls	296	−5087	—	—	—	Bothe and Brown (1999)
$Ca_5(AsO_4)_3OH$	xls	298.15	−5096.47	—	—	—	Zhu *et al*. (2006)
$Ca_5H_2(AsO_4)_4$	xls	298.15	−5636.7	—	—	—	Ryu *et al*. (2002)
$Ca_5H_2(AsO_4)_4 \cdot 9H_2O$ (ferrarisite)	xls	296	−7808	—	—	—	Bothe and Brown (1999)
$Ca_5H_2(AsO_4)_4 \cdot 9H_2O$ (guerinite)	xls	296	−7803	—	—	—	Bothe and Brown (1999)
$CaH(AsO_4) \cdot H_2O$	xls	296	−1533	—	—	—	Bothe and Brown (1999)
$CaHAsO_4^0$	aq	298.15	—	−1446.0	—	—	Wagman *et al*. (1982)
$Cd_3(AsO_4)_2$	xls	298.15	−1716.1	—	—	—	Wagman *et al*. (1982)
$Cd_3(AsO_4)_2$	xls	298.15	−1712.0	−1934.3	301.71	258.82	Barin (1995)
Cd_3As_2	xls	298.15	—	−41.8	—	—	Wagman *et al*. (1982)
Cd_3As_2	xls	298.15	−35.885	−41.840	206.83	125.30	Barin (1995)
$CdAs_2$	xls	298.15	—	−17.6	—	—	Wagman *et al*. (1982)
CoAs	xls	298.15	—	−40.6	—	—	Wagman *et al*. (1982)
CoAs (modderite)	xls	298.15	−49	−51	59	—	Naumov, Ryzhenko and Khodakovsky (1974)
$CoAs_2$	xls	298.15	—	−61.5	—	—	Wagman *et al*. (1982)
$CoAs_2$ (safflorite)	xls	298.15	−97	−83	100	—	Naumov, Ryzhenko and Khodakovsky (1974)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
Co_2As	xls	298.15	—	−39.7	—	—	Wagman *et al*. (1982)
Co_2As_3	xls	298.15	—	−97.5	—	—	Wagman *et al*. (1982)
Co_3As_2	xls	298.15	—	−81.2	—	—	Wagman *et al*. (1982)
Co_5As_2	xls	298.15	—	−79.5	—	—	Wagman *et al*. (1982)
$Co_3(AsO_4)_2$	xls	298.15	−1620.8	—	—	—	Wagman *et al*. (1982)
$Co_3(AsO_4)_2$	xls	298.15	−1671.9	−1864.3	337.02	264.31	Barin (1995)
$CrAsO_4$	xls	298.15	−968.36	−1062.1	155.35	119.10	Barin (1995)
$Cr_3(AsO_4)_2$	xls	298.15	−2027.0	−2218.2	321.42	261.83	Barin (1995)
Cs_3AsO_4	xls	298.15	−1543.9	−1668.5	283.59	176.22	Barin (1995)
Cu_3As	xls	298.15	—	−11.7	—	—	Wagman *et al*. (1982)
Cu_3As	xls	298.15	−12.322	−11.715	137.24	93.080	Barin (1995)
$Cu_3(AsO_4)$	xls	298.15	−624.04	−710.36	255.98	176.36	Barin (1995)
—	xls	298.15	−1300.7	—	—	—	Wagman *et al*. (1982)
$Cu_3(AsO_4)_2$	xls	298.15	−1301.32	—	—	—	Davis *et al*. (1996)
$Cu_3(AsO_4)_2$	xls	298.15	−1316.0	−1522.6	298.61	258.21	Barin (1995)
$Cu_3(AsO_4)_2 \cdot 6H_2O$	xls	298.15	−2733.04	—	—	—	Davis *et al*. (1996)
Cu_3AsS_4 (enargite)	xls	298.15	−206.74	−179.0	356.4	—	Castro and Baltierra (2005) and Kantar (2002)
Cu_3AsS_4 (enargite)	xls	298.15	—	—	257.6	190.4	Seal *et al*. (1996)
Cu_3AsS_4 (enargite)	xls	298.15	−437.26	—	—	—	Davis *et al*. (1996)
$Fe_3(AsO_4)_2$	xls	298.15	−1753.93	—	—	—	Davis *et al*. (1996)
$Fe_3(AsO_4)_2 \cdot 8H_2O$ (symplesite)	xls	298.15	−3687.26	—	—	—	Davis *et al*. (1996)
FeAs (westerveldite)	xls	298.15	−43.36	−43.51	62.5	50.36	Perfetti *et al*. (2008)
$FeAs_2$ (loellingite)	xls	298.15	−52.09	−43.5	127		Naumov, Ryzhenko and Khodakovsky (1974)

