

Supporting Information

High throughput identification of complex rutile alloys for the acidic oxygen evolution reaction

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Physical Vapor Deposition (PVD) library Synthesis

Each composition library (Mn-Sb-O, Mn-Sb-Sn-O, Mn-Sb-Ti-O, Mn-Sb-Sn-Ti-O, and Mn-Sb-Co-O) was synthesized via reactive RF magnetron co-sputtering from elemental metal targets (Mn, Sb, Sn, Ti, and Co) in a custom-designed combinatorial sputtering system, and post-deposition annealed in air at 700 °C for 3 h, followed by free cooling to near-ambient temperature. The deposition atmosphere was composed of 4.8 mTorr Ar and 1.2 mTorr O₂. The RF powers, as shown in Table S1, were adjusted to obtain designed composition in the wafer center and the non-confocal geometry of sputter sources provided a continuous composition gradient across 100 mm-diameter Si wafer with thermal oxide, Ti adhesion layer, and Pt conducting layer (Pt/Ti/SiO₂/Si substrates).

Table S1. Summary of RF powers used on each sputter source for 5 composition libraries.

Plate	Elements	RF power supply (W)				
		Mn	Sb	Sn	Ti	Co
5411	MnSbSnTi	155	24	12	120	-
5412	MnSbSn	155	25	11	-	-
5413	MnSbTi	155	25	-	124	-
5414	MnSb	155	23	-	-	-
5029	MnSbCo	150	42	-	-	108

Composition and Structure Characterization

X-ray fluorescence (XRF) was used to determine the spatial map of composition, which detects all elements except oxygen. It was performed on an EDAX Orbis Micro-XRF system with an x-ray beam approximately 2 mm in diameter. The Mn K, Sb L, Sn L, Ti K, and Co K XRF peak intensities were extracted from the Orbis software and converted to normalized compositions using the sensitivity factor for each element calibrated by commercial XRF calibration standards (Micromatter). Note that due to 10 nm Ti adhesion layer on the Si wafer, Ti metal concentration in the Mn-Sb-Ti-O and Mn-Sb-Sn-Ti-O thin film libraries may be 2-5 at.% higher than the actual value. Since the uncertainty in correcting these values would be as large as the corrections themselves, and since this systematic, small composition shift does not impact the conclusions of the work, we report the compositions without a correction for the Ti adhesion layer.

X-ray diffraction (XRD) was used to characterize the phase behavior of composition libraries. It was performed on a Bruker DISCOVER D8 diffractometer with Cu K α radiation from a Bruker I μ S source. Diffraction images were collected using a two-dimensional VÅNTEC-500 detector and integrated into one-dimensional patterns using DIFFRAC.SUITE EVA software. Using ICDD phases as prototypes, the phase constitution as well as the lattice parameters of each phase were determined via a novel XRD analysis tool, CrystalShift. The results are summarized in Table S2.

Neither oxygen stoichiometry nor thickness were measured. We expect the oxygen stoichiometry to reflect the equilibration of the respective thin film composition with air at 700 °C and to be best characterized by phase identification, which as noted in Fig. 2, Fig. S1, and Table S2 involved predominantly rutile-type structures where the metal-to-oxygen ratio is approximately 2. The film

thickness is on the order of 200 nm and varies with composition as a result of the co-sputter deposition using the natural gradients in deposition rate from each source. The XRF results include calibration of the molar loading of each element. The full XRF analysis can be found at <https://data.caltech.edu/doi/10.22002/tg041-j4g80>.

Scanning Droplet Cell (SDC) OER catalytic measurements

The OER performance of the $\text{Mn}_{1-x-y-z}\text{Sb}_x\text{Sn}_y\text{Ti}_z\text{-O}$ catalysts was evaluated using a customized SDC instrumentation in 1 M H_2SO_4 aqueous electrolyte saturated with bubbled 1 atm O_2 gas. The 3-electrode cell includes a Pt counter electrode, Ag/AgCl reference electrode, Gamry G300 potentiostat, and custom LabVIEW software. The measured potentials were converted to the reversible hydrogen electrode (RHE) scale according to the Nernst equation. Two cyclic voltammograms (CVs) from 1.23 to 1.79 V vs RHE was performed at a sweep rate of 0.02 V s^{-1} , and in between two CVs, each catalyst was characterized by a 200 seconds chronoamperometry (CA) at 1.72 V vs RHE, where the current over 1 s at the duration of 20 s and final 200 s were averaged to represent the activity metric at the beginning and end of CA. The current at 1.79 V vs RHE from the initial and post CA CV measurement is also used to represent the activity metric of the catalyst. Table S3 summarizes the 4 OER activity metrics obtained from 182 OER catalytic measurements. The geometric surface area of 0.02 cm^2 was used to convert current into current density in the SDC experiments.

