

Table S1 The calculated $1000\ln(\beta)$ ($^{124/116}\text{Sn}$ and $^{122/116}\text{Sn}$) of 10 configurations for each Sn-bearing aqueous species

$(^{124/116}\text{Sn}) \text{Sn}^{2+}\text{CO}_3\cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	4.370	4.370	4.181	4.171	4.171	4.390	4.102	4.181	4.102	4.171	4.221
25	3.703	3.703	3.544	3.534	3.534	3.723	3.474	3.544	3.474	3.534	3.577
50	3.175	3.175	3.045	3.035	3.035	3.195	2.986	3.045	2.986	3.035	3.071
75	2.756	2.756	2.646	2.637	2.637	2.766	2.587	2.637	2.587	2.637	2.665
100	2.417	2.417	2.317	2.307	2.307	2.427	2.267	2.317	2.267	2.307	2.335
125	2.128	2.128	2.038	2.038	2.038	2.138	1.998	2.038	1.998	2.038	2.058
150	1.888	1.888	1.818	1.808	1.808	1.898	1.778	1.818	1.778	1.808	1.829
175	1.699	1.699	1.629	1.619	1.619	1.699	1.589	1.629	1.589	1.619	1.639
200	1.529	1.529	1.459	1.459	1.459	1.529	1.429	1.459	1.429	1.459	1.474
225	1.379	1.379	1.319	1.319	1.319	1.389	1.299	1.319	1.299	1.319	1.334
250	1.249	1.249	1.199	1.199	1.199	1.259	1.179	1.199	1.179	1.199	1.211
275	1.139	1.139	1.099	1.089	1.089	1.149	1.079	1.099	1.079	1.089	1.105
300	1.049	1.049	1.009	1.000	1.000	1.049	0.990	1.009	0.990	1.000	1.015
325	0.960	0.960	0.930	0.920	0.920	0.970	0.910	0.930	0.910	0.920	0.933
350	0.890	0.890	0.850	0.850	0.850	0.890	0.840	0.850	0.840	0.850	0.860
375	0.820	0.820	0.790	0.790	0.790	0.830	0.770	0.790	0.780	0.790	0.797
400	0.760	0.760	0.730	0.730	0.730	0.770	0.720	0.730	0.720	0.730	0.738
$(^{122/116}\text{Sn}) \text{Sn}^{2+}\text{CO}_3\cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	3.334	3.334	3.195	3.185	3.185	3.344	3.125	3.185	3.125	3.175	3.219
25	2.826	2.826	2.706	2.696	2.696	2.836	2.646	2.706	2.646	2.696	2.728
50	2.427	2.427	2.317	2.317	2.317	2.437	2.277	2.317	2.277	2.307	2.342

75	2.098	2.098	2.018	2.008	2.008	2.108	1.968	2.018	1.968	2.008	2.030
100	1.838	1.838	1.758	1.758	1.758	1.848	1.729	1.758	1.729	1.758	1.777
125	1.619	1.619	1.559	1.549	1.549	1.629	1.529	1.559	1.529	1.549	1.569
150	1.439	1.439	1.379	1.379	1.379	1.449	1.359	1.379	1.359	1.379	1.394
175	1.289	1.289	1.239	1.229	1.239	1.299	1.209	1.239	1.209	1.229	1.247
200	1.159	1.159	1.109	1.109	1.109	1.169	1.089	1.109	1.089	1.109	1.121
225	1.049	1.049	1.009	1.009	1.009	1.059	0.990	1.009	0.990	1.000	1.017
250	0.960	0.960	0.920	0.910	0.910	0.960	0.900	0.920	0.900	0.910	0.925
275	0.870	0.870	0.840	0.830	0.830	0.880	0.820	0.840	0.820	0.830	0.843
300	0.800	0.800	0.770	0.760	0.760	0.800	0.750	0.770	0.750	0.760	0.772
325	0.730	0.730	0.710	0.700	0.700	0.740	0.690	0.710	0.690	0.700	0.710
350	0.680	0.680	0.650	0.650	0.650	0.680	0.640	0.650	0.640	0.650	0.657
375	0.630	0.630	0.600	0.600	0.600	0.630	0.590	0.600	0.590	0.600	0.607
400	0.580	0.580	0.560	0.560	0.560	0.590	0.550	0.560	0.550	0.560	0.565