$FeAsO_4$	xls	298.15	−772.39	−865.34	161.54	117.05	Barin (1995)
$FeAsO_4$	xls	298.15	−772.62	—	—	—	Ryu *et al*. (2002)
$FeAsO_4{\cdot}2H_2O$ (scorodite)	xls	298.15	−1280.1	—	—	—	Ryu *et al*. (2002)
$FeAsO_4{\cdot}2H_2O$ (scorodite)	xls	296	−1279.2	—	—	—	Krause and Ettel (1988)
$FeAsO_4{\cdot}2H_2O$ (scorodite)	xls	298.15	−1267.69	—	—	—	Davis *et al*. (1996)
$Fe_3(AsO_4)_2$	xls	298.15	−1766.0	−1955.0	339.91	264.64	Barin (1995)
FeAsS (arsenopyrite)	xls	298	−136.45	−144.36	68.5	68.44	Perfetti *et al*. (2008)
FeAsS (arsenopyrite)	xls	298	−141.6	—	—	—	Pokrovski, Kara and Roux (2002)
FeAsS (arsenopyrite)	xls	298.15	−127.25	—	—	—	Davis *et al*. (1996)
$FeAsS_2$ (loellingite)	xls	298.15	−80.23	−85.77	80.1	70.83	Perfetti *et al*. (2008)
$FeAsS_2$ (loellingite)	xls	298.15	−52.116	—	—	—	Davis *et al*. (1996)
GaAs (gallium arsenide)	xls	298.15	−67.8	−71	64.18	46.23	Wagman *et al*. (1982)
GaAs (gallium arsenide)	xls	298.15	−70.374	−74.057	64.183	46.858	Barin (1995)
GaAs (gallium arsenide)	xls	298.15	−67.8	−71	64.2	—	Naumov, Ryzhenko and Khodakovsky (1974)
$GaAsO_4$	xls	298.15	−901.85	−1002.2	150.12	118.26	Barin (1995)
$H_3AsO_3^0$	aq	298.15	−639.8	−737.3	212.4	85.0	Perfetti *et al*. (2008)
$H_3AsO_3^0$	aq	298.15	−640.03	−742.36	195.8	—	Nordstrom and Archer (2003)
$H_3AsO_3^0$	aq	298.15	−639.78	−740.82	200	197	Pokrovski *et al*. (1996)
$H_2AsO_3^-$	aq	298.15	−587.13	−714.79	110.5	—	Wagman *et al*. (1982)
$H_2AsO_3^-$	aq	298.15	−587.66	−714.74	112.79	—	Nordstrom and Archer (2003)
$HAsO_3^{2-}$	aq	298.15	−524	−689	−15	—	Dove and Rimstidt (1985)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
$HAsO_3^{2-}$	aq	298.15	−524.3	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
AsO_3^{3-}	aq	298.15	−448	−664	−187	—	Dove and Rimstidt (1985)
AsO_3^{3-}	aq	298.15	−447.7	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$H_3AsO_4^0$	aq	298.15	−766.3	−898.6	198.3	105.0	Perfetti *et al*. (2008)
$H_3AsO_4^0$	aq	298.15	−766.75	−903.45	183.07	—	Nordstrom and Archer (2003)
$H_2AsO_4^-$	aq	298.15	−753.17	−909.56	117	—	Wagman *et al*. (1982)
$H_2AsO_4^-$	aq	298.15	−753.65	−911.42	112.38	—	Nordstrom and Archer (2003)
$HAsO_4^{2-}$	aq	298.15	−713.73	−908.41	−11.42	—	Nordstrom and Archer (2003)
$HAsO_4^{2-}$	aq	298.15	−714.60	−906.34	—	—	Wagman *et al*. (1982)
AsO_4^{3-}	aq	298.15	−646.36	−890.21	−176.31	—	Nordstrom and Archer (2003)
$HAsO_3F^-$	aq	298.15	−1060.96	—	—	—	Wagman *et al*. (1982)
AsO_3F^{2-}	aq	298.15	−1027.45	—	—	—	Wagman *et al*. (1982)
$Hg_3(AsO_4)_2$	xls	298.15	−1033.6	−1271.0	323.47	261.72	Barin (1995)
InAs (indium arsenide)	xls	298.15	−53.6	−58.6	75.7	47.78	Wagman *et al*. (1982)
InAs (indium arsenide)	xls	298.15	−53.286	−58.601	75.701	47.780	Barin (1995)
InAs (indium arsenide)	xls	298.15	−52.7	−57.7	75.7	—	Naumov, Ryzhenko and Khodakovsky (1974)
$InAsO_4$	xls	298.15	−874.26	−978.30	154.85	119.32	Barin (1995)
KAs	xls	298.15	—	−102.9	—	—	Wagman *et al*. (1982)