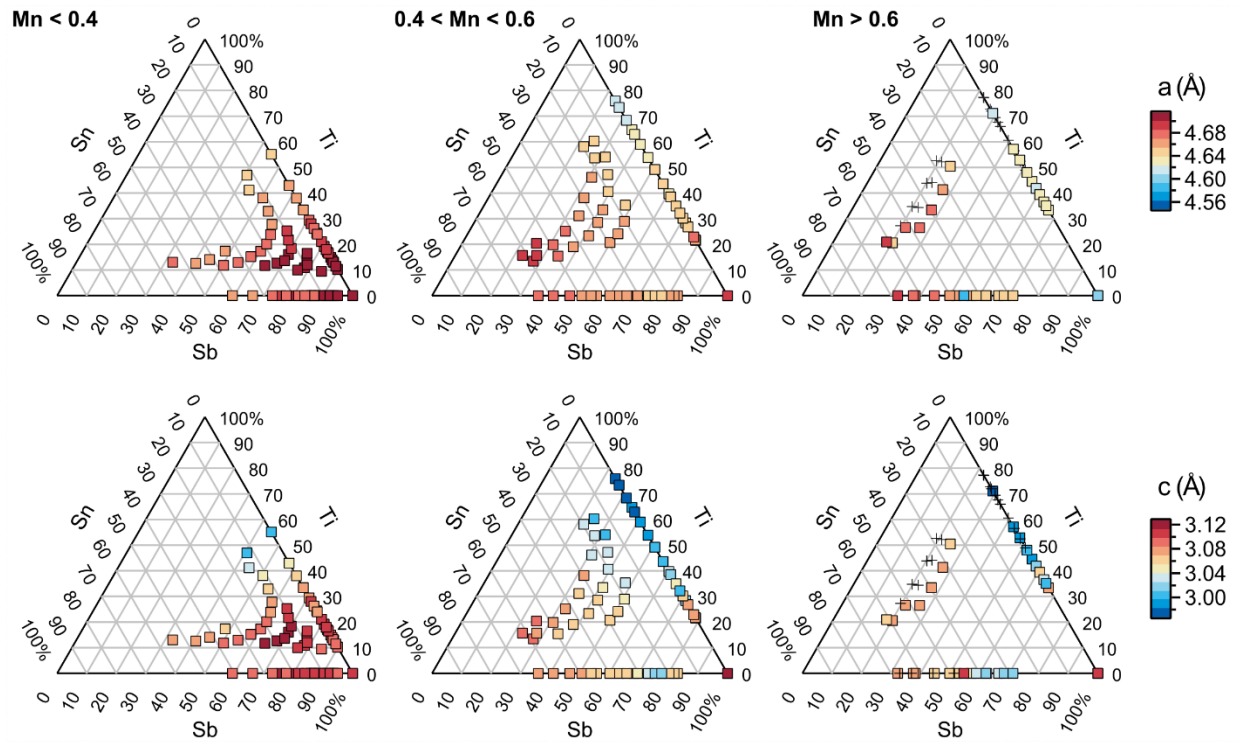


Fig. S1 Summary of the 203 XRD measurements from the 4 composition libraries (same data from Fig. 2) with compositions binned by the Mn concentration. Within each composition bin, the data are shown using re-normalized Sb-Sn-Ti compositions. Top and bottom panel corresponds to the rutile lattice parameter a and c , respectively. Solid squares are pure rutile phases while the “+” marker represents mixed-phase samples, which only appear for Mn concentration > 0.6 .

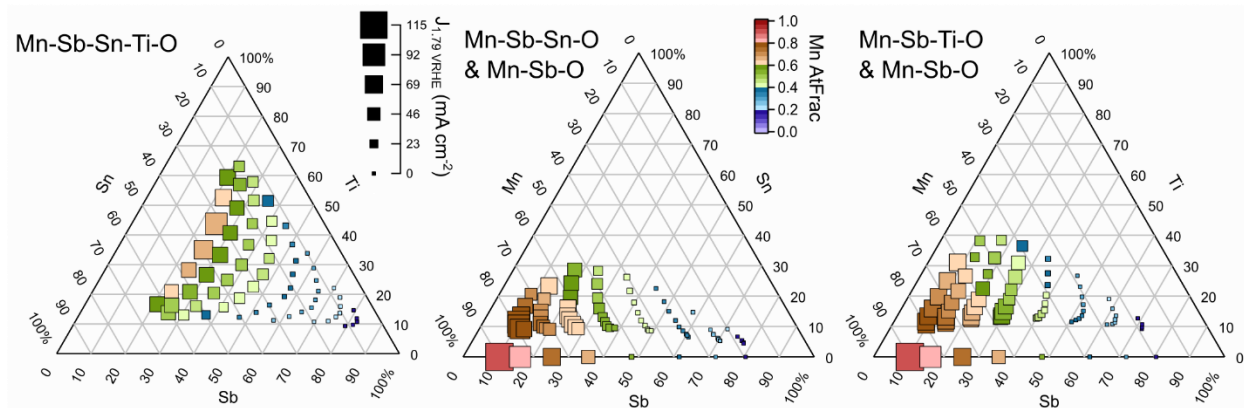


Fig. S2 An alternative composition plot of Fig. 4, which summarizes 182 OER activity measurements from the 4 composition libraries: Mn-Sb-Sn-Ti-O, Mn-Sb-Sn-O, Mn-Sb-Ti-O, and Mn-Sb-O, as labelled on each composition plot. The Mn concentration is illustrated by the marker color and the size of each data marker indicates its catalytic activity. For Mn-Sb-Sn-Ti-O library, the data is shown using re-normalized Sb-Sn-Ti compositions.

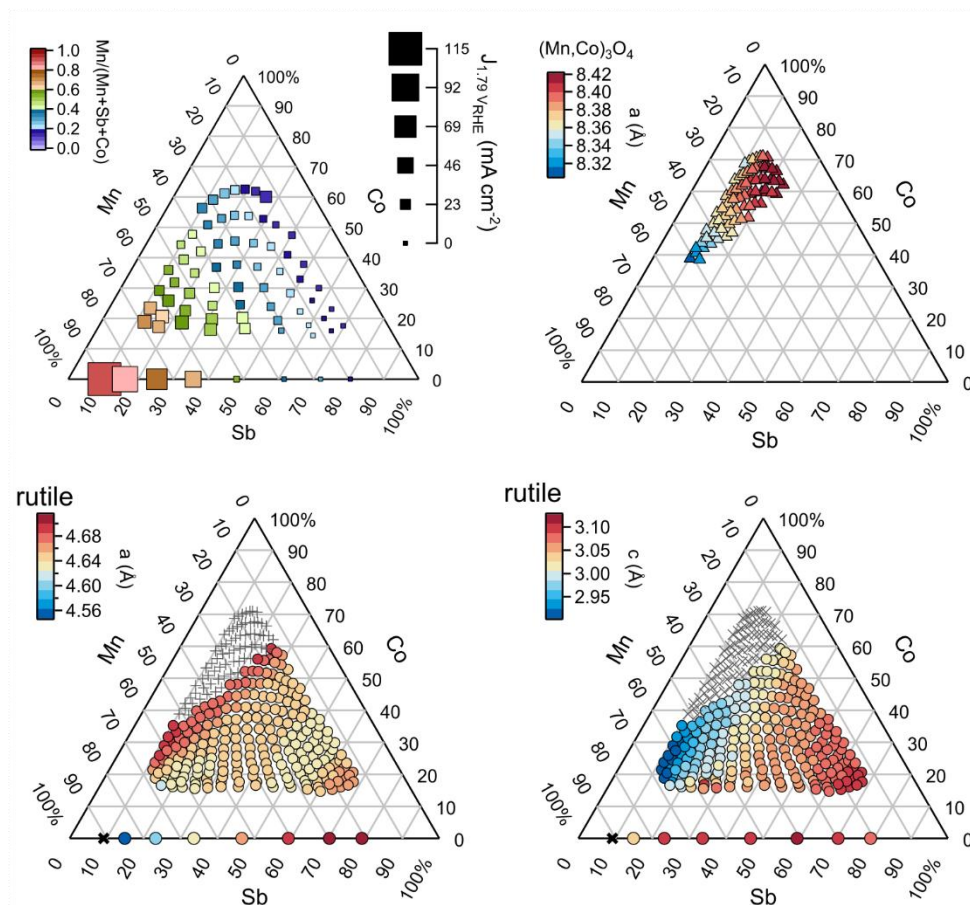


Fig. S3 The OER activity (top left) and XRD characterization (top-right and bottom) of the Mn-Sb-Co-O and Mn-Sb-O composition libraries. In the top-left OER activity composition plot, the Mn concentration is illustrated by the marker color and the size of each data marker indicates its catalytic activity. The top-right composition plot shows the lattice parameter a for the cubic $(\text{Mn,Co})_3\text{O}_4$ phase, while the bottom ones represent lattice parameters a and c for rutile phase. Grey markers in the bottom panel indicate the $(\text{Mn,Co})_3\text{O}_4$ samples.

