Bureau International des Poids et Mesures

Guide to the Realization of the ITS-90

Fixed Points: Influence of Impurities

APPENDIX 2: *Distribution coefficients and liquidus-line slopes*

Consultative Committee for Thermometry
under the auspices of the
International Committee for Weights and Measures

APPENDIX 2

Distribution coefficients and liquidus-line slopes

This appendix contains a collation of the distribution coefficients and liquidus-line slopes of impurities in the fixed-point substances of the ITS-90. It will be a permanent task of the Consultative Committee for Thermometry to update this collation at short intervals.

The distribution-coefficient values k_0^i given in Table A2.1 are taken from the comprehensive review prepared by Pearce [2014]. These values are tabulated for two reasons. First, they show how effectively purification can be achieved by zone refining. Second, for many systems, liquidus-line slopes m_l^i can be estimated from k_0^i by applying the approximate Equation (6). But this should be done with caution. Depending on the data basis, the k_0^i values have a quite different confidence. This is discussed in detail in [Pearce 2014]. For values based on the mean of several determinations, the standard deviations are mostly smaller than 0.1, but in a few cases, they are even larger than one.

Table A2.2 shows aggregate values of liquidus-line slope values m_l^i published by Pearce *et al.* [2016], in terms of mass fraction concentration of the impurity. These values have been compiled from literature surveys and thermodynamic calculations. Expression of the liquidus-line slopes in terms of mass fraction is preferred in this table because chemical assays are typically expressed in terms of mass fraction. Further discussion of the values and their derivation is given in the associated publication.

Table A2.3 is based on the "*Critical review of information relevant to the correction of the effect of chemical impurities in gases used for the realization of ITS-90 fixed points*" published by Pavese [2009] and Appendix C *Reference Data on Gases* of the book "*Modern Gas-Based Temperature and Pressure Measurements*" written by Pavese and Molinar [2013]. Data for nitrogen is additionally included because the triple point of nitrogen is an often-used reference point in secondary scales. The two references give also general comments on the influence of further impurities not contained in Table A2.3.

Last updated 1 January 2018

References

Pavese F 2009 *Metrologia* **46** 47-61

Pavese F, Molinar Min Beciet G 2013 *Modern Gas-Based Temperature and Pressure Measurements* (Springer Science + Business Media, New York)

Pearce J V 2014 *Int. J. Thermophys*. **35** 628–635

Pearce J V, Gisby J A, Steur P P M 2016 *Metrologia* **53** 1101-1114

Table A2.1: Distribution-coefficient values k_0^i for impurities in the fixed-point materials of the ITS-90 taken from the comprehensive review prepared by Pearce [2014].

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
1	H						0.020			0.360
2	He		0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
3	Li			0.060	0.010	0.200	0.961	0.370	0.580	0.215
4	Be					0.103	0.177	0.227	0.018	0.270
5	B						0.099	0.002		0.051
6	C						0.001		0.009	0.127
7	N					0.451	0.019			0.000
8	O				0.000		0.654	0.050		0.017
9	F		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
10	Ne		0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000
11	Na		0.100	1.240	0.353	0.087	0.010	0.030	0.010	0.058
12	Mg			1.210	0.053	0.012	0.356	0.540	0.560	0.116
13	Al		0.050	0.000	0.368	0.390	1.000	0.660	0.205	0.965
14	Si		0.003	0.000	0.050	0.001	0.089	0.069	0.012	0.388
15	P		0.000	0.000	0.000	0.070	0.011	0.022	0.010	0.119
16	S		0.000	0.000	0.000	0.000	0.002	0.030	0.010	0.016
17	Cl		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
18	Ar		0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000
19	K		0.100	0.000	0.000	0.000	0.280	0.000	0.000	0.000
20	Ca		0.950	0.134	0.020	0.000	0.031	0.076	0.088	0.027
21	Sc		0.205	0.205	0.029	0.000	0.479	0.420	0.700	0.064
22	Ti		0.842	0.842	0.041	0.002	6.741	0.843	1.291	0.294
23	V		0.460	0.882	0.019	0.000	4.940	0.934	1.700	1.492
24	Cr		0.675	0.675	0.000	0.023	1.968	0.864	1.357	0.505
25	Mn		0.429	0.429	0.009	0.000	0.743	0.687	0.590	0.472
26	Fe		0.350	0.542	0.015	0.274	0.183	0.939	0.870	1.490
27	Co		0.100	0.000	0.031	0.388	0.016	2.195	0.893	1.443
28	Ni		0.100		0.027	0.503	0.195	0.734	0.700	2.942
29	Cu		0.003	0.030	0.014	1.361	0.367	0.521	0.383	1.000
30	Zn	1.000	0.075	0.303	0.068	1.000	0.512	0.449	0.428	0.705
31	Ga	0.000	1.000	0.192	0.192	0.088	0.146	0.375	0.110	0.580

