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High-pressure crystal chemistry of $KAlSi_3O_8$ hollandite

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For deposit: Table 5

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Table 5A
$KAlSi_3O_8$ hollandite at 0 GPa in cell

h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	0	0	24.681	25.847	6	5	1	14.687	14.120
4	0	0	29.251	30.353	8	5	1	36.869	37.614
6	0	0	92.173	93.442	10	5	1	7.675	3.293
1	1	0	14.218	14.253	7	6	1	13.738	13.221
3	1	0	53.004	50.898	9	6	1	2.583	8.445
5	1	0	51.495	51.033	11	6	1	6.576	0.250
7	1	0	1.990	5.454	10	7	1	4.706	4.107
9	1	0	20.610	21.871	6	6	2	40.310	40.371
2	2	0	33.466	34.763	5	5	2	9.505	10.595
4	2	0	17.921	17.980	3	5	2	20.761	19.663
6	2	0	10.750	12.218	4	2	2	17.836	17.448
8	2	0	2.206	1.454	3	1	2	34.455	32.787
10	2	0	35.876	37.313	5	1	2	28.476	28.148
3	3	0	16.265	14.877	0	0	2	110.618	107.982
5	3	0	11.418	10.863	4	0	2	23.884	22.333
7	3	0	50.051	51.583	6	0	2	68.428	66.383
9	3	0	16.727	18.234	8	0	2	4.552	1.282
11	3	0	2.554	1.164	1	1	2	8.609	7.515
4	4	0	27.417	27.930	3	1	2	34.455	32.793
6	4	0	2.075	0.740	5	1	2	28.476	28.154
8	4	0	38.620	38.665	7	1	2	5.764	3.467
10	4	0	4.919	9.034	9	1	2	16.182	16.422
12	4	0	3.006	9.775	0	2	2	15.380	14.197
5	5	0	16.462	15.041	2	2	2	21.480	20.340
7	5	0	23.401	23.106	4	2	2	17.836	17.450
9	5	0	27.505	28.419	6	2	2	9.104	10.994
11	5	0	8.015	13.786	8	2	2	2.516	0.317
6	6	0	52.612	53.507	10	2	2	27.784	28.725
8	6	0	14.540	15.252	3	3	2	6.119	5.295
10	6	0	25.347	26.961	5	3	2	7.937	9.005
9	7	0	23.446	24.619	7	3	2	40.053	39.135
11	7	0	23.072	25.016	9	3	2	13.268	13.965
8	7	1	2.516	0.611	4	4	2	20.879	21.874
5	6	1	10.971	12.071	6	4	2	2.449	0.614
4	5	1	35.889	34.189	8	4	2	28.166	27.839
3	4	1	6.309	1.499	10	4	2	7.170	7.085
4	1	1	59.812	58.035	7	5	2	16.671	16.878
3	0	1	79.179	81.770	9	5	2	20.697	21.898
5	0	1	14.131	12.769	8	6	2	10.723	11.862
7	0	1	15.839	17.490	6	5	3	6.960	8.048
0	1	1	21.554	21.213	4	5	3	19.981	17.609
2	1	1	18.000	19.203	5	4	3	51.430	49.246
4	1	1	59.812	58.062	3	4	3	2.635	1.473
6	1	1	37.483	37.322	3	2	3	6.980	15.300
8	1	1	5.402	9.834	4	1	3	32.121	31.402
1	2	1	43.586	44.853	6	1	3	18.006	20.772
3	2	1	30.089	29.229	3	0	3	29.657	31.918
5	2	1	41.040	41.813	5	0	3	2.618	5.528
7	2	1	16.792	19.682	7	0	3	14.967	10.447
9	2	1	32.589	34.340	0	1	3	8.940	9.758
11	2	1	16.532	16.443	2	1	3	18.718	15.882
2	3	1	1.751	6.939	4	1	3	32.121	31.405
4	3	1	18.567	17.353	6	1	3	18.006	20.773
6	3	1	28.451	28.541	8	1	3	3.177	6.818
8	3	1	13.534	14.567	1	2	3	28.748	27.059
10	3	1	5.836	3.657	3	2	3	15.742	15.300
12	3	1	1.557	2.930	5	2	3	23.399	22.470
5	4	1	89.326	88.570	7	2	3	13.665	12.066
7	4	1	14.591	15.716	4	3	3	12.985	8.463
9	4	1	6.700	7.010	6	3	3	14.951	14.482
11	4	1	49.213	51.249	7	4	3	6.111	8.743