Table S2. Summary of phase constitution as well as the lattice parameters of each phase for total 203 samples from 4 composition libraries determined via the CrystalShift algorithm. Most samples contain a single phase, resulting in a single row in the table. Mixed-phase samples correspond to multiple rows with the same composition and the respective values for phase label, lattice constants, and phase fraction.

plate	elements	Mn	Sb	Sn	Ti	phase label	a	b	c	phase fraction
5411	MnSbSnTi	0.36	0.26	0.30	0.08	Rutile	4.664	4.664	3.082	1
5411	MnSbSnTi	0.33	0.40	0.15	0.12	Rutile	4.674	4.674	3.088	1
5411	MnSbSnTi	0.41	0.29	0.17	0.12	Rutile	4.660	4.660	3.062	1
5411	MnSbSnTi	0.26	0.50	0.14	0.09	Rutile	4.700	4.700	3.117	1
5411	MnSbSnTi	0.30	0.35	0.26	0.08	Rutile	4.673	4.673	3.094	1
5411	MnSbSnTi	0.27	0.52	0.10	0.12	Rutile	4.700	4.700	3.114	1
5411	MnSbSnTi	0.34	0.39	0.09	0.18	Rutile	4.668	4.668	3.072	1
5411	MnSbSnTi	0.21	0.62	0.07	0.11	Rutile	4.703	4.703	3.101	1
5411	MnSbSnTi	0.41	0.30	0.12	0.17	Rutile	4.654	4.654	3.043	1
5411	MnSbSnTi	0.26	0.52	0.12	0.10	Rutile	4.700	4.700	3.116	1
5411	MnSbSnTi	0.32	0.34	0.08	0.26	Rutile	4.657	4.657	3.046	1
5411	MnSbSnTi	0.41	0.30	0.15	0.14	Rutile	4.659	4.659	3.055	1
5411	MnSbSnTi	0.21	0.60	0.06	0.13	Rutile	4.699	4.699	3.100	1
5411	MnSbSnTi	0.20	0.63	0.09	0.09	Rutile	4.707	4.707	3.104	1
5411	MnSbSnTi	0.33	0.37	0.08	0.22	Rutile	4.662	4.662	3.065	1
5411	MnSbSnTi	0.38	0.25	0.08	0.29	Rutile	4.647	4.647	3.008	1
5411	MnSbSnTi	0.27	0.51	0.08	0.13	Rutile	4.696	4.696	3.112	1
5411	MnSbSnTi	0.32	0.37	0.22	0.09	Rutile	4.674	4.674	3.094	1
5411	MnSbSnTi	0.25	0.48	0.18	0.09	Rutile	4.699	4.699	3.118	1
5411	MnSbSnTi	0.27	0.49	0.08	0.16	Rutile	4.692	4.692	3.107	1
5411	MnSbSnTi	0.39	0.29	0.21	0.11	Rutile	4.656	4.656	3.063	1
5411	MnSbSnTi	0.34	0.40	0.13	0.13	Rutile	4.672	4.672	3.084	1
5411	MnSbSnTi	0.37	0.28	0.26	0.09	Rutile	4.660	4.660	3.070	1
5411	MnSbSnTi	0.40	0.27	0.09	0.25	Rutile	4.650	4.650	3.029	1
5411	MnSbSnTi	0.20	0.63	0.07	0.10	Rutile	4.706	4.706	3.103	1
5411	MnSbSnTi	0.27	0.48	0.07	0.18	Rutile	4.684	4.684	3.102	1
5411	MnSbSnTi	0.32	0.39	0.18	0.10	Rutile	4.674	4.674	3.089	1
5411	MnSbSnTi	0.15	0.72	0.05	0.08	Rutile	4.706	4.706	3.092	1
5411	MnSbSnTi	0.34	0.40	0.10	0.16	Rutile	4.670	4.670	3.080	1
5411	MnSbSnTi	0.20	0.61	0.11	0.08	Rutile	4.707	4.707	3.107	1
5411	MnSbSnTi	0.41	0.28	0.10	0.21	Rutile	4.653	4.653	3.035	1
5411	MnSbSnTi	0.43	0.20	0.28	0.09	Rutile	4.669	4.669	3.069	1
5411	MnSbSnTi	0.67	0.07	0.09	0.17	Rutile	4.641	4.641	3.034	0.336971
5411	MnSbSnTi	0.67	0.07	0.09	0.17	Mn2O3	9.426	9.426	9.426	0.663029
5411	MnSbSnTi	0.68	0.07	0.17	0.09	Rutile	4.674	4.674	3.069	1
5411	MnSbSnTi	0.45	0.20	0.09	0.26	Rutile	4.651	4.651	3.028	1
5411	MnSbSnTi	0.55	0.14	0.10	0.21	Rutile	4.656	4.656	3.038	1
5411	MnSbSnTi	0.40	0.20	0.33	0.08	Rutile	4.673	4.673	3.077	1
5411	MnSbSnTi	0.62	0.10	0.18	0.10	Rutile	4.676	4.676	3.082	1
5411	MnSbSnTi	0.46	0.15	0.32	0.07	Rutile	4.685	4.685	3.087	1
5411	MnSbSnTi	0.69	0.07	0.13	0.11	Rutile	4.658	4.658	3.071	0.329172
5411	MnSbSnTi	0.69	0.07	0.13	0.11	Mn2O3	9.426	9.426	9.426	0.670828
5411	MnSbSnTi	0.63	0.10	0.15	0.12	Rutile	4.669	4.669	3.072	1
5411	MnSbSnTi	0.49	0.14	0.29	0.08	Rutile	4.684	4.684	3.082	1
5411	MnSbSnTi	0.46	0.21	0.23	0.10	Rutile	4.668	4.668	3.065	1
5411	MnSbSnTi	0.69	0.06	0.16	0.08	Rutile	4.670	4.670	3.080	0.311909
5411	MnSbSnTi	0.69	0.06	0.16	0.08	Mn2O3	9.426	9.426	9.426	0.688091
5411	MnSbSnTi	0.58	0.10	0.23	0.08	Rutile	4.690	4.690	3.087	1
5411	MnSbSnTi	0.58	0.09	0.08	0.24	Rutile	4.647	4.647	3.026	1
5411	MnSbSnTi	0.48	0.13	0.08	0.31	Rutile	4.648	4.648	3.002	1
5411	MnSbSnTi	0.56	0.15	0.15	0.14	Rutile	4.663	4.663	3.063	1
5411	MnSbSnTi	0.52	0.15	0.23	0.09	Rutile	4.680	4.680	3.081	1
5411	MnSbSnTi	0.55	0.10	0.28	0.07	Rutile	4.695	4.695	3.091	1

