

Supporting Information on:

Combinatorial Study of the Li-Ni-Mn-Co Oxide  
Pseudo-Quaternary System for use in Li-ion  
Batteries

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**Table S.1:** List of hexagonal lattice parameters retrieved from the XRD fits for all single-phase layered compositions in this work. The list provides the  $a_{\text{hex}}$  and  $c_{\text{hex}}$  parameters along with their calculated errors  $\delta a_{\text{hex}}$  and  $\delta c_{\text{hex}}$ . The compositions are written in the format (Li, Ni, Mn, Co), where each atomic symbol represents the metallic fraction dispensed in the sample and their values have been rounded to three decimal places. As the initial compositions of these materials lie within the single-phase layered region of this system, the loss of the lithium during synthesis is noticeable but not severe and the final compositions are expected to be within 5% of the reported dispensed compositions. Sample cooling rate is indicated by ‘Q’ for quenching and ‘RC’ for regular-cooling.

Single-Phase Hexagonal Layered					
Dispensed Composition (Li, Ni, Mn, Co)	<b>a</b> (Å)	<b>δa</b> (Å)	<b>c</b> (Å)	<b>δc</b> (Å)	<b>Cooling Rate</b> (Q or RC)
(0.590, 0.311, 0.000, 0.100)	2.864	0.001	14.171	0.009	RC
(0.558, 0.342, 0.000, 0.100)	2.879	0.001	14.207	0.022	RC
(0.527, 0.374, 0.000, 0.100)	2.868	0.001	14.189	0.014	RC
(0.495, 0.405, 0.000, 0.100)	2.872	0.001	14.194	0.008	RC
(0.450, 0.450, 0.000, 0.100)	2.926	0.003	14.364	0.027	RC
(0.360, 0.540, 0.000, 0.100)	2.927	0.009	14.363	0.052	RC
(0.270, 0.630, 0.000, 0.100)	2.937	0.002	14.398	0.005	RC
(0.180, 0.720, 0.000, 0.100)	2.942	0.007	14.443	0.039	RC
(0.090, 0.810, 0.000, 0.100)	2.951	0.006	14.476	0.02	RC
(0.000, 0.900, 0.000, 0.100)	2.955	0.001	14.496	0.001	RC
(0.590, 0.279, 0.032, 0.100)	2.860	0.001	14.176	0.012	RC
(0.558, 0.311, 0.032, 0.100)	2.864	0.001	14.194	0.007	RC
(0.527, 0.342, 0.032, 0.100)	2.869	0.001	14.199	0.008	RC
(0.495, 0.374, 0.032, 0.100)	2.873	0.001	14.203	0.01	RC
(0.590, 0.248, 0.063, 0.100)	2.861	0.001	14.192	0.013	RC
(0.558, 0.279, 0.063, 0.100)	2.860	0.001	14.189	0.009	RC
(0.527, 0.311, 0.063, 0.100)	2.869	0.001	14.208	0.013	RC
(0.495, 0.342, 0.063, 0.100)	2.872	0.001	14.207	0.01	RC
(0.450, 0.360, 0.090, 0.100)	2.914	0.002	14.302	0.027	RC
(0.180, 0.630, 0.090, 0.100)	2.946	0.003	14.483	0.017	RC
(0.090, 0.720, 0.090, 0.100)	2.949	0.003	14.466	0.02	RC
(0.590, 0.216, 0.095, 0.100)	2.854	0.001	14.188	0.007	RC
(0.558, 0.248, 0.095, 0.100)	2.860	0.001	14.207	0.002	RC
(0.527, 0.279, 0.095, 0.100)	2.865	0.001	14.215	0.006	RC

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**Table S.1 – continued from previous page**