$(^{124/116}\text{Sn}) \text{Sn}^{2+}\text{Cl}_3^- \cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	3.477	3.229	3.229	2.995	3.142	3.384	2.976	2.836	3.045	2.956	3.127
25	2.937	2.726	2.726	2.527	2.651	2.856	2.507	2.397	2.567	2.497	2.639
50	2.512	2.332	2.332	2.161	2.267	2.447	2.148	2.048	2.198	2.128	2.257
75	2.173	2.017	2.017	1.868	1.960	2.118	1.858	1.768	1.898	1.838	1.952
100	1.898	1.761	1.761	1.632	1.712	1.848	1.619	1.549	1.659	1.609	1.705
125	1.672	1.552	1.552	1.437	1.508	1.629	1.429	1.359	1.459	1.419	1.502
150	1.484	1.377	1.377	1.275	1.337	1.449	1.269	1.209	1.299	1.259	1.334
175	1.325	1.230	1.230	1.139	1.194	1.289	1.139	1.079	1.159	1.119	1.190
200	1.191	1.106	1.106	1.023	1.073	1.159	1.019	0.970	1.039	1.009	1.070

225	1.076	1.000	1.000	0.925	0.970	1.049	0.920	0.880	0.940	0.910	0.967
250	0.978	0.908	0.908	0.840	0.881	0.950	0.840	0.800	0.850	0.830	0.879
275	0.892	0.828	0.828	0.766	0.803	0.870	0.760	0.730	0.780	0.750	0.801
300	0.817	0.758	0.758	0.701	0.736	0.800	0.700	0.670	0.710	0.690	0.734
325	0.750	0.697	0.697	0.645	0.676	0.730	0.640	0.610	0.660	0.630	0.674
350	0.692	0.643	0.643	0.594	0.623	0.670	0.590	0.560	0.600	0.590	0.621
375	0.640	0.594	0.594	0.550	0.577	0.620	0.550	0.520	0.560	0.540	0.575
400	0.594	0.551	0.551	0.510	0.535	0.580	0.510	0.480	0.520	0.500	0.533

$(^{122/116}\text{Sn}) \text{ Sn}^{2+}\text{Cl}_3^- \cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	2.650	2.461	2.461	2.282	2.395	2.577	2.267	2.168	2.317	2.247	2.383
25	2.237	2.078	2.078	1.926	2.021	2.178	1.918	1.828	1.958	1.898	2.012
50	1.914	1.777	1.777	1.647	1.729	1.868	1.639	1.559	1.679	1.629	1.722
75	1.656	1.538	1.538	1.424	1.494	1.609	1.419	1.349	1.449	1.399	1.488
100	1.447	1.343	1.343	1.243	1.305	1.409	1.239	1.179	1.269	1.229	1.301
125	1.274	1.183	1.183	1.095	1.149	1.239	1.089	1.039	1.109	1.079	1.144
150	1.130	1.049	1.049	0.972	1.019	1.099	0.970	0.920	0.990	0.960	1.016
175	1.010	0.938	0.938	0.868	0.911	0.990	0.860	0.820	0.880	0.860	0.908
200	0.908	0.843	0.843	0.780	0.819	0.890	0.780	0.740	0.790	0.770	0.816
225	0.821	0.762	0.762	0.705	0.740	0.800	0.700	0.670	0.720	0.690	0.737
250	0.745	0.692	0.692	0.640	0.671	0.730	0.640	0.610	0.650	0.630	0.670
275	0.680	0.631	0.631	0.584	0.612	0.660	0.580	0.550	0.590	0.580	0.610
300	0.622	0.578	0.578	0.535	0.561	0.610	0.530	0.510	0.540	0.530	0.559
325	0.572	0.531	0.531	0.491	0.515	0.560	0.490	0.470	0.500	0.480	0.514
350	0.527	0.490	0.490	0.453	0.475	0.510	0.450	0.430	0.460	0.450	0.474