5411	MnSbSnTi	0.56	0.14	0.13	0.17	Rutile	4.656	4.656	3.071	1
5411	MnSbSnTi	0.43	0.18	0.08	0.31	Rutile	4.647	4.647	3.006	1
5411	MnSbSnTi	0.55	0.15	0.19	0.11	Rutile	4.673	4.673	3.075	1
5411	MnSbSnTi	0.48	0.21	0.11	0.21	Rutile	4.651	4.651	3.040	1
5411	MnSbSnTi	0.52	0.14	0.09	0.26	Rutile	4.652	4.652	3.031	1
5411	MnSbSnTi	0.71	0.06	0.13	0.10	Rutile	4.657	4.657	3.079	0.279126
5411	MnSbSnTi	0.71	0.06	0.13	0.10	Mn2O3	9.430	9.430	9.430	0.720874
5411	MnSbSnTi	0.48	0.21	0.13	0.17	Rutile	4.658	4.658	3.046	1
5411	MnSbSnTi	0.71	0.06	0.10	0.13	Rutile	4.650	4.650	3.043	0.282745
5411	MnSbSnTi	0.71	0.06	0.10	0.13	Mn2O3	9.428	9.428	9.428	0.717255
5411	MnSbSnTi	0.49	0.21	0.15	0.15	Rutile	4.664	4.664	3.061	1
5411	MnSbSnTi	0.48	0.22	0.18	0.12	Rutile	4.665	4.665	3.064	1
5411	MnSbSnTi	0.68	0.06	0.09	0.17	Rutile	4.643	4.643	3.023	0.288492
5411	MnSbSnTi	0.68	0.06	0.09	0.17	Mn2O3	9.429	9.429	9.429	0.711508
5411	MnSbSnTi	0.62	0.10	0.09	0.19	Rutile	4.653	4.653	3.060	1
5411	MnSbSnTi	0.63	0.10	0.12	0.15	Rutile	4.660	4.660	3.072	1
5411	MnSbSnTi	0.64	0.07	0.21	0.07	Rutile	4.649	4.649	3.082	1
5411	MnSbSnTi	0.69	0.07	0.11	0.14	Rutile	4.648	4.648	3.064	0.322948
5411	MnSbSnTi	0.69	0.07	0.11	0.14	Mn2O3	9.429	9.429	9.429	0.677052
5411	MnSbSnTi	0.66	0.06	0.21	0.07	Rutile	4.687	4.687	3.065	1
5412	MnSbSn	0.16	0.80	0.05	0.00	Rutile	4.710	4.710	3.087	1
5412	MnSbSn	0.29	0.65	0.06	0.00	Rutile	4.707	4.707	3.119	1
5412	MnSbSn	0.30	0.59	0.11	0.00	Rutile	4.705	4.705	3.125	1
5412	MnSbSn	0.23	0.66	0.11	0.00	Rutile	4.709	4.709	3.112	1
5412	MnSbSn	0.30	0.62	0.08	0.00	Rutile	4.708	4.708	3.121	1
5412	MnSbSn	0.30	0.61	0.09	0.00	Rutile	4.707	4.707	3.124	1
5412	MnSbSn	0.22	0.71	0.07	0.00	Rutile	4.710	4.710	3.102	1
5412	MnSbSn	0.29	0.64	0.07	0.00	Rutile	4.707	4.707	3.120	1
5412	MnSbSn	0.21	0.73	0.05	0.00	Rutile	4.710	4.710	3.099	1
5412	MnSbSn	0.31	0.52	0.17	0.00	Rutile	4.696	4.696	3.123	1
5412	MnSbSn	0.21	0.74	0.05	0.00	Rutile	4.709	4.709	3.097	1
5412	MnSbSn	0.30	0.56	0.14	0.00	Rutile	4.702	4.702	3.124	1
5412	MnSbSn	0.22	0.70	0.08	0.00	Rutile	4.710	4.710	3.106	1
5412	MnSbSn	0.17	0.77	0.06	0.00	Rutile	4.709	4.709	3.098	1
5412	MnSbSn	0.15	0.81	0.04	0.00	Rutile	4.708	4.708	3.095	1
5412	MnSbSn	0.49	0.40	0.11	0.00	Rutile	4.659	4.659	3.067	1
5412	MnSbSn	0.38	0.54	0.08	0.00	Rutile	4.684	4.684	3.108	1
5412	MnSbSn	0.48	0.43	0.09	0.00	Rutile	4.663	4.663	3.065	1
5412	MnSbSn	0.48	0.33	0.19	0.00	Rutile	4.657	4.657	3.065	1
5412	MnSbSn	0.38	0.53	0.09	0.00	Rutile	4.682	4.682	3.107	1
5412	MnSbSn	0.38	0.41	0.21	0.00	Rutile	4.666	4.666	3.087	1
5412	MnSbSn	0.38	0.37	0.25	0.00	Rutile	4.667	4.667	3.084	1
5412	MnSbSn	0.39	0.47	0.14	0.00	Rutile	4.674	4.674	3.093	1
5412	MnSbSn	0.40	0.49	0.11	0.00	Rutile	4.676	4.676	3.100	1
5412	MnSbSn	0.49	0.35	0.16	0.00	Rutile	4.657	4.657	3.067	1
5412	MnSbSn	0.49	0.37	0.14	0.00	Rutile	4.657	4.657	3.064	1
5412	MnSbSn	0.48	0.42	0.09	0.00	Rutile	4.661	4.661	3.068	1
5412	MnSbSn	0.49	0.41	0.10	0.00	Rutile	4.662	4.662	3.067	1
5412	MnSbSn	0.46	0.30	0.24	0.00	Rutile	4.660	4.660	3.069	1
5412	MnSbSn	0.44	0.28	0.28	0.00	Rutile	4.664	4.664	3.070	1
5412	MnSbSn	0.38	0.54	0.08	0.00	Rutile	4.683	4.683	3.109	1
5412	MnSbSn	0.39	0.44	0.16	0.00	Rutile	4.670	4.670	3.090	1
5412	MnSbSn	0.39	0.51	0.10	0.00	Rutile	4.680	4.680	3.102	1
5412	MnSbSn	0.59	0.30	0.11	0.00	Rutile	4.652	4.652	3.035	1
5412	MnSbSn	0.64	0.16	0.20	0.00	Rutile	4.670	4.670	3.068	1
5412	MnSbSn	0.56	0.24	0.20	0.00	Rutile	4.666	4.666	3.060	1
5412	MnSbSn	0.60	0.28	0.12	0.00	Rutile	4.657	4.657	3.046	1
5412	MnSbSn	0.58	0.15	0.27	0.00	Rutile	4.682	4.682	3.074	1
5412	MnSbSn	0.69	0.19	0.12	0.00	Rutile	4.650	4.650	3.040	1
5412	MnSbSn	0.61	0.15	0.24	0.00	Rutile	4.677	4.677	3.073	1
5412	MnSbSn	0.69	0.21	0.10	0.00	Rutile	4.650	4.650	3.028	1
5412	MnSbSn	0.59	0.31	0.10	0.00	Rutile	4.645	4.645	3.023	1
5412	MnSbSn	0.68	0.18	0.14	0.00	Rutile	4.655	4.655	3.041	1