<b>Dispensed Composition (Li, Ni, Mn, Co)</b>	<b>a (Å)</b>	<b>δa (Å)</b>	<b>c (Å)</b>	<b>δc (Å)</b>	<b>Cooling Rate (Q or RC)</b>
(0.621, 0.153, 0.126, 0.100)	2.865	0.001	14.23	0.008	RC
(0.590, 0.185, 0.126, 0.100)	2.878	0.001	14.293	0.009	RC
(0.558, 0.216, 0.126, 0.100)	2.861	0.001	14.212	0.005	RC
(0.527, 0.248, 0.126, 0.100)	2.885	0.002	14.312	0.014	RC
(0.495, 0.279, 0.126, 0.100)	2.875	0.001	14.24	0.013	RC
(0.653, 0.090, 0.158, 0.100)	2.843	0.001	14.193	0.011	RC
(0.621, 0.122, 0.158, 0.100)	2.863	0.001	14.246	0.008	RC
(0.590, 0.153, 0.158, 0.100)	2.87	0.001	14.261	0.008	RC
(0.558, 0.185, 0.158, 0.100)	2.864	0.001	14.226	0.008	RC
(0.527, 0.216, 0.158, 0.100)	2.883	0.001	14.303	0.009	RC
(0.495, 0.248, 0.158, 0.100)	2.877	0.001	14.252	0.009	RC
(0.630, 0.090, 0.180, 0.100)	2.852	0.002	14.213	0.014	RC
(0.585, 0.135, 0.180, 0.100)	2.861	0.001	14.242	0.009	RC
(0.540, 0.180, 0.180, 0.100)	2.869	0.001	14.267	0.007	RC
(0.495, 0.225, 0.180, 0.100)	2.869	0.001	14.249	0.007	RC
(0.675, 0.000, 0.225, 0.100)	2.834	0.001	14.198	0.011	RC
(0.630, 0.045, 0.225, 0.100)	2.846	0.001	14.22	0.01	RC
(0.585, 0.090, 0.225, 0.100)	2.851	0.001	14.225	0.007	RC
(0.540, 0.135, 0.225, 0.100)	2.859	0.001	14.247	0.008	RC
(0.450, 0.450, 0.000, 0.100)	2.879	0.001	14.212	0.005	Q
(0.360, 0.540, 0.000, 0.100)	2.904	0.003	14.236	0.023	Q
(0.270, 0.630, 0.000, 0.100)	2.919	0.019	14.311	0.051	Q
(0.180, 0.720, 0.000, 0.100)	2.942	0.003	14.424	0.015	Q
(0.090, 0.810, 0.000, 0.100)	2.943	0.001	14.368	0.005	Q
(0.000, 0.900, 0.000, 0.100)	2.947	0.002	14.478	0.006	Q
(0.540, 0.270, 0.090, 0.100)	2.855	0.001	14.174	0.005	Q
(0.450, 0.360, 0.090, 0.100)	2.871	0.001	14.204	0.005	Q
(0.180, 0.630, 0.090, 0.100)	2.94	0.006	14.438	0.027	Q
(0.090, 0.720, 0.090, 0.100)	2.943	0.001	14.364	0.005	Q
(0.585, 0.135, 0.180, 0.100)	2.847	0.001	14.197	0.006	Q
(0.540, 0.180, 0.180, 0.100)	2.861	0.001	14.214	0.009	Q
(0.495, 0.225, 0.180, 0.100)	2.868	0.001	14.256	0.009	Q

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**Table S.1 – continued from previous page**

<b>Dispensed Composition (Li, Ni, Mn, Co)</b>	<b>a (Å)</b>	<b>δa (Å)</b>	<b>c (Å)</b>	<b>δc (Å)</b>	<b>Cooling Rate (Q or RC)</b>
(0.585, 0.045, 0.270, 0.100)	2.843	0.001	14.205	0.01	Q
(0.540, 0.090, 0.270, 0.100)	2.85	0.002	14.228	0.012	Q
(0.560, 0.240, 0.000, 0.200)	2.851	0.001	14.157	0.009	RC
(0.160, 0.640, 0.000, 0.200)	2.932	0.005	14.391	0.045	RC
(0.080, 0.720, 0.000, 0.200)	2.947	0.011	14.447	0.104	RC
(0.000, 0.800, 0.000, 0.200)	2.964	0.003	14.521	0.009	RC
(0.560, 0.160, 0.080, 0.200)	2.849	0.001	14.172	0.01	RC
(0.480, 0.240, 0.080, 0.200)	2.863	0.001	14.216	0.012	RC
(0.160, 0.560, 0.080, 0.200)	2.929	0.003	14.37	0.051	RC
(0.600, 0.040, 0.160, 0.200)	2.837	0.001	14.171	0.011	RC
(0.560, 0.080, 0.160, 0.200)	2.846	0.001	14.197	0.009	RC
(0.520, 0.120, 0.160, 0.200)	2.854	0.001	14.232	0.007	RC
(0.600, 0.000, 0.200, 0.200)	2.83	0.001	14.178	0.013	RC
(0.480, 0.320, 0.000, 0.200)	2.859	0.001	14.168	0.013	Q
(0.160, 0.640, 0.000, 0.200)	2.844	0.01	14.238	0.013	Q
(0.080, 0.720, 0.000, 0.200)	2.94	0.011	14.429	0.032	Q
(0.000, 0.800, 0.000, 0.200)	2.965	0.001	14.529	0.004	Q
(0.560, 0.160, 0.080, 0.200)	2.841	0.001	14.15	0.012	Q
(0.240, 0.480, 0.080, 0.200)	2.935	0.004	14.35	0.021	Q
(0.160, 0.560, 0.080, 0.200)	2.946	0.004	14.437	0.017	Q
(0.600, 0.040, 0.160, 0.200)	2.838	0.001	14.173	0.01	Q
(0.560, 0.080, 0.160, 0.200)	2.846	0.001	14.182	0.013	Q
(0.520, 0.120, 0.160, 0.200)	2.852	0.002	14.189	0.026	Q
(0.600, 0.000, 0.200, 0.200)	2.827	0.002	14.125	0.026	Q
(0.560, 0.040, 0.200, 0.200)	2.836	0.001	14.189	0.007	Q
(0.520, 0.080, 0.200, 0.200)	2.846	0.001	14.23	0.005	Q
(0.560, 0.140, 0.000, 0.300)	2.832	0.001	14.108	0.01	RC
(0.490, 0.210, 0.000, 0.300)	2.84	0.001	14.134	0.014	RC
(0.070, 0.630, 0.000, 0.300)	2.953	0.03	14.468	0.101	RC
(0.000, 0.700, 0.000, 0.300)	2.967	0.008	14.558	0.044	RC
(0.560, 0.070, 0.070, 0.300)	2.828	0.001	14.13	0.008	RC
(0.490, 0.140, 0.070, 0.300)	2.846	0.001	14.17	0.01	RC
(0.560, 0.000, 0.140, 0.300)	2.825	0.001	14.147	0.017	RC