Table A2.1: (Continued)

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
32	Ge		0.002	0.000	1.045	0.108	0.055	0.176	0.026	0.356
33	As		0.000	0.000	0.760	0.797	0.009	0.185	1.122	0.177
34	Se	0.000	0.000	0.000	0.000	0.000	0.003	0.109	0.010	0.006
35	Br	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002
36	Kr	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000
37	Rb	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000
38	Sr	0.000	0.000	0.000	0.000	0.000	0.026	0.008	0.010	0.009
39	Y	0.000	0.000	0.000	0.000	0.000	0.019	0.125	0.000	0.033
40	Zr		0.571	0.571	0.000	0.000	2.406	0.455	1.142	0.033
41	Nb		1.053	1.053	1.053	0.000	2.963	0.860	2.240	3.385
42	Mo		1.105	1.105	1.105	0.000	2.117	0.286	3.160	3.000
43	Tc		1.454	1.454	1.454	1.454	0.100	1.670	3.160	0.450
44	Ru		0.890	0.890	0.890	0.890	0.077	2.078	1.372	1.465
45	Rh		0.969	0.969	0.969	0.969	0.053	2.300	1.826	2.480
46	Pd		0.791	0.791	0.791	1.595	0.044	2.807	2.345	2.230
47	Ag	0.096	0.450	0.045	0.027	1.862	0.435	1.000	0.974	0.354
48	Cd	3.034	0.050	0.444	0.322	0.111	0.287	0.657	0.500	0.159
49	In		0.015	1.000	0.345	0.072	0.139	0.559	0.380	0.346
50	Sn		0.000	0.752	1.000	0.074	0.020	0.358	0.141	0.118
51	Sb		0.000	0.005	2.040	0.052	0.267	0.234	0.027	0.116
52	Te		0.000	2.820	0.000	0.000	0.035	0.080	0.002	0.011
53	J	0.020	0.020	0.020	0.020	0.000	0.020	0.020	0.020	0.020
54	Xe	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.000	0.000
55	Cs	0.020	0.020	0.020	0.020	0.020	0.003	0.000	0.000	0.000
56	Ba	0.020	0.020	0.020	0.020	0.020	0.003	0.001	0.000	0.003
57	La	0.020	0.020	0.020	0.020	0.020	0.010	0.005	0.009	0.060
58	Ce	0.020	0.020	0.020	0.029	0.020	0.002	0.021	0.007	0.030
59	Pr	0.020	0.020	0.020	0.020	0.020	0.002	0.003	0.000	0.080
60	Nd	0.020	0.020	0.020	0.020	0.167	0.001	0.020	0.012	0.035
61	Pm	0.020	0.020	0.020	0.020	0.020	0.000	0.000	0.000	0.070
62	Sm	0.020	0.020	0.020	0.020	0.020	0.020	0.038	0.017	0.108

Table A2.1: (Continued)