5412	MnSbSn	0.59	0.27	0.14	0.00	Rutile	4.659	4.659	3.055	1
5412	MnSbSn	0.51	0.20	0.29	0.00	Rutile	4.674	4.674	3.072	1
5412	MnSbSn	0.68	0.22	0.10	0.00	Rutile	4.648	4.648	3.024	1
5412	MnSbSn	0.54	0.21	0.25	0.00	Rutile	4.669	4.669	3.073	1
5412	MnSbSn	0.67	0.23	0.09	0.00	Rutile	4.649	4.649	3.012	1
5412	MnSbSn	0.58	0.25	0.17	0.00	Rutile	4.664	4.664	3.064	1
5412	MnSbSn	0.67	0.17	0.16	0.00	Rutile	4.662	4.662	3.057	1
5412	MnSbSn	0.58	0.32	0.09	0.00	Rutile	4.641	4.641	3.020	1
5412	MnSbSn	0.77	0.13	0.11	0.00	Rutile	4.590	4.590	3.103	1
5412	MnSbSn	0.74	0.11	0.15	0.00	Rutile	4.665	4.665	3.071	0.35612
5412	MnSbSn	0.74	0.11	0.15	0.00	Mn2O3	9.418	9.418	9.418	0.64388
5412	MnSbSn	0.68	0.10	0.22	0.00	Rutile	4.686	4.686	3.075	1
5412	MnSbSn	0.80	0.08	0.13	0.00	Mn2O3	9.439	9.439	9.439	0.792226
5412	MnSbSn	0.80	0.08	0.13	0.00	Rutile	4.667	4.667	3.077	0.207774
5412	MnSbSn	0.76	0.15	0.09	0.00	Rutile	4.649	4.649	3.017	1
5412	MnSbSn	0.71	0.11	0.18	0.00	Rutile	4.678	4.678	3.071	1
5412	MnSbSn	0.76	0.08	0.16	0.00	Mn2O3	9.426	9.426	9.426	0.745528
5412	MnSbSn	0.76	0.08	0.16	0.00	Rutile	4.678	4.678	3.087	0.254472
5412	MnSbSn	0.77	0.14	0.10	0.00	Rutile	4.651	4.651	3.033	1
5412	MnSbSn	0.81	0.08	0.11	0.00	Mn2O3	9.443	9.443	9.443	1
5412	MnSbSn	0.82	0.08	0.10	0.00	Mn2O3	9.448	9.448	9.448	1
5412	MnSbSn	0.82	0.09	0.09	0.00	Mn2O3	9.440	9.440	9.440	0.795904
5412	MnSbSn	0.82	0.09	0.09	0.00	Rutile	4.649	4.649	3.034	0.204096
5412	MnSbSn	0.75	0.12	0.12	0.00	Rutile	4.663	4.663	3.066	1
5413	MnSbTi	0.77	0.11	0.00	0.12	Mn2O3	9.463	9.463	9.463	0.759483
5413	MnSbTi	0.77	0.11	0.00	0.12	Rutile	4.601	4.601	3.040	0.240517
5413	MnSbTi	0.58	0.10	0.00	0.32	Rutile	4.619	4.619	2.974	1
5413	MnSbTi	0.75	0.07	0.00	0.18	Mn2O3	9.449	9.449	9.449	0.732607
5413	MnSbTi	0.75	0.07	0.00	0.18	Rutile	4.611	4.611	3.001	0.267393
5413	MnSbTi	0.69	0.10	0.00	0.20	Rutile	4.620	4.620	2.997	0.339524
5413	MnSbTi	0.69	0.10	0.00	0.20	Mn2O3	9.444	9.444	9.444	0.660476
5413	MnSbTi	0.70	0.17	0.00	0.13	Rutile	4.624	4.624	2.989	1
5413	MnSbTi	0.70	0.07	0.00	0.24	Rutile	4.613	4.613	2.989	0.322198
5413	MnSbTi	0.70	0.07	0.00	0.24	Mn2O3	9.443	9.443	9.443	0.677802
5413	MnSbTi	0.64	0.10	0.00	0.25	Rutile	4.621	4.621	2.975	1
5413	MnSbTi	0.68	0.17	0.00	0.16	Rutile	4.626	4.626	3.002	1
5413	MnSbTi	0.73	0.11	0.00	0.17	Rutile	4.615	4.615	3.009	0.297472
5413	MnSbTi	0.73	0.11	0.00	0.17	Mn2O3	9.449	9.449	9.449	0.702528
5413	MnSbTi	0.70	0.17	0.00	0.12	Rutile	4.619	4.619	3.012	1
5413	MnSbTi	0.75	0.11	0.00	0.14	Mn2O3	9.457	9.457	9.457	0.740398
5413	MnSbTi	0.75	0.11	0.00	0.14	Rutile	4.609	4.609	3.025	0.259602
5413	MnSbTi	0.78	0.05	0.00	0.17	Mn2O3	9.447	9.447	9.447	0.765415
5413	MnSbTi	0.78	0.05	0.00	0.17	Rutile	4.602	4.602	2.974	0.234585
5413	MnSbTi	0.71	0.18	0.00	0.12	Rutile	4.626	4.626	3.062	1
5413	MnSbTi	0.80	0.07	0.00	0.12	Mn2O3	9.453	9.453	9.453	1
5413	MnSbTi	0.82	0.05	0.00	0.13	Mn2O3	9.437	9.437	9.437	0.789388
5413	MnSbTi	0.82	0.05	0.00	0.13	Rutile	4.605	4.605	3.011	0.210612
5413	MnSbTi	0.78	0.07	0.00	0.15	Mn2O3	9.450	9.450	9.450	0.784465
5413	MnSbTi	0.78	0.07	0.00	0.15	Rutile	4.608	4.608	3.007	0.215535
5413	MnSbTi	0.82	0.08	0.00	0.11	Mn2O3	9.454	9.454	9.454	1
5413	MnSbTi	0.77	0.12	0.00	0.11	Mn2O3	9.464	9.464	9.464	0.764583
5413	MnSbTi	0.77	0.12	0.00	0.11	Rutile	4.594	4.594	3.037	0.235417
5413	MnSbTi	0.43	0.20	0.00	0.37	Rutile	4.627	4.627	2.987	1
5413	MnSbTi	0.47	0.22	0.00	0.31	Rutile	4.629	4.629	2.990	1
5413	MnSbTi	0.59	0.25	0.00	0.16	Rutile	4.630	4.630	3.033	1
5413	MnSbTi	0.51	0.23	0.00	0.27	Rutile	4.635	4.635	2.995	1
5413	MnSbTi	0.54	0.23	0.00	0.23	Rutile	4.634	4.634	3.001	1
5413	MnSbTi	0.60	0.25	0.00	0.14	Rutile	4.629	4.629	3.032	1
5413	MnSbTi	0.63	0.25	0.00	0.12	Rutile	4.633	4.633	3.069	1
5413	MnSbTi	0.57	0.24	0.00	0.19	Rutile	4.634	4.634	3.002	1
5413	MnSbTi	0.61	0.25	0.00	0.14	Rutile	4.631	4.631	3.004	1
5413	MnSbTi	0.53	0.15	0.00	0.32	Rutile	4.622	4.622	2.974	1
5413	MnSbTi	0.58	0.16	0.00	0.27	Rutile	4.625	4.625	2.982	1