Table 5B
$KAlSi_3O_8$ hollandite at 1.64 GPa in cell

h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	3	1	3.112	6.380	6	5	1	16.417	14.526
2	0	0	25.605	26.409	8	5	1	39.476	39.151
4	0	0	28.954	30.305	10	5	1	6.156	3.248
6	0	0	92.531	95.369	7	6	1	10.988	12.754
1	1	0	14.135	14.105	9	6	1	6.770	7.933
3	1	0	54.421	52.245	11	6	1	4.258	0.214
5	1	0	53.758	51.477	10	7	1	3.857	3.450
7	1	0	1.951	5.248	6	6	2	40.366	41.374
9	1	0	21.412	23.191	3	5	2	20.590	19.271
2	2	0	32.943	34.644	2	4	2	36.012	33.949
4	2	0	16.266	17.698	5	1	2	28.835	28.810
6	2	0	13.884	11.917	0	0	2	110.457	111.045
8	2	0	4.384	1.970	4	0	2	23.543	22.757
10	2	0	36.496	38.439	6	0	2	69.930	68.259
3	3	0	16.231	14.991	3	1	2	34.622	33.833
5	3	0	9.979	9.657	1	1	2	6.070	7.841
7	3	0	51.720	52.218	3	1	2	34.622	33.839
9	3	0	18.965	18.588	5	1	2	28.835	28.816
11	3	0	2.415	2.550	7	1	2	5.340	3.308
4	4	0	27.046	28.842	9	1	2	18.222	17.757
6	4	0	7.353	1.274	0	2	2	15.800	14.660
8	4	0	37.929	39.623	2	2	2	22.023	20.263
10	4	0	7.984	9.052	4	2	2	18.761	17.090
12	4	0	9.148	10.399	6	2	2	11.062	10.961
5	5	0	15.440	15.452	8	2	2	4.990	0.718
7	5	0	22.229	23.745	10	2	2	30.197	29.840
9	5	0	27.251	29.317	3	3	2	4.116	5.010
11	5	0	11.547	14.701	5	3	2	8.254	8.359
6	6	0	54.028	54.238	7	3	2	40.642	39.897
8	6	0	12.802	14.883	9	3	2	14.709	14.439
10	6	0	27.926	28.736	4	4	2	23.479	22.555
9	7	0	23.735	26.151	6	4	2	2.410	0.276
11	7	0	26.773	26.763	8	4	2	28.747	29.151
8	7	1	6.019	1.539	10	4	2	6.670	7.072
4	5	1	35.940	35.659	5	5	2	7.633	10.919
4	1	1	61.093	58.754	7	5	2	16.171	17.797
3	0	1	84.128	83.352	9	5	2	19.834	22.827
5	0	1	14.466	13.726	8	6	2	11.078	11.695
7	0	1	16.613	17.527	6	5	3	8.413	8.705
0	1	1	21.518	21.407	4	5	3	19.348	19.383
2	1	1	18.750	19.290	5	4	3	51.567	51.636
4	1	1	61.093	58.788	3	4	3	4.633	1.128
6	1	1	39.598	38.659	3	2	3	8.071	15.561
8	1	1	11.308	9.941	4	1	3	34.878	32.275
1	2	1	43.310	44.910	3	0	3	35.720	33.580
3	2	1	29.079	29.211	5	0	3	2.654	6.294
5	2	1	43.160	42.877	7	0	3	14.052	10.475
7	2	1	18.768	19.924	0	1	3	11.392	9.984
9	2	1	34.013	35.945	2	1	3	16.090	16.381
4	3	1	17.814	17.427	4	1	3	34.878	32.279
6	3	1	29.794	29.218	6	1	3	22.537	22.178
8	3	1	12.582	13.271	8	1	3	8.830	6.792
10	3	1	6.239	4.169	1	2	3	29.366	27.248
12	3	1	9.294	2.808	3	2	3	15.033	15.561
3	4	1	1.829	0.657	5	2	3	24.643	23.917
5	4	1	90.469	90.515	7	2	3	9.757	12.101
7	4	1	15.967	16.030	4	3	3	9.012	8.606
9	4	1	6.210	6.585	6	3	3	16.992	15.403
11	4	1	51.823	53.337	7	4	3	11.859	9.327