KAs_2	xls	298.15	—	−127.2	—	—	Wagman *et al*. (1982)
K_3As	xls	298.15	—	−186.2	—	—	Wagman *et al*. (1982)
K_5As_4	xls	298.15	—	−452.7	—	—	Wagman *et al*. (1982)
KH_2AsO_4	xls	298.15	−1035.9	−1180.7	155.02	126.73	Wagman *et al*. (1982)
KH_2AsO_4	xls	298.15	−1041.6	−1186.2	155	—	Naumov, Ryzhenko and Khodakovsky (1974)
$K_3(AsO_4)$	xls	298.15	−1548.8	−1668.7	237.82	172.29	Barin (1995)
KUO_2AsO_4	xls	298.15	−2021.1	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$LaAsO_4$	xls	298.15	−1455.7	−1556.9	163.47	117.89	Barin (1995)
$Li_3(AsO_4)$	xls	298.15	−1595.0	−1702.4	173.13	161.84	Barin (1995)
$MgAs_4$	xls	298.15	—	−126	—	—	Wagman *et al*. (1982)
Mg_3As_2	xls	298.15	—	−371.5	—	—	Wagman *et al*. (1982)
$Mg_3(AsO_4)_2$	xls	298.15	—	−3092.8	—	—	Wagman *et al*. (1982)
$Mg_3(AsO_4)_2$	xls	298.15	−2775	—	—	—	Ryu *et al*. (2002)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
$Mg_3(AsO_4)_2$	xls	298.15	−2831.7	−3059.8	225.10	236.31	Barin (1995)
$Mg_3(AsO_4)_2 \cdot 10H_2O$	xls	298.15	−5147.2	—	—	—	Ryu *et al*. (2002)
$MgHAsO_4$	xls	298.15	−1187	—	—	—	Ryu *et al*. (2002)
$MgHAsO_4 \cdot 7H_2O$ (roesslerite)	xls	298.15	−2848	—	—	—	Ryu *et al*. (2002)
$MgNH_4AsO_4 \cdot 6H_2O$	xls	298.15	—	−3316.7	—	—	Wagman *et al*. (1982)
MnAs (α)	xls	298.15	−61.636	−51.861	107.00	71.116	Barin (1995)
MnAs (β)	xls	298.15	−59.865	−53.297	91.442	70.340	Barin (1995)
MnAs (γ)	xls	298.15	−59.691	−56.902	77.069	70.164	Barin (1995)
MnAs	xls	298.15	—	−59	—	—	Wagman *et al*. (1982)
MnAs (kaneite)	xls	298.15	−55.2	−57.3	60	—	Naumov, Ryzhenko and Khodakovsky (1974)
$Mn_3(AsO_4)_2$	xls	298.15	−2167.4	—	—	—	Ryu *et al*. (2002)
$Mn_3(AsO_4)_2$	xls	298.15	—	−2145.6	—	—	Wagman *et al*. (1982)
$Mn_3(AsO_4)_2$	xls	298.15	−2167.0	−2366.3	319.62	261.79	Barin (1995)
$Mn_3(AsO_4)_2 \cdot 8H_2O$	xls	298.15	−4055	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$MnHAsO_4$	xls	298.15	—	−1102.5	—	—	Wagman *et al*. (1982)
$MoAsO_4$	xls	298.15	−817.79	−910.69	163.01	120.06	Barin (1995)
NaAs	xls	298.15	−89.1	−96.2	62.8	—	Wagman *et al*. (1982)
$NaAs_2$	xls	298.15	−100.4	−106.7	100	—	Wagman *et al*. (1982)
Na_3As	xls	298.15	−187.4	−205	130	—	Wagman *et al*. (1982)
Na_3As	xls	298.15	−187.10	−205.02	130.00	97.769	Barin (1995)