5413	MnSbTi	0.48	0.14	0.00	0.38	Rutile	4.621	4.621	2.969	1
5413	MnSbTi	0.65	0.16	0.00	0.18	Rutile	4.629	4.629	2.986	1
5413	MnSbTi	0.62	0.16	0.00	0.22	Rutile	4.630	4.630	2.986	1
5413	MnSbTi	0.21	0.67	0.00	0.12	Rutile	4.701	4.701	3.091	1
5413	MnSbTi	0.22	0.67	0.00	0.11	Rutile	4.704	4.704	3.093	1
5413	MnSbTi	0.23	0.67	0.00	0.10	Rutile	4.703	4.703	3.099	1
5413	MnSbTi	0.16	0.75	0.00	0.09	Rutile	4.702	4.702	3.084	1
5413	MnSbTi	0.22	0.67	0.00	0.10	Rutile	4.704	4.704	3.096	1
5413	MnSbTi	0.21	0.65	0.00	0.14	Rutile	4.698	4.698	3.090	1
5413	MnSbTi	0.17	0.74	0.00	0.09	Rutile	4.701	4.701	3.094	1
5413	MnSbTi	0.16	0.75	0.00	0.10	Rutile	4.699	4.699	3.092	1
5413	MnSbTi	0.37	0.45	0.00	0.19	Rutile	4.669	4.669	3.079	1
5413	MnSbTi	0.29	0.57	0.00	0.14	Rutile	4.695	4.695	3.108	1
5413	MnSbTi	0.32	0.39	0.00	0.29	Rutile	4.656	4.656	3.053	1
5413	MnSbTi	0.28	0.57	0.00	0.15	Rutile	4.693	4.693	3.105	1
5413	MnSbTi	0.31	0.57	0.00	0.12	Rutile	4.692	4.692	3.109	1
5413	MnSbTi	0.32	0.57	0.00	0.11	Rutile	4.689	4.689	3.108	1
5413	MnSbTi	0.27	0.53	0.00	0.21	Rutile	4.685	4.685	3.097	1
5413	MnSbTi	0.30	0.57	0.00	0.13	Rutile	4.694	4.694	3.109	1
5413	MnSbTi	0.35	0.43	0.00	0.22	Rutile	4.666	4.666	3.074	1
5413	MnSbTi	0.33	0.41	0.00	0.25	Rutile	4.660	4.660	3.067	1
5413	MnSbTi	0.28	0.55	0.00	0.18	Rutile	4.690	4.690	3.101	1
5413	MnSbTi	0.38	0.46	0.00	0.16	Rutile	4.671	4.671	3.079	1
5413	MnSbTi	0.84	0.05	0.00	0.11	Mn2O3	9.439	9.439	9.439	0.792956
5413	MnSbTi	0.84	0.05	0.00	0.11	Rutile	4.592	4.592	2.954	0.207044
5413	MnSbTi	0.52	0.34	0.00	0.14	Rutile	4.641	4.641	3.023	1
5413	MnSbTi	0.53	0.35	0.00	0.13	Rutile	4.639	4.639	3.069	1
5413	MnSbTi	0.43	0.45	0.00	0.12	Rutile	4.663	4.663	3.065	1
5413	MnSbTi	0.42	0.46	0.00	0.13	Rutile	4.667	4.667	3.078	1
5413	MnSbTi	0.40	0.46	0.00	0.14	Rutile	4.669	4.669	3.079	1
5413	MnSbTi	0.39	0.46	0.00	0.15	Rutile	4.671	4.671	3.082	1
5413	MnSbTi	0.46	0.33	0.00	0.21	Rutile	4.649	4.649	3.023	1
5413	MnSbTi	0.43	0.32	0.00	0.25	Rutile	4.644	4.644	3.009	1
5413	MnSbTi	0.48	0.34	0.00	0.18	Rutile	4.644	4.644	3.043	1
5413	MnSbTi	0.41	0.30	0.00	0.29	Rutile	4.643	4.643	3.000	1
5413	MnSbTi	0.38	0.28	0.00	0.34	Rutile	4.639	4.639	3.002	1
5413	MnSbTi	0.51	0.34	0.00	0.15	Rutile	4.643	4.643	3.062	1
5413	MnSbTi	0.50	0.34	0.00	0.16	Rutile	4.647	4.647	3.011	1
5414	MnSb	0.21	0.79	0.00	0.00	Rutile	4.713	4.713	3.083	1
5414	MnSb	0.91	0.09	0.00	0.00	Mn2O3	9.472	9.472	9.472	1
5414	MnSb	0.66	0.34	0.00	0.00	Rutile	4.624	4.624	3.091	1
5414	MnSb	0.53	0.47	0.00	0.00	Rutile	4.665	4.665	3.091	1
5414	MnSb	0.85	0.15	0.00	0.00	Rutile	4.549	4.549	3.029	1
5414	MnSb	0.41	0.59	0.00	0.00	Rutile	4.695	4.695	3.116	1
5414	MnSb	0.77	0.23	0.00	0.00	Rutile	4.597	4.597	3.101	1
5414	MnSb	0.30	0.70	0.00	0.00	Rutile	4.708	4.708	3.105	1

Table S3. Summary of the 182 OER activity measurements in 1 M H₂SO₄ electrolyte where the current density (with respect to the estimated geometric area of the electrode-electrolyte contact area) was recorded at a potential of 1.79 V vs RHE, the high-potential endpoint of a cyclic voltammogram.