Table 5C
$KAlSi_3O_8$ hollandite at 2.95 GPa in cell

h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	0	0	25.920	26.260	4	5	1	36.944	35.127
4	0	0	30.229	29.754	6	5	1	17.090	14.647
6	0	0	97.677	96.988	8	5	1	39.701	39.449
1	1	0	13.889	14.466	10	5	1	7.413	3.099
3	1	0	53.143	52.335	7	6	1	14.846	14.006
5	1	0	50.461	51.566	9	6	1	10.804	9.021
7	1	0	7.897	5.088	11	6	1	8.109	0.253
2	2	0	36.364	35.477	10	7	1	6.964	4.152
4	2	0	18.963	18.091	5	5	2	8.552	11.814
6	2	0	13.149	12.827	2	4	2	35.040	33.225
8	2	0	2.311	1.300	0	0	2	111.444	112.325
10	2	0	36.647	38.386	4	0	2	22.126	22.120
3	3	0	16.617	15.790	6	0	2	71.399	68.909
5	3	0	9.426	10.058	5	1	2	28.392	28.917
7	3	0	53.244	53.547	1	1	2	10.279	7.630
9	3	0	18.060	17.425	3	1	2	35.247	33.990
11	3	0	2.724	2.263	5	1	2	28.392	28.922
4	4	0	27.411	28.757	7	1	2	7.629	3.504
6	4	0	5.981	1.669	9	1	2	13.924	18.009
8	4	0	37.444	39.534	0	2	2	15.502	14.142
10	4	0	8.346	9.363	2	2	2	21.688	20.842
12	4	0	15.056	11.474	4	2	2	19.496	17.669
5	5	0	16.296	16.478	6	2	2	11.996	11.248
7	5	0	21.998	24.374	8	2	2	2.643	0.333
9	5	0	26.378	28.968	10	2	2	30.465	29.904
11	5	0	11.511	15.412	1	3	2	50.701	50.268
6	6	0	53.981	55.137	3	3	2	7.689	4.443
8	6	0	16.097	15.849	5	3	2	11.668	8.874
10	6	0	25.962	27.144	7	3	2	39.342	40.919
9	7	0	23.002	26.219	9	3	2	14.430	13.355
11	7	0	26.069	27.189	4	4	2	23.603	22.762
3	0	1	86.725	84.578	6	4	2	8.990	0.423
5	0	1	14.835	13.344	8	4	2	28.906	29.139
7	0	1	18.921	18.433	10	4	2	10.853	7.517
0	1	1	22.081	21.689	7	5	2	19.414	17.985
2	1	1	19.189	19.757	9	5	2	22.731	22.684
4	1	1	56.517	58.420	8	6	2	13.666	12.637
6	1	1	38.987	39.049	6	5	3	8.861	8.403
8	1	1	9.605	9.399	3	4	3	6.259	0.803
1	2	1	44.199	45.591	4	1	3	33.147	32.324
3	2	1	30.494	29.223	3	0	3	35.247	33.809
5	2	1	41.810	41.758	5	0	3	2.796	5.657
7	2	1	20.910	19.535	0	1	3	13.992	10.535
9	2	1	36.292	35.104	4	1	3	33.147	32.328
11	2	1	15.773	16.434	6	1	3	21.804	22.695
2	3	1	9.208	6.861	1	2	3	28.214	27.818
4	3	1	19.715	18.086	1	2	3	28.214	27.817
6	3	1	28.238	29.862	3	2	3	13.153	15.985
8	3	1	13.400	14.250	5	2	3	22.795	22.838
10	3	1	4.562	2.962	7	2	3	13.923	12.219
12	3	1	7.502	2.487	2	3	3	6.430	4.708
3	4	1	5.405	0.783	4	3	3	9.970	9.229
5	4	1	88.681	90.503	6	3	3	16.967	15.947
7	4	1	14.386	15.431	5	4	3	50.446	51.385
9	4	1	9.088	6.247	7	4	3	12.981	8.570
11	4	1	56.039	53.906					

