

Table S1. Powder X-ray diffraction data ( $d$  in Å) for haywoodite. Only calculated lines with  $I > 0.5$  are listed.

$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$	$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$	$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$
8	18.02	18.2537	4	0 0 1			3.0698	1	1 2 4			1.9193	1	2 4 4
		12.5977	2	0 1 0	10	3.063	3.0567	1	1 1 5			1.9164	1	-3-2 5
100	10.62	10.6038	100	0-1 1			3.0457	1	2-3 3			1.9040	1	3-5 5
		10.1477	1	0 1 1			3.0262	2	-2 0 4	14	1.9047	1.9008	1	-3-3 3
		9.1269	1	0 0 2			3.0036	1	2-2 4			1.8919	1	3-6 3
22	7.99	7.9326	6	1 0 0	24	2.975	2.9638	2	2 2 0			1.8864	1	3-1 7
		7.5618	1	0-1 2			2.9586	3	-2 4 0			1.8772	1	2 5 0
		7.3336	2	-1 0 1			2.8504	1	-1-2 5			1.8746	1	-2 7 0
		7.2900	3	1-1 1			2.8202	1	1 0 6	18	1.8693	1.8696	3	1 6 1
45	7.26	7.2479	1	-1 1 1			2.7497	2	-1-1 6			1.8585	1	3 3 3
		7.2313	8	0 1 2			2.7400	2	-2 3 4			1.8113	1	2-7 3
		7.2184	2	1 0 1	51	2.731	2.7370	2	1-2 6	9	1.8044	1.7934	1	4-5 3
		6.0846	8	0 0 3			2.7317	2	3-1 1			1.7757	1	-1 1 1 0
		6.0525	1	-1 0 2			2.7293	7	1 2 5			1.7705	1	1 0 1 0
		6.0425	1	0-2 1			2.6743	11	-2 2 5	15	1.7733	1.7673	3	0-6 6
40	6.04	6.0072	1	1-1 2			2.6655	1	1 1 6			1.7587	1	-4 0 5
		5.9603	2	-1 1 2			2.6576	1	2 0 5			1.7344	1	4-6 1
		5.9276	4	1 1 0	93	2.652	2.6558	2	1 4 0	9	1.7352	1.7322	1	0-5 8
		5.9172	2	-1 2 0			2.6509	2	0-4 4			1.7109	1	-1-6 5
		5.7023	2	-1-1 1			2.6464	11	3-2 2	20	1.7082	1.7045	4	-2-2 9
		5.6756	1	1-2 1			2.6442	3	3 0 0			1.7034	2	1-3 1 0
13	5.71	5.5832	2	-1 2 1			2.6319	3	-2 4 3			1.6766	3	3-6 6
		5.5754	1	1 1 1			2.6214	6	1 3 4	18	1.6756	1.6738	3	-3-4 4
		5.3809	1	0 1 3	12	2.604	2.5777	2	0-1 7			1.6510	3	2-8 1
35	5.32	5.3019	22	0-2 2			2.5192	1	-1 5 2			1.6473	2	1 7 0
		5.0739	1	0 2 2	13	2.498	2.5094	1	-1-3 5			1.6314	1	-1 0 1 1
		5.0605	1	-1-1 2			2.4802	2	0 5 1			1.6286	1	-4 1 7
9	5.01	5.0297	1	1-2 2			2.4712	2	-1 1 7	12	1.6142	1.6167	1	4-3 7
		4.9028	1	-1 2 2			2.4675	4	-2 1 6			1.6149	1	3-3 9
		4.8865	1	1 1 2			2.4615	1	1 0 7			1.5849	1	0 7 5
		4.8792	1	-1 0 3	32	2.451	2.4506	1	2-1 6			1.5808	4	-5 4 3
14	4.836	4.8076	1	-1 1 3			2.4445	2	-3 0 3			1.5801	1	3 5 1
		4.7782	1	1 0 3			2.4300	4	3-3 3	60	1.5781	1.5794	3	-1 5 9
		4.3567	1	0-1 4			2.4190	1	3-4 1			1.5762	1	5-1 3
		4.3295	1	-1-1 3			2.4104	2	0 3 6			1.5746	3	4 1 6
5	4.362	4.3114	1	-1 3 0	37	2.402	2.4005	1	2 3 2			1.5711	3	-1 4 1 0
		4.3026	1	1-2 3			2.3951	1	-1 5 3			1.5676	2	-5 3 4
		4.1839	2	-1 2 3			2.3933	7	1 4 3			1.5623	2	4 0 7
24	4.180	4.1669	3	1 1 3	4	2.252	2.2439	1	-2-3 4	29	1.5589	1.5594	1	-5 5 2
		4.1613	1	1 2 1			2.2324	1	2-5 4			1.5528	3	4 2 5
		4.0648	1	2-1 1			2.2030	1	3-2 5			1.5224	1	-5 2 5
		3.9931	1	-1 0 4	23	2.201	2.2009	5	-2 0 7	9	1.5250	1.5182	1	4-1 8
11	3.968	3.9682	2	1-1 4			2.1900	1	1 2 7			1.5148	1	0-7 7
		3.9191	1	1 0 4			2.1793	2	3 2 1			1.5080	1	-2-3 1 0
		3.8445	1	-1 3 2			2.1648	2	-2-2 6			1.5074	3	1-4 1 1
8	3.854	3.8385	1	1 2 2	25	2.164	2.1632	4	3-4 4	19	1.5070	1.5022	1	-5-1 2
		3.6848	1	-1-1 4			2.1596	1	-3-2 2			1.5008	1	5-5 4
		3.6450	1	2-2 2			2.1513	1	2-4 6			1.4850	1	3-7 7
		3.6157	1	0 2 4			2.1318	1	-2 6 1	8	1.4842	1.4827	2	-3-5 5
8	3.592	3.5799	1	1-3 3			2.1250	2	1 5 2			1.4634	2	2-9 2
		3.5346	2	0-3 3	16	2.114	2.1221	1	-2-4 2	8	1.4597	1.4606	2	-1-8 1
21	3.420	3.4040	3	-2 3 1			2.1153	1	2-6 2	7	1.4319	1.4218	1	3-2 1 1
		3.3826	2	0 3 3			2.0882	1	-4 2 0			1.3700	1	-4 6 8
		3.3440	3	-1 0 5	7	2.068	2.0667	1	-2 3 7	6	1.3743	1.3658	1	6-2 2
		3.3258	3	1-1 5			2.0282	1	0 0 9			1.3595	1	2 3 1 1
48	3.306	3.3076	1	1 3 0	8	2.018	2.0035	1	1 3 7	18	1.3596	1.3543	1	6-1 1
		3.2899	9	-2-1 2			1.9705	1	-2 2 8			1.3530	1	-4 7 7
		3.2717	6	2-3 2	10	1.9696	1.9566	1	0 6 3			1.3443	1	1-5 1 2
		3.2279	6	-1 4 1			1.9419	1	-1-1 9	9	1.3430	1.3327	1	2 2 1 2
		3.2250	2	0-2 5			1.9374	1	-2-1 8			1.3298	1	5 3 2
53	3.219	3.2078	6	-1-2 4	16	1.9350	1.9353	2	1-2 9			1.3255	1	0-8 8
		3.1926	6	1-3 4			1.9255	1	2-3 8	15	1.3271	1.3238	1	-3-6 6
		3.1566	1	-1-3 2			1.9223	1	-2 6 4			1.3221	1	6 0 0
20	3.138	3.1470	1	1-4 2								1.3160	1	-4 8 6
		3.1283	9	0-4 1						4	1.3034	1.3076	1	2-10 3