

No	Sample	Heating (°C)	Holding_T (h)	M2+ atom	MI3+ atom	MII3+ atom	M2+ radii (Å)	MI3+ radii (Å)	MII3+ radii (Å)	$\chi$ of M2+	$\chi$ of MI3+	$\chi$ of MII3+	Weighted (Å)	Weighted (mg/g)	log10(Kd) (ml/g)	M2+ elutic (mg/L)	Success	data_label	
1	Mg-Al-017	60	22	0.83	0.17	0	0.72	0.535	0	1.31	1.61	0	0.68855	1.361	3.105	2.3277	9.94	1	training
2	Mg-Al-018	60	22	0.82	0.18	0	0.72	0.535	0	1.31	1.61	0	0.6867	1.364	2.985	2.307	9.62	1	training
3	Mg-Al-019	60	22	0.81	0.19	0	0.72	0.535	0	1.31	1.61	0	0.68485	1.367	3.863	2.4457	8.16	1	training
4	Mg-Al-020	140	22	0.8	0.2	0	0.72	0.535	0	1.31	1.61	0	0.683	1.37	13.905	3.4522	7.74	1	training
5	Mg-Al-025	140	22	0.75	0.25	0	0.72	0.535	0	1.31	1.61	0	0.67375	1.385	16.204	3.9014	5.22	1	training
6	Mg-Al-033	140	22	0.67	0.33	0	0.72	0.535	0	1.31	1.61	0	0.65895	1.409	17.805	4.6149	9.32	1	training
7	Mg-Fe-020	100	12	0.8	0.2	0	0.72	0.645	0	1.31	1.83	0	0.705	1.414	12.048	3.2311	6.7	1	training
8	Mg-Fe-021	100	12	0.75	0.25	0	0.72	0.645	0	1.31	1.83	0	0.70125	1.44	14.919	3.55	11	1	training
9	Mg-Fe-030	100	12	0.7	0.3	0	0.72	0.645	0	1.31	1.83	0	0.6975	1.466	11.759	3.2031	10.9	1	training
10	Mg-Fe-022	140	12	0.8	0.2	0	0.72	0.645	0	1.31	1.83	0	0.705	1.414	3.923	2.4117	4.04	1	training
11	Mg-Fe-023	140	12	0.75	0.25	0	0.72	0.645	0	1.31	1.83	0	0.70125	1.44	10.851	3.1178	6.2	1	training
12	Mg-Fe-031	140	12	0.7	0.3	0	0.72	0.645	0	1.31	1.83	0	0.6975	1.466	10.723	3.106	5.32	1	training
13	Zn-Al-20	100	12	0.8	0.2	0	0.74	0.535	0	1.65	1.61	0	0.699	1.642	10.247	3.0623	17.4	1	training
14	Zn-Al-033	100	12	0.67	0.33	0	0.74	0.535	0	1.65	1.61	0	0.67235	1.6368	18.969	5.0877	12.9	1	training
15	Cu-Cr-033	100	12	0.67	0.33	0	0.73	0.615	0	1.9	1.66	0	0.69205	1.8208	15.42	3.7139	8.17	1	training
16	Zn-Cr-033	100	12	0.67	0.33	0	0.74	0.615	0	1.65	1.66	0	0.69875	1.6533	17.729	4.4218	15.5	1	training
17	Zn-Al-035	110	13	0.65	0.35	0	0.74	0.535	0	1.65	1.61	0	0.66825	1.636	19.04	4.9309	12.9	1	training
18	Mg-Al-033	110	14	0.67	0.33	0	0.67	0.72	0	1.31	1.61	0	0.6865	1.409	18.779	4.5884	21.2	1	training
19	Zn-Cr-035	90	14	0.65	0.35	0	0.74	0.615	0	1.65	1.66	0	0.69625	1.6535	18.068	4.1795	14.9	1	training
20	Mg-Fe-40	100	20	0.6	0.4	0	0.72	0.645	0	1.31	1.83	0	0.69	1.518	1.104	1.784	8.35	1	training