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**Table S.1 – continued from previous page**

<b>Dispensed Composition (Li, Ni, Mn, Co)</b>	<b>a (Å)</b>	<b>δa (Å)</b>	<b>c (Å)</b>	<b>δc (Å)</b>	<b>Cooling Rate (Q or RC)</b>
(0.525, 0.035, 0.140, 0.300)	2.831	0.001	14.171	0.012	RC
(0.490, 0.070, 0.140, 0.300)	2.837	0.001	14.194	0.01	RC
(0.490, 0.210, 0.000, 0.300)	2.838	0.001	14.118	0.009	Q
(0.140, 0.560, 0.000, 0.300)	2.931	0.005	14.362	0.027	Q
(0.000, 0.700, 0.000, 0.300)	2.968	0.008	14.568	0.043	Q
(0.560, 0.070, 0.070, 0.300)	2.829	0.001	14.128	0.01	Q
(0.490, 0.140, 0.070, 0.300)	2.839	0.001	14.145	0.007	Q
(0.210, 0.420, 0.070, 0.300)	2.937	0.008	14.417	0.069	Q
(0.560, 0.000, 0.140, 0.300)	2.828	0.001	14.156	0.018	Q
(0.490, 0.070, 0.140, 0.300)	2.837	0.001	14.196	0.008	Q
(0.525, 0.035, 0.140, 0.300)	2.834	0.001	14.177	0.012	Q
(0.490, 0.035, 0.175, 0.300)	2.832	0.001	14.2	0.003	Q

**Table S.2:** List of cubic lattice parameters retrieved from fitting the XRD patterns of all single-phase cubic spinel compositions in this work. The list provides the  $a_{\text{cub}}$  parameters along with their calculated error  $\delta a_{\text{cub}}$ . The compositions are written in the format (Li, Ni, Mn, Co), where each atomic symbol represents the metallic fraction dispensed in the sample, which have been rounded to three decimal places. Due to lithium loss during synthesis being negligible for these materials, the final compositions are expected to be within 3% of the reported dispensed compositions. Sample cooling rate is indicated by ‘Q’ for quenching and ‘RC’ for regular-cooling.

### Single-Phase Cubic Spinel

Dispensed Composition (Li, Ni, Mn, Co)	$a$ (Å)	$\delta a$ (Å)	Cooling Rate (Q or RC)
(0.171, 0.225, 0.504, 0.100)	8.261	0.002	RC
(0.137, 0.252, 0.511, 0.100)	8.276	0.002	RC
(0.103, 0.279, 0.518, 0.100)	8.308	0.002	RC
(0.068, 0.306, 0.526, 0.100)	8.317	0.002	RC
(0.034, 0.333, 0.533, 0.100)	8.336	0.002	RC
(0.000, 0.360, 0.540, 0.100)	8.354	0.003	RC
(0.171, 0.198, 0.531, 0.100)	8.281	0.002	RC
(0.137, 0.225, 0.538, 0.100)	8.299	0.002	RC
(0.103, 0.252, 0.545, 0.100)	8.323	0.003	RC
(0.068, 0.279, 0.553, 0.100)	8.34	0.003	RC
(0.034, 0.306, 0.560, 0.100)	8.341	0.002	RC
(0.000, 0.333, 0.567, 0.100)	8.367	0.003	RC
(0.171, 0.171, 0.558, 0.100)	8.27	0.003	RC
(0.364, 0.036, 0.500, 0.100)	8.151	0.002	RC
(0.329, 0.072, 0.499, 0.100)	8.167	0.002	RC
(0.295, 0.108, 0.497, 0.100)	8.189	0.002	RC
(0.261, 0.144, 0.495, 0.100)	8.21	0.002	RC
(0.227, 0.180, 0.493, 0.100)	8.229	0.002	RC
(0.364, 0.000, 0.536, 0.100)	8.153	0.002	RC
(0.329, 0.036, 0.535, 0.100)	8.164	0.002	RC
(0.295, 0.072, 0.533, 0.100)	8.198	0.002	RC