Table 5D
$KAlSi_3O_8$ hollandite at 3.60 GPa in cell

h	k	l	Fo	Fc	h	k	l	Fo	Fc
8	1	3	2.999	6.879	12	3	1	5.561	2.971
7	0	3	15.044	11.548	5	4	1	95.179	90.134
6	1	3	24.077	23.230	7	4	1	18.185	14.900
9	1	2	22.660	17.737	9	4	1	7.930	6.857
8	0	2	9.337	1.403	11	4	1	51.900	54.113
7	0	1	17.288	18.743	6	5	1	18.476	15.064
4	1	1	58.524	58.355	8	5	1	40.558	39.645
2	0	0	25.634	26.194	10	5	1	12.117	3.027
4	0	0	30.119	29.862	9	6	1	6.617	9.524
6	0	0	97.195	96.622	11	6	1	2.931	0.508
1	1	0	14.444	14.407	8	6	2	9.607	13.081
3	1	0	55.888	52.081	6	6	2	39.779	42.212
5	1	0	50.353	51.298	5	5	2	10.712	12.187
7	1	0	2.185	5.691	3	5	2	21.302	19.821
2	2	0	32.939	35.454	4	4	2	22.793	23.058
4	2	0	17.433	18.469	2	4	2	34.223	32.847
6	2	0	15.093	13.515	5	1	2	28.952	28.752
10	2	0	35.981	38.731	0	0	2	110.007	111.784
3	3	0	17.987	15.945	2	0	2	14.736	14.063
5	3	0	8.989	9.709	4	0	2	23.423	22.264
7	3	0	52.993	53.619	6	0	2	71.249	68.906
9	3	0	17.153	17.165	3	1	2	35.482	34.091
11	3	0	6.257	2.797	1	1	2	5.246	7.702
4	4	0	26.554	29.091	3	1	2	35.300	34.092
6	4	0	4.872	2.023	5	1	2	28.952	28.758
8	4	0	38.141	39.248	7	1	2	4.895	3.950
10	4	0	4.433	9.171	2	2	2	20.338	20.815
12	4	0	5.535	11.726	4	2	2	17.480	18.016
5	5	0	18.330	17.019	6	2	2	12.845	11.810
7	5	0	23.784	25.222	8	2	2	6.470	0.461
9	5	0	27.924	29.269	3	3	2	8.453	4.603
11	5	0	17.330	16.216	5	3	2	6.992	8.759
8	6	0	11.134	16.295	7	3	2	43.194	41.098
10	6	0	25.588	27.367	9	3	2	12.057	13.254
11	7	0	26.044	27.217	6	4	2	8.739	0.704
10	7	1	3.075	4.197	8	4	2	29.837	28.886
7	6	1	15.252	13.954	10	4	2	10.424	7.452
4	5	1	32.839	34.735	7	5	2	16.118	18.710
3	4	1	5.138	1.174	9	5	2	22.280	22.979
3	0	1	84.097	84.024	6	5	3	9.656	8.742
5	0	1	16.621	13.955	4	5	3	17.413	18.439
0	1	1	21.025	21.811	7	4	3	14.683	8.257
2	1	1	21.867	20.171	5	4	3	51.517	51.544
4	1	1	58.524	58.412	3	4	3	9.551	0.997
6	1	1	38.855	39.493	4	3	3	2.794	8.968
8	1	1	9.881	9.932	2	3	3	4.983	5.106
10	1	1	25.741	23.396	4	1	3	33.853	32.571
1	2	1	41.599	45.459	3	0	3	32.469	33.733
3	2	1	29.918	29.167	5	0	3	3.146	5.933
5	2	1	41.663	41.221	2	1	3	17.350	16.628
7	2	1	19.698	19.080	0	1	3	11.681	10.739
9	2	1	34.691	34.922	2	1	3	17.350	16.628
11	2	1	15.341	15.645	4	1	3	33.853	32.572
2	3	1	8.362	7.310	6	1	3	24.077	23.231
4	3	1	19.402	17.592	3	2	3	17.397	16.135
6	3	1	29.489	29.677	5	2	3	19.289	22.775
8	3	1	15.217	14.702	7	2	3	11.992	12.017
10	3	1	9.828	2.987	6	3	3	20.313	15.790