375	0.488	0.453	0.453	0.419	0.439	0.480	0.420	0.400	0.430	0.410	0.439
400	0.453	0.420	0.420	0.389	0.408	0.440	0.390	0.370	0.400	0.380	0.407

$(^{124/116}\text{Sn}) \text{ Sn}^{2+}\text{F}_3\cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	5.455	5.172	5.505	5.485	5.187	5.515	5.316	5.236	5.505	5.127	5.350
25	4.619	4.378	4.659	4.639	4.390	4.669	4.500	4.440	4.659	4.341	4.529
50	3.962	3.753	4.002	3.982	3.763	4.002	3.863	3.803	3.992	3.723	3.885
75	3.434	3.252	3.464	3.444	3.265	3.474	3.344	3.295	3.464	3.225	3.366
100	3.005	2.844	3.025	3.015	2.856	3.035	2.926	2.876	3.025	2.826	2.943
125	2.646	2.508	2.666	2.656	2.517	2.676	2.577	2.537	2.666	2.487	2.594
150	2.357	2.228	2.367	2.357	2.237	2.377	2.287	2.257	2.367	2.208	2.304
175	2.108	1.991	2.118	2.108	1.998	2.128	2.048	2.018	2.118	1.978	2.061
200	1.888	1.791	1.908	1.898	1.798	1.918	1.838	1.808	1.908	1.778	1.853
225	1.709	1.619	1.729	1.719	1.619	1.729	1.669	1.639	1.719	1.609	1.676
250	1.559	1.471	1.569	1.559	1.479	1.569	1.509	1.489	1.569	1.459	1.523
275	1.419	1.342	1.429	1.419	1.349	1.439	1.379	1.359	1.429	1.329	1.389
300	1.299	1.229	1.309	1.299	1.229	1.309	1.269	1.239	1.309	1.219	1.271
325	1.199	1.130	1.199	1.199	1.129	1.209	1.159	1.139	1.199	1.119	1.168
350	1.099	1.042	1.109	1.099	1.049	1.119	1.069	1.059	1.109	1.039	1.079
375	1.019	0.965	1.029	1.019	0.970	1.029	0.990	0.980	1.029	0.960	0.999
400	0.950	0.895	0.950	0.950	0.900	0.960	0.920	0.910	0.950	0.890	0.928

$(^{122/116}\text{Sn}) \text{ Sn}^{2+}\text{F}_3\cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	4.151	3.942	4.201	4.181	3.952	4.201	4.052	3.992	4.191	3.912	4.078

25	3.524	3.337	3.554	3.534	3.344	3.564	3.434	3.384	3.554	3.315	3.454
50	3.015	2.861	3.045	3.035	2.866	3.055	2.946	2.896	3.045	2.836	2.960
75	2.617	2.478	2.637	2.627	2.487	2.646	2.547	2.507	2.637	2.457	2.564
100	2.287	2.168	2.307	2.297	2.178	2.317	2.228	2.198	2.307	2.148	2.244
125	2.018	1.911	2.038	2.028	1.918	2.038	1.968	1.938	2.038	1.898	1.979
150	1.798	1.698	1.808	1.798	1.699	1.818	1.748	1.719	1.808	1.689	1.758
175	1.599	1.518	1.619	1.609	1.519	1.619	1.559	1.539	1.619	1.509	1.571
200	1.439	1.365	1.449	1.449	1.369	1.459	1.409	1.379	1.449	1.359	1.413
225	1.309	1.234	1.309	1.309	1.239	1.319	1.269	1.249	1.309	1.229	1.278
250	1.189	1.121	1.189	1.189	1.119	1.199	1.149	1.129	1.189	1.109	1.158
275	1.079	1.022	1.089	1.079	1.029	1.089	1.049	1.039	1.089	1.019	1.058
300	0.990	0.937	1.000	0.990	0.940	1.000	0.960	0.950	1.000	0.930	0.970
325	0.910	0.862	0.920	0.910	0.860	0.920	0.890	0.870	0.920	0.860	0.892
350	0.840	0.795	0.850	0.840	0.800	0.850	0.820	0.800	0.850	0.790	0.824
375	0.780	0.735	0.780	0.780	0.740	0.790	0.760	0.740	0.780	0.730	0.762
400	0.720	0.682	0.730	0.720	0.680	0.730	0.700	0.690	0.730	0.680	0.706