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
63	Eu	0.020	0.020	0.020	0.020	0.020	0.000	0.000	0.000	0.000
64	Gd	0.020	0.020	0.020	0.020	0.020	0.010	0.062	0.049	0.000
65	Tb	0.020	0.020	0.020	0.020	0.020	0.017	0.090	0.060	0.000
66	Dy	0.020	0.020	0.020	0.020	0.020	0.020	0.090	0.150	0.000
67	Ho	0.020	0.020	0.020	0.020	0.020	0.020	0.110	0.260	0.003
68	Er	0.020	0.020	0.020	0.020	0.020	0.020	0.210	0.190	0.000
69	Tm	0.020	0.020	0.020	0.020	0.020	0.008	0.215	0.250	0.000
70	Yb	0.020	0.020	0.020	0.020	0.020	0.040	0.115	0.240	0.002
71	Lu	0.020	0.020	0.020	0.020	0.020	0.000	0.280	0.330	0.000
72	Hf		0.840	0.840	0.840	0.000	4.087	0.100	0.898	0.057
73	Ta		1.687	1.687	1.687	0.000	8.555	0.700	0.570	8.000
74	W		1.432	1.432	1.432	1.432	2.557	1.290	0.850	3.300
75	Re		1.639	1.639	1.639	1.639	1.000	1.890	1.130	3.000
76	Os		1.407	1.407	1.407	1.407	0.031	2.487	1.410	2.764
77	Ir		0.992	0.992	0.992	0.992	0.030	2.017	1.690	2.528
78	Pt		0.003	0.260	0.807	0.807	0.310	3.240	1.971	1.875
79	Au			0.005	0.032	1.510	0.109	1.250	1.000	0.456
80	Hg	1.000	0.040	0.590	0.152	0.247	0.130	0.580	0.220	0.134
81	Tl		0.003	1.060	0.044	0.568	0.020	0.363	0.077	0.060
82	Pb	6.678	0.002	0.733	0.131	0.087	0.093	0.253	0.039	0.075
83	Bi	0.000	0.002	0.350	0.244	0.084	0.082	0.096	0.004	0.002
84	Po	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
85	At	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
86	Rn	0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.000	0.000
87	Fr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
88	Ra	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
89	Ac	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.025
90	Th	0.020	0.020	0.020	0.020	0.020	0.053	0.105	0.001	0.037
91	Pa	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020
92	U	0.020	0.020	0.020	0.020	0.289	0.004	0.205	0.025	0.025
93	Np	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020
94	Pu	0.020	0.020	0.020	0.020	0.020	0.004	0.050	0.020	0.014

Table A2.2: Liquidus-line slopes m_l^i for chemical impurities in fixed-point materials of the ITS-90 taken from Pearce *et al.* [2016]. The m_l^i values are given in units of mK / (mg kg^{-1}). Values are uniformly presented to two decimal places to improve readability, but they are not necessarily all significant.

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
1	H						-11.92			-55.81
2	He		-2.38	-13.46	-8.78		-4.53	-30.24	-58.60	
3	Li	-5.54	-1.37	-4.37	-4.03	-4.20	-0.79	-7.00	-16.94	-11.31
4	Be	-4.43	-1.05	-5.95	-3.97	-0.16	-2.09	-9.69	-18.04	-5.58
5	B	0.00	0.00	0.00	-3.31	-1.65	-2.25	-8.00	-20.95	-4.96
6	C	0.00	0.00	0.00	0.00	0.00	-0.75	10.00	-22.95	-2.81
7	N	0.00	0.00	0.00	0.00	-2.54	-1.28	-4.32	-16.67	-5.31
8	O	-2.47	-0.59	-3.35	-2.23	-1.11	-0.40	-14.88	19.95	-2.63
9	F					0.00				
10	Ne		-0.47	-2.67	-1.74		-0.90	-6.00	-11.62	
11	Na	-2.24	-0.39	-0.89	-1.16	-1.51	-0.78	-3.49	-6.34	-1.71
12	Mg	-1.63	-0.40	0.32	-1.44	-1.03	-0.49	-2.33	-4.91	-2.96
13	Al	0.00	-0.26	-1.98	-0.87	-0.92	0.00	-1.87	-14.56	-0.21
14	Si	0.00	-0.17	0.00	-0.75	-1.28	-0.63	-4.20	-10.17	-1.76
15	P	-1.29	0.00	0.00	-1.15	-1.15	-0.83	-5.76	-7.23	-2.11
16	S	-1.24	-0.15	-0.84	-1.11	-0.56	0.17	-3.34	-5.02	-2.73
17	Cl							-0.30		
18	Ar		-0.24	-1.35	-0.88		-0.45	-3.03	-5.87	
19	K	-1.01	-0.23	-1.37	-0.90	-0.91	-0.26	-1.66	-3.29	-1.02
20	Ca	-0.99	-0.13	-1.34	-1.02	2.42	-0.40	-2.81	-4.45	-1.99
21	Sc	-0.89	-0.21	-1.19	-0.80	-0.79	-0.22	-0.93	-0.95	-1.54
22	Ti	-0.83	0.00	-1.12	-0.70	-0.81	3.63	-0.26	2.04	-1.06
23	V	-0.79	-0.14	-1.05	0.00	-0.70	2.36	-0.16	1.56	0.87
24	Cr	-0.83	-0.19	-0.52	0.00	-1.64	0.84	1.26	2.25	-0.76
25	Mn	-0.24	-0.17	-0.98	-0.65	-0.60	0.02	-0.38	-0.85	-0.73
26	Fe	-0.72	-0.14	-0.96	-0.52	-0.58	-0.33	-0.58	-1.14	0.49
27	Co	-0.69	-0.15	-0.38	-0.59	-0.61	-0.28	1.98	-0.94	0.67
28	Ni	-0.68	-0.16	-0.92	-0.57	-0.60	-0.32	-0.67	-1.31	1.98
29	Cu	-0.63	-0.15	-0.75	-0.57	0.27	-0.25	-0.95	-1.48	0.00
30	Zn	-0.34	-0.13	-0.41	-0.50	0.00	-0.11	-1.17	-3.68	-0.30
31	Ga	-0.51	0.00	-0.49	-0.40	-0.51	-0.19	-0.95	-3.27	-0.51

