Synthesis, Characterization and Chemical Bonding Analysis of the Quaternary Cyanamides $Li_2MnHf_2(NCN)_6$ and $Li_2MnZr_2(NCN)_6$

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Supporting Information

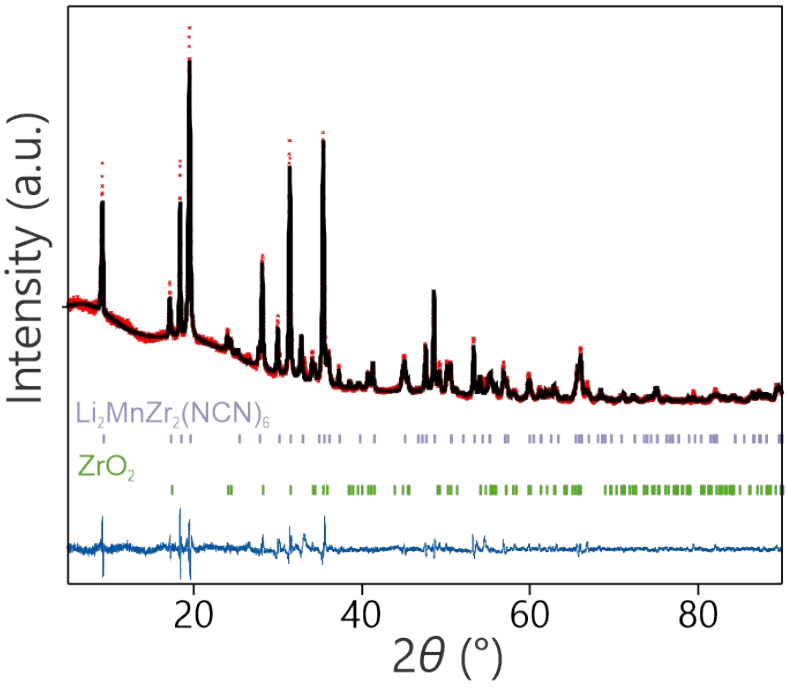

Figure S1. Rietveld fit of $Li_2MnZr_2(NCN)_6$ to PXRD data (Cu $K_{\alpha1}$), showing observed (red), calculated (black) and difference (blue) intensities. Bragg positions of $Li_2MnZr_2(NCN)_6$ (violet) and 20.1(1) wt% ZrO_2 baddeleyite $P2_1/c$ (blue) are denoted by vertical markers.

Table S1. CHN results of $Li_2MnHf_2(NCN)_6$ using ZnNCN and $Li_2MnZr_2(NCN)_6$ compared to theoretical values corrected for the presence of HfO_2 and ZrO_2.

		C	H	N
$Li_2MnHf_2(NCN)_6$	Theoretical (wt. %)	9.9	0	23.2
	Experimental (wt. %)	8.8	0	18.9
$Li_2MnZr_2(NCN)_6$	Theoretical (wt. %)	12.8	0	29.9
	Experimental (wt. %)	12.9	0	26.3

Table S2. Crystallographic data and fractional coordinates for $Li_2MnZr_2(NCN)_6$.[a]

Atom		*x*	*y*	*z*	*occ.*	U_{iso} (10^2 Å^2)
Li1	2*d*	⅓	⅔	½	0.944(1)	0.92(4)
Zr2	2*d*	⅓	⅔	½	0.056(1)	0.92(4)
Mn	1*b*	0	0	½	1	1.38(14)
Zr1	2*c*	⅓	⅔	0	0.944(1)	0.92(4)
Li2	2*c*	⅓	⅔	0	0.056(1)	0.92(4)
N1	6*k*	0.5945(15)	0	0.8687(7)	1	2.9(2)
N2	6*k*	0.3217(14)	0	0.3849(8)	1	2.9(2)
C	6*k*	0.628(3)	0	0.736(1)	1	2.9(2)
Trigonal, $P\bar{3}1m$ (No. 162), $Z = 1$, $a = 5.94791(12)$ Å, $c = 9.6403(3)$ Å; $R_{wp} = 5.84\%$, $R_p = 4.14\%$, $\chi^2 = 4.647$, $R_{wpb} = 8.45\ \%$						

[a] Standard deviations are given in parentheses.