$(^{124/116}\text{Sn}) \text{Sn}^{2+}(\text{OH})_2 \cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	4.948	5.090	5.177	5.137	5.017	5.614	5.047	5.196	5.435	5.276	5.194
25	4.191	4.318	4.390	4.360	4.251	4.769	4.281	4.410	4.619	4.480	4.407
50	3.603	3.707	3.773	3.743	3.653	4.092	3.673	3.783	3.962	3.843	3.783
75	3.125	3.217	3.275	3.245	3.165	3.554	3.195	3.285	3.444	3.334	3.284
100	2.736	2.817	2.866	2.846	2.776	3.115	2.796	2.876	3.015	2.926	2.877
125	2.417	2.486	2.527	2.507	2.447	2.746	2.467	2.537	2.656	2.577	2.537
150	2.148	2.211	2.247	2.228	2.178	2.447	2.188	2.257	2.367	2.297	2.257

175	1.918	1.978	2.008	1.998	1.948	2.188	1.958	2.018	2.118	2.058	2.019
200	1.729	1.780	1.808	1.798	1.748	1.968	1.768	1.818	1.908	1.848	1.817
225	1.559	1.610	1.639	1.629	1.589	1.778	1.599	1.649	1.719	1.669	1.644
250	1.419	1.464	1.489	1.479	1.439	1.619	1.449	1.499	1.569	1.519	1.495
275	1.299	1.336	1.359	1.349	1.319	1.479	1.329	1.369	1.429	1.389	1.366
300	1.189	1.224	1.249	1.239	1.209	1.359	1.209	1.249	1.309	1.269	1.251
325	1.089	1.125	1.149	1.139	1.109	1.249	1.119	1.149	1.209	1.169	1.151
350	1.009	1.038	1.059	1.049	1.019	1.149	1.029	1.059	1.109	1.079	1.060
375	0.930	0.962	0.980	0.970	0.950	1.059	0.950	0.980	1.029	1.000	0.981
400	0.870	0.893	0.910	0.900	0.880	0.990	0.890	0.910	0.960	0.930	0.913

$(^{122/116}\text{Sn}) \text{ Sn}^{2+}(\text{OH})_2 \cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	3.763	3.879	3.942	3.912	3.823	4.281	3.853	3.962	4.141	4.022	3.958
25	3.195	3.291	3.344	3.324	3.245	3.633	3.265	3.364	3.514	3.414	3.359
50	2.746	2.826	2.876	2.856	2.786	3.115	2.806	2.886	3.025	2.936	2.886
75	2.377	2.452	2.497	2.477	2.417	2.706	2.427	2.507	2.627	2.547	2.503
100	2.088	2.147	2.188	2.168	2.118	2.367	2.128	2.188	2.297	2.228	2.192
125	1.838	1.895	1.928	1.908	1.868	2.098	1.878	1.938	2.028	1.968	1.935
150	1.639	1.685	1.719	1.699	1.659	1.858	1.669	1.719	1.798	1.748	1.719
175	1.459	1.508	1.529	1.519	1.479	1.669	1.499	1.539	1.609	1.569	1.538
200	1.319	1.357	1.379	1.369	1.339	1.499	1.349	1.389	1.449	1.409	1.386
225	1.189	1.227	1.249	1.239	1.209	1.359	1.219	1.249	1.309	1.269	1.252
250	1.079	1.115	1.139	1.129	1.099	1.229	1.109	1.139	1.189	1.159	1.139
275	0.990	1.018	1.039	1.029	1.000	1.129	1.009	1.039	1.089	1.059	1.040
300	0.910	0.933	0.950	0.940	0.920	1.029	0.930	0.950	1.000	0.970	0.953