$NaAsO_2$	xls	298.15	—	−660.53	—	—	Wagman *et al*. (1982)
$NaUO_2AsO_4 \cdot 4H_2O$	xls	298.15	−2944.6	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
Na_3AsO_4	xls	298.15	—	−1540	—	—	Wagman *et al*. (1982)
Na_3AsO_4	xls	298.15	−1426.0	−1540.0	217.94	170.13	Barin (1995)
$Na_3AsO_4 \cdot 12H_2O$	xls	298.15	—	−5092	—	—	Wagman *et al*. (1982)
NiAs (nickeline, niccolite)	xls	298.15	—	—	61	—	Naumov, Ryzhenko and Khodakovsky (1974)
NiAs	xls	298.15	−67.268	−73.291	45.380	56.001	Barin (1995)
$Ni_3(AsO_4)_2$	xls	298.15	−1579.3	—	—	—	Wagman *et al*. (1982)
$Ni_3(AsO_4)_2$	xls	298.15	−1659.4	−1849.2	344.80	265.41	Barin (1995)
$Ni_3(AsO_4)_2 \cdot 8H_2O$ (Annabergite)	xls	298.15	−3482	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
Ni_5As_2	xls	298.15	−242.11	−251.10	190.63	215.98	Barin (1995)
$Ni_{11}As_8$	xls	298.15	−762.63	−774.04	468.88	552.00	Barin (1995)
$NH_4H_2AsO_4$	xls	298.15	−832.9	−1059.8	172.05	151.17	Wagman *et al*. (1982)

(*continued overleaf*)

Table C.1 *(continued)*

Chemical species	Phase	Temperature (K)	Gibbs free energy (G_i) (kJ mol^{-1})	Enthalpy (H_i) (kJ mol^{-1})	Entropy (S_i) (J mol^{-1}·K^{-1})	Heat Capacity (Cp_i) (J mol^{-1}·K^{-1})	Reference
$NH_4H_2AsO_4$	xls	298.15	−837.34	−1064.1	172	—	Naumov, Ryzhenko and Khodakovsky (1974)
$(NH_4)_2HAsO_4$	xls	298.15	—	−1181.6	—	—	Wagman *et al*. (1982)
$(NH_4)_3AsO_4$	xls	298.15	—	−1286.2	—	—	Wagman *et al*. (1982)
$(NH_4)_3AsO_4 \cdot 3H_2O$	xls	298.15	—	−2166.9	—	—	Wagman *et al*. (1982)
$Pb_3(AsO_4)_2$	xls	298.15	−1553.1	−1780.2	324.60	258.00	Barin (1995)
$Pb_3(AsO_4)_2$	xls	298.15	−1580.01	—	—	—	Davis *et al*. (1996)
$Pb_3(AsO_4)_2$	xls	298.15	−1579.3	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$Pb_5(AsO_4)_3Cl$ (mimetite)	xls	298.15	−2616.25	—	—	—	Davis *et al*. (1996)
$Pb_5(AsO_4)_3OH$	xls	298.15	−2659	—	—	—	Lee and Nriagu (2007)
$PbHAsO_4$	xls	298.15	−805.66	—	—	—	Lee and Nriagu (2007)
$Rb_3(AsO_4)$	xls	298.15	−1547.0	−1669.0	267.06	175.28	Barin (1995)
Re_3As_7	xls	298.15	−88.624	−95.395	336.81	248.64	Barin (1995)
$ReAsO_4$	xls	298.15	−678.39	−771.57	170.00	121.37	Barin (1995)
$Sn_3(AsO_4)_2$	xls	298.15	−1564.6	−1785.8	303.93	259.1	Barin (1995)
$Sr_3(AsO_4)_2$	xls	298.15	−3094.4	−3317.1	312.1	257.6	Barin (1995)
$Ti_3(AsO_4)_2$	xls	298.15	−2547.3	−2617.3	339.4	264.5	Barin (1995)

$TlAsO_4$	xls	298.15	−885.81	−948.56	299.74	145.69	Barin (1995)
$YAsO_4$	xls	298.15	−1416.8	−1515.1	160.54	120.75	Barin (1995)
$Zn_3(AsO_4)_2$	xls	298.15	−1895.91	—	—	—	Davis *et al*. (1996)
$Zn_3(AsO_4)_2$	xls	298.15	−1895	—	—	—	Wagman *et al*. (1982)
$Zn_3(AsO_4)_2$	xls	298.15	−1915.6	−2134.7	281.92	255.28	Barin (1995)
$Zn_3(AsO_4)_2{\cdot}2.5H_2O$ (legrandite)	xls	298.15	−2611	—	—	—	Naumov, Ryzhenko and Khodakovsky (1974)
$ZnAs_2$	xls	298.15	—	−41.8	—	—	Wagman *et al*. (1982)
Zn_3As_2	xls	298.15	−125.46	−133.89	168.04	125.23	Barin (1995)
Zn_3As_2	xls	298.15	—	−32.2	—	—	Wagman *et al*. (1982)

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