Table A2.2: (Continued)

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
32	Ge	0.00	-0.13	-0.74	-0.36	-0.43	-0.23	-1.46	-3.95	-0.67
33	As	-0.54	0.00	0.00	-0.27	-0.46	-0.19	-1.32	-3.24	-0.85
34	Se	-0.50	-0.12	-0.68	-0.45	-0.23	-0.13	-1.67	-2.05	-1.06
35	Br					0.00	-0.23			-0.94
36	Kr		-0.11	-0.64	-0.42		-0.22	-1.44	-2.80	
37	Rb	-0.47	-0.11	-0.63	-0.42	-0.42	-0.16	-0.78	-1.83	-0.48
38	Sr	-0.45	-0.11	-0.62	-0.41	0.00	-0.21	-0.89	-3.50	-0.80
39	Y	-0.45	-0.11	-0.60	-0.40	-0.40	-0.20	-0.92	-0.50	-0.87
40	Zr	-0.45	-0.10	-0.59	-0.41	-1.64	1.11	-1.57	0.18	-0.79
41	Nb	0.00	-0.10	-0.58	0.00	-0.38	4.70	0.54	1.91	1.18
42	Mo	0.00	0.00	-0.56	-0.36	-0.37	0.79	-0.90	3.53	0.48
43	Tc	0.00	-0.10	-0.55	-0.37	-0.36	0.05	1.22	3.42	0.04
44	Ru	0.00	-0.09	-0.53	0.00	-0.35	0.86	0.49	0.32	0.58
45	Rh	-0.39	-0.09	-0.52	-0.35	-0.35	0.02	0.40	1.30	0.76
46	Pd	-0.37	-0.09	-0.50	-0.51	0.17	-0.10	1.50	3.64	0.73
47	Ag	-0.31	-0.10	-0.39	-0.33	0.30	-0.06	0.00	-0.07	-0.46
48	Cd	0.73	-0.07	-0.15	-0.21	-0.34	-0.15	-0.38	-1.45	-0.52
49	In	0.45	-0.08	0.00	-0.18	-0.38	-0.17	-0.47	-1.73	-0.48
50	Sn	2.10	-0.09	-0.09	0.00	-0.31	-0.15	-0.45	-2.19	-0.58
51	Sb	-0.33	0.00	-0.55	0.30	-0.33	-0.16	-0.89	-2.63	-0.55
52	Te	-0.31	-0.04	0.17	-0.28	0.47	-0.21	-0.74	-1.73	-0.34
53	J									
54	Xe		-0.07	-0.41	-0.27		-0.14	-0.92	-1.79	
55	Cs	-0.41	-0.07	-0.40	-0.30	-0.27	-0.10	-0.52	-0.54	-0.32
56	Ba	-0.29	-0.07	-0.39	-0.26	0.09	-0.17	-0.86	-0.59	-0.51
57	La	-0.29	-0.07	-0.41	-0.42	-0.26	-0.14	-0.78	-1.60	-0.68
58	Ce	-0.29	-0.07	-0.38	-0.40	-0.20	-0.15	-0.86	-1.96	-0.72
59	Pr	-0.28	-0.07	-0.38	-0.25	-0.31	-0.08	-0.85	-1.57	-0.58
60	Nd	-0.28	-0.07	-0.37	-0.25	-0.25	-0.14	-0.71	-0.89	-0.60
61	Pm									-0.47
62	Sm	-0.27	-0.06	-0.36	-0.62	-0.24	-0.12	-0.73	-1.53	-0.51

Table A2.2: (Continued)