325	0.830	0.858	0.870	0.870	0.840	0.950	0.850	0.880	0.920	0.890	0.876
350	0.770	0.792	0.810	0.800	0.780	0.880	0.790	0.810	0.850	0.820	0.810
375	0.710	0.733	0.750	0.740	0.720	0.810	0.730	0.750	0.790	0.760	0.749
400	0.660	0.681	0.690	0.690	0.670	0.750	0.670	0.700	0.730	0.710	0.695

$(^{124/116}\text{Sn}) \text{ Sn}^{4+}\text{Cl}_4 \cdot 50\text{H}_2\text{O}$											
T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	9.059	9.009	9.089	8.999	8.930	8.960	8.940	9.049	8.950	8.940	8.993
25	7.680	7.641	7.710	7.631	7.581	7.591	7.581	7.680	7.591	7.581	7.627
50	6.588	6.558	6.618	6.558	6.509	6.509	6.499	6.588	6.509	6.509	6.545
75	5.714	5.684	5.743	5.684	5.644	5.644	5.644	5.714	5.644	5.644	5.676
100	4.997	4.978	5.027	4.978	4.938	4.938	4.938	5.007	4.938	4.938	4.968
125	4.410	4.390	4.440	4.390	4.360	4.360	4.360	4.420	4.360	4.360	4.385
150	3.922	3.902	3.942	3.902	3.882	3.872	3.872	3.922	3.872	3.872	3.896
175	3.504	3.494	3.534	3.494	3.474	3.464	3.464	3.514	3.464	3.464	3.487
200	3.155	3.145	3.175	3.145	3.125	3.115	3.115	3.155	3.115	3.115	3.136
225	2.856	2.846	2.876	2.846	2.826	2.816	2.816	2.856	2.816	2.816	2.837
250	2.597	2.587	2.607	2.587	2.567	2.557	2.557	2.597	2.567	2.567	2.579
275	2.367	2.357	2.387	2.357	2.347	2.337	2.337	2.367	2.337	2.337	2.353
300	2.168	2.158	2.188	2.158	2.148	2.138	2.138	2.168	2.138	2.148	2.155
325	1.998	1.988	2.008	1.988	1.978	1.968	1.968	1.998	1.968	1.968	1.983
350	1.838	1.828	1.848	1.828	1.818	1.818	1.818	1.838	1.818	1.818	1.827
375	1.699	1.699	1.719	1.699	1.689	1.679	1.679	1.709	1.679	1.679	1.693
400	1.579	1.569	1.589	1.569	1.569	1.559	1.559	1.579	1.559	1.559	1.569

$$(^{122/116}\text{Sn}) \text{ Sn}^{4+}\text{Cl}_4 \cdot 50\text{H}_2\text{O}$$

T(°C)	1	2	3	4	5	6	7	8	9	10	Mean
0	6.906	6.866	6.926	6.856	6.807	6.827	6.807	6.896	6.827	6.817	6.854
25	5.853	5.823	5.883	5.823	5.773	5.783	5.773	5.853	5.783	5.773	5.812
50	5.017	4.997	5.047	4.997	4.958	4.968	4.958	5.017	4.968	4.958	4.989
75	4.351	4.331	4.380	4.331	4.301	4.301	4.301	4.360	4.301	4.301	4.326
100	3.813	3.793	3.833	3.793	3.763	3.763	3.763	3.813	3.763	3.763	3.786
125	3.364	3.344	3.384	3.344	3.324	3.324	3.324	3.364	3.324	3.324	3.342
150	2.986	2.976	3.005	2.976	2.956	2.956	2.946	2.996	2.956	2.956	2.971
175	2.676	2.666	2.686	2.666	2.646	2.637	2.637	2.676	2.646	2.646	2.658
200	2.407	2.397	2.417	2.397	2.377	2.377	2.377	2.407	2.377	2.377	2.391
225	2.178	2.168	2.188	2.168	2.148	2.148	2.148	2.178	2.148	2.148	2.162
250	1.978	1.968	1.988	1.968	1.958	1.948	1.948	1.978	1.948	1.958	1.964
275	1.808	1.798	1.818	1.798	1.788	1.778	1.778	1.808	1.778	1.778	1.793
300	1.649	1.649	1.669	1.649	1.639	1.629	1.629	1.659	1.629	1.629	1.643
325	1.519	1.509	1.529	1.509	1.509	1.499	1.499	1.519	1.499	1.499	1.509
350	1.399	1.399	1.409	1.399	1.389	1.379	1.379	1.399	1.389	1.389	1.393
375	1.299	1.289	1.309	1.289	1.289	1.279	1.279	1.299	1.279	1.279	1.289
400	1.199	1.199	1.209	1.199	1.189	1.189	1.189	1.209	1.189	1.189	1.196

