Supplementary Information

Paper Ref.: B301189E

For deposition with RSC Electronic Supplementary Information service

Table S1 Anisotropic displacement parameters[a] ($Å^2$) in $Li_2Mg_2(MoO_4)_3$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo1	0.0080(1)	0.0071(1)	0.0065(1)	0	0.0001(1)	0
Mo2	0.00933(9)	0.00716(8)	0.00785(8)	0.00082(9)	0.00038(9)	-0.00100(7)
O1	0.0134(9)	0.0113(9)	0.0113(8)	-0.0021(8)	-0.0001(7)	0.0006(8)
O2	0.014(1)	0.013(1)	0.006(1)	0	0.002(1)	0
O3	0.0102(8)	0.0094(8)	0.0119(8)	0.0010(7)	0.0010(7)	-0.0021(7)
O4	0.011(1)	0.010(1)	0.011(1)	0	0.000(1)	0
O5	0.0113(8)	0.0096(8)	0.0110(7)	0.0004(8)	0.0015(7)	-0.0026(7)
O6	0.0108(9)	0.0139(9)	0.0101(8)	0.0004(8)	0.0020(7)	0.0009(7)
O7	0.0145(9)	0.0148(9)	0.0143(9)	0.0024(8)	-0.0004(8)	0.0038(8)

[a]The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2 (h^2a^{*2} U_{11} + k^2b^{*2} U_{22} + l^2c^{*2} U_{33} + 2hka^*b^* U_{12} + 2hla^*c^* U_{13} + 2klb^*c^* U_{23})]$

For deposition with ICDD

Table S2 X-ray powder diffraction data* for $Li_2Mg_2(MoO_4)_3$

h	*k*	*l*	d_{obs}(Å)	d_{cal}(Å)	I_{obs}(%)	I_{rel}(%)	*h*	*k*	*l*	d_{obs}(Å)	d_{cal} (Å)	I_{obs}(%)	I_{rel}(%)
0	2	0	5.220	5.232	10	7	1	4	4	2.051	2.059	7	9
0	1	3	5.107	5.122	12	7	2	2	4	2.038	2.038	5	5
0	2	2	4.498	4.498	15	10	2	3	3	1.943	1.946	6	10
1	1	1	-	4.448	-	20	2	0	6	1.925	1.929	6	6
1	0	2	4.425	4.425	30	11	1	5	1	1.922	1.925	8	9
0	3	1	3.411	3.422	16	17	1	3	7	1.891	1.896	6	9
1	2	2	3.367	3.379	100	100	1	2	8	1.883	1.887	7	16
0	2	4		3.370		20	1	5	3	1.834	1.839	5	9
0	1	5	3.335	3.340	55	16	2	4	0	1.828	1.829	7	14
1	0	4		3.339		57	1	4	6	1.824	1.825	9	11
0	3	3	2.986	2.999	8	8	2	2	6	1.807	1.810	12	24
0	0	6	2.928	2.937	6	6	1	1	9	-	1.801	-	9
1	3	1	2.833	2.844	6	6	0	5	5	1.797	1.799	7	9
0	4	0	2.608	2.616	7	10	0	0	10	-	1.762	-	7
1	3	3	2.579	2.587	12	17	1	6	2	1.619	1.622	6	13
0	2	6	2.560	2.561	17	16	1	4	8	1.598	1.601	4	8
2	0	0		2.558		14	2	3	7	1.593	1.595	7	8
1	0	6	2.537	2.547	8	10	3	2	2		1.594		10
1	4	1	2.301	2.309	5	7	3	0	4	1.588	1590	8	6
2	2	2	2.217	2.224	6	9	1	2	10		1.587		7

**Reflections with $I_{rel} < 5$ have been omitted*