plate	elements	Mn	Sb	Sn	Ti	J_1.79Vrhe (mA/cm ²)
5411	MnSbSnTi	0.58	0.09	0.26	0.07	57.30
5411	MnSbSnTi	0.62	0.09	0.22	0.08	50.90
5411	MnSbSnTi	0.65	0.09	0.17	0.10	55.60
5411	MnSbSnTi	0.66	0.09	0.14	0.12	75.00
5411	MnSbSnTi	0.65	0.09	0.11	0.15	89.30
5411	MnSbSnTi	0.64	0.08	0.09	0.19	63.95
5411	MnSbSnTi	0.60	0.08	0.08	0.24	60.30
5411	MnSbSnTi	0.49	0.13	0.31	0.07	53.60
5411	MnSbSnTi	0.51	0.12	0.28	0.08	54.10
5411	MnSbSnTi	0.55	0.13	0.23	0.09	55.95
5411	MnSbSnTi	0.58	0.13	0.18	0.11	55.25
5411	MnSbSnTi	0.59	0.13	0.15	0.14	59.60
5411	MnSbSnTi	0.59	0.12	0.12	0.17	54.95
5411	MnSbSnTi	0.57	0.12	0.10	0.21	54.05
5411	MnSbSnTi	0.54	0.12	0.08	0.26	44.95
5411	MnSbSnTi	0.50	0.11	0.07	0.32	35.60
5411	MnSbSnTi	0.42	0.18	0.32	0.08	33.60
5411	MnSbSnTi	0.46	0.18	0.28	0.09	36.45
5411	MnSbSnTi	0.49	0.18	0.22	0.10	40.10
5411	MnSbSnTi	0.51	0.18	0.19	0.12	40.35
5411	MnSbSnTi	0.51	0.19	0.15	0.15	39.80
5411	MnSbSnTi	0.52	0.18	0.12	0.18	35.80
5411	MnSbSnTi	0.50	0.18	0.10	0.22	34.50
5411	MnSbSnTi	0.48	0.17	0.09	0.27	37.75
5411	MnSbSnTi	0.44	0.16	0.08	0.32	35.90
5411	MnSbSnTi	0.38	0.23	0.31	0.08	26.05
5411	MnSbSnTi	0.40	0.25	0.26	0.09	28.25
5411	MnSbSnTi	0.42	0.25	0.22	0.11	36.30
5411	MnSbSnTi	0.44	0.26	0.18	0.13	37.55
5411	MnSbSnTi	0.45	0.26	0.15	0.15	37.80
5411	MnSbSnTi	0.44	0.26	0.12	0.18	31.75
5411	MnSbSnTi	0.43	0.25	0.10	0.22	33.40
5411	MnSbSnTi	0.42	0.23	0.09	0.26	34.40
5411	MnSbSnTi	0.40	0.22	0.08	0.31	37.05
5411	MnSbSnTi	0.32	0.32	0.27	0.08	2.91
5411	MnSbSnTi	0.34	0.34	0.23	0.09	3.26
5411	MnSbSnTi	0.35	0.35	0.19	0.11	3.56
5411	MnSbSnTi	0.36	0.36	0.15	0.12	4.26
5411	MnSbSnTi	0.37	0.36	0.13	0.14	5.30
5411	MnSbSnTi	0.37	0.35	0.11	0.17	6.40
5411	MnSbSnTi	0.37	0.34	0.09	0.20	6.50
5411	MnSbSnTi	0.35	0.33	0.08	0.24	7.10
5411	MnSbSnTi	0.34	0.30	0.08	0.28	11.15
5411	MnSbSnTi	0.27	0.42	0.23	0.08	1.56
5411	MnSbSnTi	0.27	0.45	0.19	0.09	1.71
5411	MnSbSnTi	0.28	0.46	0.15	0.10	1.66
5411	MnSbSnTi	0.29	0.47	0.13	0.11	1.71
5411	MnSbSnTi	0.30	0.47	0.11	0.13	1.61
5411	MnSbSnTi	0.30	0.46	0.09	0.15	1.51
5411	MnSbSnTi	0.30	0.45	0.08	0.17	1.46
5411	MnSbSnTi	0.30	0.43	0.07	0.20	1.56
5411	MnSbSnTi	0.29	0.40	0.07	0.24	1.66
5411	MnSbSnTi	0.23	0.54	0.15	0.08	0.81
5411	MnSbSnTi	0.22	0.57	0.12	0.09	0.91
5411	MnSbSnTi	0.22	0.58	0.10	0.10	0.86
5411	MnSbSnTi	0.23	0.59	0.08	0.11	0.86
5411	MnSbSnTi	0.23	0.58	0.07	0.12	0.91

5411	MnSbSnTi	0.24	0.56	0.06	0.14	0.86
5411	MnSbSnTi	0.23	0.53	0.06	0.17	0.81
5411	MnSbSnTi	0.18	0.65	0.09	0.08	0.40
5411	MnSbSnTi	0.17	0.68	0.07	0.08	0.71
5411	MnSbSnTi	0.17	0.68	0.06	0.09	0.76
5411	MnSbSnTi	0.18	0.67	0.05	0.10	0.71
5411	MnSbSnTi	0.19	0.64	0.05	0.12	0.66
5412	MnSbSn	0.70	0.09	0.21	0.00	40.10
5412	MnSbSn	0.74	0.09	0.17	0.00	55.50
5412	MnSbSn	0.77	0.10	0.14	0.00	66.50
5412	MnSbSn	0.78	0.10	0.11	0.00	89.50
5412	MnSbSn	0.79	0.11	0.10	0.00	88.00
5412	MnSbSn	0.79	0.12	0.09	0.00	77.00
5412	MnSbSn	0.78	0.13	0.09	0.00	58.00
5412	MnSbSn	0.64	0.13	0.23	0.00	62.50
5412	MnSbSn	0.67	0.14	0.19	0.00	41.50
5412	MnSbSn	0.70	0.15	0.15	0.00	54.50
5412	MnSbSn	0.71	0.16	0.13	0.00	54.50
5412	MnSbSn	0.73	0.17	0.11	0.00	52.00
5412	MnSbSn	0.72	0.18	0.10	0.00	45.35
5412	MnSbSn	0.72	0.19	0.10	0.00	36.30
5412	MnSbSn	0.71	0.20	0.09	0.00	42.00
5412	MnSbSn	0.54	0.18	0.29	0.00	51.00
5412	MnSbSn	0.57	0.19	0.24	0.00	54.50
5412	MnSbSn	0.60	0.21	0.20	0.00	53.00
5412	MnSbSn	0.62	0.22	0.16	0.00	61.00
5412	MnSbSn	0.64	0.23	0.14	0.00	59.50
5412	MnSbSn	0.64	0.24	0.12	0.00	57.00
5412	MnSbSn	0.64	0.26	0.11	0.00	61.00
5412	MnSbSn	0.63	0.27	0.10	0.00	56.50
5412	MnSbSn	0.63	0.28	0.09	0.00	42.10
5412	MnSbSn	0.47	0.24	0.28	0.00	27.55
5412	MnSbSn	0.50	0.26	0.24	0.00	35.15
5412	MnSbSn	0.52	0.29	0.19	0.00	32.00
5412	MnSbSn	0.53	0.31	0.16	0.00	36.15
5412	MnSbSn	0.54	0.33	0.13	0.00	27.75
5412	MnSbSn	0.54	0.35	0.12	0.00	25.00
5412	MnSbSn	0.54	0.36	0.10	0.00	24.95
5412	MnSbSn	0.54	0.37	0.10	0.00	20.35
5412	MnSbSn	0.52	0.38	0.10	0.00	12.00
5412	MnSbSn	0.40	0.34	0.26	0.00	12.25
5412	MnSbSn	0.42	0.37	0.22	0.00	9.70
5412	MnSbSn	0.42	0.40	0.18	0.00	7.00
5412	MnSbSn	0.43	0.43	0.15	0.00	5.75
5412	MnSbSn	0.43	0.45	0.12	0.00	6.85
5412	MnSbSn	0.43	0.47	0.10	0.00	5.15
5412	MnSbSn	0.43	0.48	0.09	0.00	4.56
5412	MnSbSn	0.43	0.49	0.09	0.00	4.41
5412	MnSbSn	0.42	0.49	0.09	0.00	3.46
5412	MnSbSn	0.34	0.44	0.23	0.00	2.36
5412	MnSbSn	0.34	0.48	0.18	0.00	1.91
5412	MnSbSn	0.34	0.51	0.15	0.00	1.81
5412	MnSbSn	0.34	0.55	0.12	0.00	1.81
5412	MnSbSn	0.34	0.57	0.10	0.00	1.61
5412	MnSbSn	0.33	0.58	0.09	0.00	1.56
5412	MnSbSn	0.33	0.60	0.07	0.00	1.36
5412	MnSbSn	0.33	0.61	0.07	0.00	1.36
5412	MnSbSn	0.33	0.60	0.07	0.00	1.21
5412	MnSbSn	0.27	0.58	0.15	0.00	0.86
5412	MnSbSn	0.25	0.66	0.09	0.00	0.81
5412	MnSbSn	0.25	0.68	0.07	0.00	0.86
5412	MnSbSn	0.24	0.69	0.06	0.00	0.86
5412	MnSbSn	0.24	0.70	0.06	0.00	0.96