		Fixed-point material								
Z	Element	Hg	Ga	In	Sn	Zn	Al	Ag	Au	Cu
63	Eu	-0.26	-0.06	-0.35	-0.24	-0.24	-0.12	-0.94	-1.80	-0.64
64	Gd	-0.25	-0.06	-0.34	-0.23	-0.23	-0.08	-0.67	-0.60	-0.39
65	Tb	-0.25	-0.06	-0.34	-0.23	-0.22	-0.11	-0.79	-1.41	-0.47
66	Dy	-0.25	-0.06	-0.33	-0.56	-0.22	-0.10	-0.73	-1.91	-0.54
67	Ho	-0.26	-0.06	-0.33	-0.22	-0.22	-0.11	-0.66	-0.58	-0.45
68	Er		-0.06	-0.32	-0.21	-0.21	-0.10	-0.74	-1.26	-0.40
69	Tm	-0.24	-0.06	-0.32	-0.21	-0.21	-0.10	-0.67	-1.20	-0.44
70	Yb	-0.23	-0.06	-0.31	-0.24	-0.21	-0.04	-0.69	-1.06	-0.40
71	Lu	-0.23	-0.05	-0.31	-0.21	-0.20	-0.10	-0.62	-1.11	-0.42
72	Hf	0.00	-0.05	-0.30	-0.20	-0.20	2.39	0.00	-0.14	-0.33
73	Ta	0.00	-0.05	-0.30	-0.20	-0.20	1.61	0.12	-0.23	1.45
74	W	0.00	0.00	0.00	-0.20	-0.13	1.40	0.00	2.86	0.89
75	Re	0.00	-0.05	-0.29	-0.19	-0.10	0.10	0.62	0.96	0.54
76	Os	0.00	0.00	-0.28	-0.19	-0.19	0.40	0.25	3.69	1.11
77	Ir	0.00	-0.05	-0.28	-0.19	-0.19	0.38	0.03	3.44	0.56
78	Pt	-0.21	-0.02	-0.24	-0.31	-0.40	-0.02	1.37	1.25	0.28
79	Au	-0.23	-0.05	-0.27	-0.13	0.20	-0.10	0.15	0.00	-0.17
80	Hg	0.00	-0.04	-0.13	-0.14	-0.12	-0.05	-0.31	-1.07	-0.54
81	Tl	-0.14	-0.05	-0.07	-0.14	-0.15	-0.05	-0.48	-1.02	-0.34
82	Pb	0.49	-0.05	0.00	-0.15	-0.49	-0.05	-0.57	-1.20	-0.39
83	Bi	-0.19	-0.06	-0.16	-0.10	-0.14	-0.13	-0.62	-1.13	-0.46
84	Po				-0.11					
85	At									
86	Rn		-0.04	-0.24	-0.16		-0.08	-0.55	-1.06	
87	Fr									
88	Ra									
89	Ac									-0.32
90	Th	-0.17	-0.04	-0.23	-0.15	-0.15	-0.08	-0.10	-0.56	-0.25
91	Pa	-0.17	-0.04	-0.23	-0.16	-0.15	-0.08	-0.52	-1.01	-0.32
92	U	-0.17	-0.04	-0.23	-0.15	-0.15	-0.07	-0.25	-0.83	0.12
93	Np	-0.17	-0.04	-0.23	-0.15	-0.15	-0.08	-0.51	-0.98	-0.31
94	Pu	-0.16	-0.04	0.09	-0.15	-0.15	-0.05	-0.09	-0.96	-0.58

Table A2.3: Distribution coefficients k_0^i and liquidus-line slopes m_l^i for chemical impurities in gases used for the realization of temperature fixed points at low temperatures. The m_l^i values are given in μK / ppm[1].

	Fixed-point material								
	H_2		Ne		N_2		O_2		Ar
Impurity	m_l μK/ppm	k_0	m_l μK/ppm	k_0	m_l μK/ppm	k_0	m_l μK/ppm	k_0	m_l μK/ppm
Ar				0.8	–4.5	1	12		
CH_4				1	–3		< –30	0.3	–25
CO				4	8			0.5	–24
F_2								< 0.1	–10
H_2			–7						
He	–11						1.5		
Kr					25	0.6	–5	1	5
O_2				0.5	–15			0.6	–22
Ne	–2						–1		0
N_2		0.4	–7			0.6	–22	0.4	–22
Xe						0.3	–8		–6

[1] ppm is the abbreviation for parts per million