21	Ni-Fe-029	70	16	0.71	0.29	0	0.69	0.645	0	1.91	1.83	0	0.67695	1.8868	17.962	4.2896	11.4	1	training
22	Co-Al-021	120	17	0.79	0.21	0	0.745	0.535	0	1.88	1.61	0	0.7009	1.8233	18.245	4.4559	6.31	1	training
23	Co-Al-Cr-0	100	15	0.71	0.15	0.15	0.745	0.535	0.615	1.88	1.61	1.66	0.6957	1.809	18.322	4.5132	7.5	1	training
24	Mn-Cr-Y-0	60	22	0.67	0.1	0.23	0.83	0.615	0.9	1.55	1.66	1.22	0.8246	1.4851	5.678	2.64	2.53	0	Run 1
25	Mn-Cr-030	60	12	0.67	0.33	0	0.83	0.615	0	1.55	1.66	0	0.75905	1.5863	0	0	7.48	0	Run 2
26	Mg-Y-030	100	12	0.7	0.3	0	0.72	0.9	0	1.31	1.22	0	0.774	1.283	6.41	2.7105	0.07	0	Run 3
27	Mg-Fe-Y-0	60	12	0.8	0.1	0.1	0.72	0.645	0.9	1.31	1.83	1.22	0.7305	1.353	4.037	2.44	0	0	Run 4
28	Ni-Fe-Ga-	120	15	0.67	0.23	0.1	0.69	0.645	0.62	1.91	1.83	1.81	0.67265	1.8816	18.63	4.6389	8.41	1	Run 5
29	Ni-Y-020	120	22	0.8	0.2	0	0.69	0.9	0	1.91	1.22	0	0.732	1.772	5.962	2.6689	3.86	0	Run 6
30	Ni-Fe-Cr-0	60	22	0.67	0.1	0.23	0.69	0.645	0.615	1.91	1.83	1.66	0.66825	1.8445	16.88	3.9205	4.88	1	Run 7
31	Mg-Al-Ga-	120	22	0.67	0.1	0.23	0.72	0.535	0.62	1.31	1.61	1.81	0.6785	1.455	17.35	4.0476	7.91	1	Run 8
32	Mn-Al-Fe-	120	22	0.67	0.23	0.1	0.83	0.535	0.645	1.55	1.61	1.83	0.74365	1.5918	0.668	1.5676	0.1	0	Run 9
33	Ni-Al-Ga-0	120	12	0.67	0.1	0.23	0.69	0.535	0.62	1.91	1.61	1.81	0.6584	1.857	18.33	4.5018	2.53	1	Run 10
34	Zn-Al-Ga-	120	22	0.8	0.1	0.1	0.74	0.535	0.62	1.65	1.61	1.81	0.7075	1.662	3.582	2.365	4.51	0	Run 11
35	Zn-Al-Y-0;	120	22	0.8	0.1	0.1	0.74	0.535	0.9	1.65	1.61	1.22	0.7355	1.603	7.015	2.766	0.28	0	Run 12
36	Zn-Al-Fe-0	120	22	0.8	0.1	0.1	0.74	0.535	0.645	1.65	1.61	1.83	0.71	1.664	0.567	1.4872	2.16	0	Run 13
37	Zn-Al-Cr-0	120	22	0.8	0.1	0.1	0.74	0.535	0.615	1.65	1.61	1.66	0.707	1.647	11.568	3.1899	7.23	0	Run 14
38	Zn-Al-Ga-	60	22	0.67	0.23	0.1	0.74	0.535	0.62	1.65	1.61	1.81	0.68085	1.6568	18.523	4.5564	5.87	1	Run 15
39	Ni-Fe-Y-0;	60	22	0.67	0.23	0.1	0.69	0.645	0.9	1.91	1.61	1.22	0.70065	1.772	15.782	3.6716	3.4	1	Run 16
40	Ni-Cr-Y-0;	60	22	0.67	0.23	0.1	0.69	0.615	0.9	1.91	1.66	1.22	0.69375	1.7835	17.086	3.9191	1.48	1	Run 17

a "1" means the success of LDH structure formation, while "0" means the fail of LDH structure formation.