Table 5E
$KAlSi_3O_8$ hollandite at 4.47 GPa in cell

h	k	l	Fo	Fc	h	k	l	Fo	Fc
8	4	2	30.749	30.032	7	6	1	15.519	15.404
7	3	2	39.761	39.654	4	7	1	20.441	18.643
6	2	2	12.637	11.332	6	7	1	34.034	34.613
5	1	2	28.330	29.581	8	7	1	3.811	2.557
8	8	0	4.903	5.681	10	7	1	7.180	5.056
1	1	0	15.259	14.844	5	8	1	20.495	20.543
3	1	0	47.768	49.645	7	8	1	10.021	9.818
2	2	0	36.507	36.045	9	8	1	20.071	20.875
4	2	0	19.057	17.594	6	9	1	10.222	8.655
1	3	0	72.480	71.211	8	9	1	5.704	5.268
3	3	0	16.955	15.942	7	10	1	9.931	3.098
5	3	0	12.296	11.976	4	8	2	7.773	5.886
7	3	0	50.729	51.827	5	7	2	28.354	29.860
2	4	0	57.135	55.114	3	7	2	31.561	30.319
4	4	0	28.507	27.740	2	6	2	5.793	7.358
6	4	0	4.229	0.283	1	5	2	15.736	14.041
8	4	0	41.454	40.462	0	0	2	105.665	104.998
3	5	0	24.059	24.368	4	0	2	22.621	22.155
5	5	0	16.621	17.089	1	1	2	9.038	7.406
7	5	0	23.964	23.771	3	1	2	31.707	32.825
9	5	0	28.414	27.561	0	2	2	15.849	13.636
4	6	0	18.069	17.787	2	2	2	20.900	21.481
6	6	0	53.601	53.838	4	2	2	17.609	17.352
8	6	0	15.119	16.059	1	3	2	48.790	49.024
3	7	0	41.796	39.788	3	3	2	6.539	3.654
5	7	0	41.524	40.587	5	3	2	13.495	9.841
7	7	0	18.846	16.498	2	4	2	31.278	32.849
9	7	0	24.206	24.170	4	4	2	22.255	21.934
4	8	0	10.793	6.613	6	4	2	4.814	0.501
6	8	0	6.794	10.336	3	5	2	19.312	19.409
10	8	0	25.550	24.856	5	5	2	14.663	12.286
5	9	0	6.879	3.219	7	5	2	17.348	17.193
7	9	0	49.839	50.727	4	6	2	16.499	14.834
9	9	0	17.076	17.061	6	6	2	40.445	41.036
8	10	0	18.221	14.191	8	6	2	12.180	12.676
9	6	1	11.365	8.957	7	7	2	11.851	12.178
1	4	1	36.100	36.577	6	8	2	6.857	7.597
0	3	1	79.002	79.572	5	6	3	11.197	8.213
0	1	1	20.521	21.082	3	6	3	15.923	15.318
2	1	1	18.017	18.976	2	5	3	43.235	44.781
4	1	1	53.826	56.350	0	5	3	8.744	5.109
1	2	1	43.316	44.736	4	1	3	31.695	31.533
3	2	1	28.562	28.300	3	0	3	33.334	33.628
5	2	1	38.124	39.147	0	1	3	11.880	10.285
2	3	1	6.897	8.319	2	1	3	15.272	14.829
4	3	1	17.982	17.639	4	1	3	31.695	31.531
6	3	1	29.278	29.324	1	2	3	28.769	27.316
3	4	1	3.048	2.654	3	2	3	17.244	15.506
5	4	1	88.768	86.787	5	2	3	18.725	20.924
7	4	1	15.114	14.958	2	3	3	7.029	5.143
2	5	1	79.085	78.246	4	3	3	13.233	9.208
4	5	1	34.864	33.604	3	4	3	8.318	1.388
6	5	1	15.528	15.015	5	4	3	48.784	50.230
8	5	1	37.701	38.423	4	5	3	19.486	17.244
3	6	1	27.950	28.314	6	5	3	11.295	8.150
5	6	1	11.419	12.864					