Table S2 The calculated $1000\ln(\beta)$ values for minerals and Sn-bearing species in solution at different temperature.

Speciation	$1000\ln^{124/116}\beta$ (‰)				$1000\ln^{122/116}\beta$ (‰)			
	25 °C	100 °C	200 °C	350 °C	25 °C	100 °C	200 °C	350 °C
Cassiterite	11.128	7.244	4.570	2.666	8.474	5.525	3.484	2.028
Malayaite	11.434	7.482	4.739	2.766	8.712	5.694	3.604	2.108
Stannite	3.225	2.068	1.299	0.750	2.457	1.579	0.990	0.570
$\text{Sn}^{2+}\text{Cl}_3^-(\text{H}_2\text{O})_{50}$	2.639 ± 0.14	1.705 ± 0.09	1.070 ± 0.05	0.620 ± 0.03	2.012 ± 0.10	1.301 ± 0.06	0.816 ± 0.04	0.473 ± 0.02
$\text{Sn}^{2+}\text{CO}_3(\text{H}_2\text{O})_{50}$	3.577 ± 0.07	2.335 ± 0.05	1.474 ± 0.03	0.860 ± 0.02	2.728 ± 0.06	1.777 ± 0.04	1.121 ± 0.02	0.657 ± 0.01
Sn^{2+} $(\text{OH})_2(\text{H}_2\text{O})_{50}$	4.407 ± 0.13	2.877 ± 0.08	1.818 ± 0.05	1.060 ± 0.03	3.359 ± 0.09	2.192 ± 0.06	1.386 ± 0.04	0.810 ± 0.02
$\text{Sn}^{2+}\text{F}_3^-(\text{H}_2\text{O})_{50}$	4.530 ± 0.12	2.943 ± 0.07	1.854 ± 0.05	1.080 ± 0.02	3.454 ± 0.09	2.243 ± 0.05	1.413 ± 0.03	0.823 ± 0.02
$\text{Sn}^{4+}\text{Cl}_4(\text{H}_2\text{O})_{50}$	7.627 ± 0.04	4.968 ± 0.02	3.136 ± 0.01	1.827 ± 0.008	5.812 ± 0.03	3.786 ± 0.02	2.391 ± 0.01	1.393 ± 0.007

Table S3 $1000\ln(\alpha)^{124}\text{Sn}_{\text{A-B}}$ values between Sn-bearing species in solution and minerals at 25 °C.

	Cassiterite	Malayaite	Stannite	$\text{Sn}^{2+}\text{Cl}_3^-$	$\text{Sn}^{2+}\text{CO}_3\cdot$	$\text{Sn}^{2+}(\text{OH})_2$	$\text{Sn}^{2+}\text{F}_3^-$	$\text{Sn}^{4+}\text{Cl}_4$
Cassiterite	0	-0.306	7.903	8.489	7.511	6.721	6.598	3.501
Malayaite		0	8.209	8.795	7.857	7.027	6.904	3.807
Stannite			0	0.586	-0.352	-1.182	-1.305	-4.402
$\text{Sn}^{2+}\text{Cl}_3^-$				0	-	-	-	-
					0.938±0.09	1.768±0.19	1.891±0.15	4.988±0.13
$\text{Sn}^{2+}\text{CO}_3$					0	-	-	-
						0.830±0.14	0.953±0.13	4.050±0.07
Sn^{2+}						0	-	-
$(\text{OH})_2$							0.123±0.14	3.220±0.15
$\text{Sn}^{2+}\text{F}_3^-$							0	-
								3.097±0.11
$\text{Sn}^{4+}\text{Cl}_4$								0