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**Table S.2 – continued from previous page**

<b>Dispensed Composition (Li, Ni, Mn, Co)</b>	<b>a (Å)</b>	<b>δa (Å)</b>	<b>Cooling Rate (Q or RC)</b>
(0.329, 0.000, 0.571, 0.100)	8.144	0.004	RC
(0.295, 0.036, 0.569, 0.100)	8.203	0.002	RC
(0.261, 0.072, 0.567, 0.100)	8.213	0.002	RC
(0.270, 0.090, 0.540, 0.100)	8.199	0.002	RC
(0.180, 0.180, 0.540, 0.100)	8.258	0.002	RC
(0.090, 0.270, 0.540, 0.100)	8.304	0.002	RC
(0.000, 0.360, 0.540, 0.100)	8.354	0.002	RC
(0.315, 0.090, 0.495, 0.100)	8.145	0.002	RC
(0.270, 0.135, 0.495, 0.100)	8.167	0.003	RC
(0.315, 0.045, 0.540, 0.100)	8.131	0.003	RC
(0.270, 0.090, 0.540, 0.100)	8.196	0.002	RC
(0.315, 0.000, 0.585, 0.100)	8.159	0.004	RC
(0.270, 0.045, 0.585, 0.100)	8.192	0.003	RC
(0.270, 0.135, 0.495, 0.100)	8.2	0.002	Q
(0.270, 0.090, 0.540, 0.100)	8.222	0.001	Q
(0.180, 0.180, 0.540, 0.100)	8.264	0.002	Q
(0.090, 0.270, 0.540, 0.100)	8.314	0.001	Q
(0.000, 0.360, 0.540, 0.100)	8.356	0.002	Q
(0.270, 0.045, 0.585, 0.100)	8.209	0.002	Q
(0.270, 0.000, 0.630, 0.100)	8.226	0.001	Q
(0.180, 0.090, 0.630, 0.100)	8.239	0.006	Q
(0.240, 0.160, 0.400, 0.200)	8.167	0.002	RC
(0.320, 0.040, 0.440, 0.200)	8.12	0.002	RC
(0.280, 0.080, 0.440, 0.200)	8.149	0.002	RC
(0.240, 0.120, 0.440, 0.200)	8.193	0.002	RC
(0.320, 0.000, 0.480, 0.200)	8.139	0.002	RC
(0.280, 0.040, 0.480, 0.200)	8.175	0.001	RC
(0.240, 0.080, 0.480, 0.200)	8.213	0.001	RC
(0.160, 0.160, 0.480, 0.200)	8.244	0.002	RC
(0.240, 0.160, 0.400, 0.200)	8.206	0.002	Q
(0.240, 0.120, 0.440, 0.200)	8.198	0.002	Q
(0.160, 0.160, 0.480, 0.200)	8.233	0.001	Q
(0.240, 0.080, 0.480, 0.200)	8.207	0.002	Q
(0.280, 0.000, 0.520, 0.200)	8.208	0.002	Q
(0.240, 0.040, 0.520, 0.200)	8.229	0.002	Q
(0.240, 0.000, 0.560, 0.200)	8.244	0.003	Q
(0.160, 0.080, 0.560, 0.200)	8.287	0.002	Q

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**Table S.2 – continued from previous page**

<b>Dispensed Composition (Li, Ni, Mn, Co)</b>	<b>a (Å)</b>	<b>δa (Å)</b>	<b>Cooling Rate (Q or RC)</b>
(0.000, 0.240, 0.560, 0.200)	8.351	0.002	Q
(0.210, 0.140, 0.350, 0.300)	8.153	0.002	RC
(0.140, 0.210, 0.350, 0.300)	8.222	0.002	RC
(0.210, 0.105, 0.385, 0.300)	8.168	0.002	RC
(0.210, 0.070, 0.420, 0.300)	8.179	0.001	RC
(0.000, 0.280, 0.420, 0.300)	8.317	0.004	RC
(0.245, 0.000, 0.455, 0.300)	8.14	0.002	RC
(0.140, 0.140, 0.420, 0.300)	8.248	0.002	Q
(0.070, 0.210, 0.420, 0.300)	8.315	0.002	Q
(0.000, 0.280, 0.420, 0.300)	8.307	0.004	Q
(0.210, 0.035, 0.455, 0.300)	8.212	0.002	Q
(0.210, 0.000, 0.490, 0.300)	8.208	0.002	Q
(0.140, 0.070, 0.490, 0.300)	8.269	0.002	Q