5412	MnSbSn	0.24	0.71	0.05	0.00	0.71
5412	MnSbSn	0.20	0.71	0.09	0.00	0.56
5412	MnSbSn	0.19	0.75	0.07	0.00	0.81
5412	MnSbSn	0.18	0.77	0.05	0.00	0.91
5412	MnSbSn	0.18	0.78	0.05	0.00	0.81
5412	MnSbSn	0.18	0.78	0.04	0.00	0.71
5413	MnSbTi	0.61	0.08	0.00	0.31	64.06
5413	MnSbTi	0.71	0.14	0.00	0.15	50.64
5413	MnSbTi	0.69	0.13	0.00	0.18	53.36
5413	MnSbTi	0.65	0.13	0.00	0.22	53.74
5413	MnSbTi	0.61	0.13	0.00	0.27	50.61
5413	MnSbTi	0.55	0.12	0.00	0.33	26.72
5413	MnSbTi	0.51	0.11	0.00	0.38	30.43
5413	MnSbTi	0.66	0.22	0.00	0.12	53.65
5413	MnSbTi	0.61	0.20	0.00	0.19	54.24
5413	MnSbTi	0.58	0.20	0.00	0.22	48.65
5413	MnSbTi	0.54	0.19	0.00	0.27	26.78
5413	MnSbTi	0.49	0.18	0.00	0.32	41.26
5413	MnSbTi	0.44	0.17	0.00	0.38	30.83
5413	MnSbTi	0.57	0.30	0.00	0.13	54.14
5413	MnSbTi	0.54	0.29	0.00	0.17	55.77
5413	MnSbTi	0.52	0.29	0.00	0.19	38.91
5413	MnSbTi	0.50	0.28	0.00	0.22	38.52
5413	MnSbTi	0.47	0.27	0.00	0.26	48.33
5413	MnSbTi	0.39	0.24	0.00	0.36	35.07
5413	MnSbTi	0.47	0.40	0.00	0.13	12.94
5413	MnSbTi	0.47	0.40	0.00	0.13	14.82
5413	MnSbTi	0.45	0.41	0.00	0.14	16.15
5413	MnSbTi	0.44	0.41	0.00	0.15	12.26
5413	MnSbTi	0.42	0.40	0.00	0.18	9.52
5413	MnSbTi	0.41	0.39	0.00	0.20	12.01
5413	MnSbTi	0.39	0.38	0.00	0.24	8.12
5413	MnSbTi	0.37	0.36	0.00	0.27	8.50
5413	MnSbTi	0.34	0.34	0.00	0.32	7.96
5413	MnSbTi	0.38	0.51	0.00	0.12	2.27
5413	MnSbTi	0.36	0.52	0.00	0.12	1.86
5413	MnSbTi	0.35	0.52	0.00	0.13	1.75
5413	MnSbTi	0.34	0.53	0.00	0.14	1.54
5413	MnSbTi	0.33	0.52	0.00	0.15	1.32
5413	MnSbTi	0.32	0.51	0.00	0.17	1.09
5413	MnSbTi	0.31	0.49	0.00	0.20	0.88
5413	MnSbTi	0.30	0.47	0.00	0.23	0.72
5413	MnSbTi	0.29	0.45	0.00	0.27	0.78
5413	MnSbTi	0.28	0.61	0.00	0.11	0.77
5413	MnSbTi	0.27	0.63	0.00	0.11	0.82
5413	MnSbTi	0.26	0.63	0.00	0.11	0.83
5413	MnSbTi	0.25	0.63	0.00	0.12	0.86
5413	MnSbTi	0.24	0.62	0.00	0.14	0.77
5413	MnSbTi	0.24	0.60	0.00	0.16	0.74
5413	MnSbTi	0.23	0.57	0.00	0.19	0.51
5413	MnSbTi	0.19	0.72	0.00	0.09	0.68
5413	MnSbTi	0.19	0.72	0.00	0.10	0.35
5413	MnSbTi	0.18	0.71	0.00	0.11	0.40
5413	MnSbTi	0.18	0.69	0.00	0.13	0.53
5414	MnSb	0.90	0.10	0.00	0.00	115.15
5414	MnSb	0.84	0.16	0.00	0.00	84.30
5414	MnSb	0.75	0.25	0.00	0.00	66.15
5414	MnSb	0.64	0.36	0.00	0.00	46.75
5414	MnSb	0.52	0.48	0.00	0.00	6.70
5414	MnSb	0.38	0.62	0.00	0.00	1.11
5414	MnSb	0.28	0.72	0.00	0.00	0.71
5414	MnSb	0.20	0.80	0.00	0.00	0.35