Supporting Information

"Computational Screening of Dual Cation Metal Ammine Borohydrides by Density Functional Theory"

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Table S1. Crystallographic details of the lowest energy structures of $M_1M_2(BH_4)_3(NH_3)_{2-6}$ considered in the screening.

System	a	b	c	α	β	γ	Symmetry
$NaMg(BH_4)_3(NH_3)_2$	8.025	8.025	8.140	90.0	90.0	120.0	$P6_3/m$ (176)
$NaCa(BH_4)_3(NH_3)_2$	8.104	8.443	8.336	90.0	118.4	90.0	$P2_1$ (4)
$NaNi(BH_4)_3(NH_3)_2$	6.906	7.050	8.245	79.5	73.0	89.0	$P1$ (1)
$NaMn(BH_4)_3(NH_3)_2$	8.010	7.960	8.037	90.0	118.8	90.0	Pm (6)
$NaSr(BH_4)_3(NH_3)_2$	8.083	8.515	9.162	82.9	78.7	63.5	$P\bar{1}$ (2)
$NaZn(BH_4)_3(NH_3)_2$	7.976	7.976	10.043	90.0	90.0	120.0	$P\bar{6}$ (174)
$LiMg(BH_4)_3(NH_3)_2$	7.855	7.855	8.505	90.0	90.0	120.0	$P6_3/m$ (176)
$LiCa(BH_4)_3(NH_3)_2$	8.124	8.853	8.243	90.0	119.3	90.0	$P2_1/m$ (11)
$LiNi(BH_4)_3(NH_3)_2$	6.949	6.990	8.170	71.8	77.3	87.8	$P\bar{1}$ (2)
$LiMn(BH_4)_3(NH_3)_2$	7.879	7.879	8.611	90.0	90.0	120.0	$P6_3$ (173)
$LiSr(BH_4)_3(NH_3)_2$	7.682	8.392	9.020	81.5	77.4	64.1	$P\bar{1}$ (2)
$LiZn(BH_4)_3(NH_3)_2$	6.272	6.324	8.768	86.4	87.6	61.4	$P1$ (1)
$KMg(BH_4)_3(NH_3)_2$	8.230	8.230	8.128	90.0	90.0	120.0	$P6_3$ (173)
$KCa(BH_4)_3(NH_3)_2$	8.365	8.365	8.504	90.0	90.0	120.0	$P6_3/m$ (176)
$KNi(BH_4)_3(NH_3)_2$	7.296	7.732	8.090	62.5	68.2	88.8	$P\bar{1}$ (2)
$KMn(BH_4)_3(NH_3)_2$	8.206	8.217	8.219	89.6	60.4	88.3	$P1$ (1)
$KSr(BH_4)_3(NH_3)_2$	8.417	8.417	8.700	90.0	90.0	120.0	$P6_3/m$ (176)
$KZn(BH_4)_3(NH_3)_2$	6.334	6.424	8.856	92.4	90.7	118.9	$P1$ (1)
$NaMg(BH_4)_3(NH_3)_3$	7.808	8.970	9.225	66.6	84.4	81.9	$P1$ (1)
$NaCa(BH_4)_3(NH_3)_3$	8.216	8.474	10.956	83.5	83.3	62.5	$P1$ (1)
$NaNi(BH_4)_3(NH_3)_3$	7.387	6.826	8.178	90.0	93.4	90.0	$P2_1$ (4)
$NaMn(BH_4)_3(NH_3)_3$	8.068	9.047	9.103	64.3	82.8	77.3	$P1$ (1)
$NaSr(BH_4)_3(NH_3)_3$	8.105	8.992	9.022	63.1	76.7	80.8	$P1$ (1)
$NaZn(BH_4)_3(NH_3)_3$	7.534	8.408	10.332	86.6	89.5	66.8	$P1$ (1)
$LiMg(BH_4)_3(NH_3)_3$	7.463	9.413	9.534	83.1	80.1	72.6	$P1$ (1)
$LiCa(BH_4)_3(NH_3)_3$	7.966	8.395	8.508	90.0	97.5	90.0	$P2_1$ (4)
$LiNi(BH_4)_3(NH_3)_3$	7.923	8.306	9.852	71.5	84.9	68.7	$P1$ (1)
$LiMn(BH_4)_3(NH_3)_3$	7.326	8.037	10.100	86.4	86.9	66.6	$P1$ (1)
$LiSr(BH_4)_3(NH_3)_3$	7.770	8.401	10.134	81.7	75.5	82.1	$P1$ (1)
$LiZn(BH_4)_3(NH_3)_3$	6.997	6.211	7.329	90.0	93.7	90.0	$P2_1$ (4)
$KMg(BH_4)_3(NH_3)_3$	7.314	8.794	10.878	81.9	89.4	72.9	$P1$ (1)
$KCa(BH_4)_3(NH_3)_3$	8.174	8.991	9.057	64.7	76.7	81.8	$P1$ (1)
$KNi(BH_4)_3(NH_3)_3$	8.100	8.885	8.914	68.9	71.9	72.4	$P1$ (1)
$KMn(BH_4)_3(NH_3)_3$	7.552	7.886	10.505	90.1	91.7	113.4	$P1$ (1)
$KSr(BH_4)_3(NH_3)_3$	9.045	8.733	9.379	90.0	107.3	90.0	$P2_1$ (4)
$KZn(BH_4)_3(NH_3)_3$	6.496	6.730	8.668	88.0	88.6	64.6	$P1$ (1)
$NaMg(BH_4)_3(NH_3)_4$	7.361	9.426	9.963	62.5	84.2	80.3	$P1$ (1)
$NaCa(BH_4)_3(NH_3)_4$	7.783	8.438	9.774	89.2	85.1	81.7	$P1$ (1)
$NaNi(BH_4)_3(NH_3)_4$	7.320	7.920	7.927	80.2	87.3	89.7	$P1$ (1)
$NaMn(BH_4)_3(NH_3)_4$	7.163	8.847	9.811	95.8	96.1	99.6	$P1$ (1)
$NaSr(BH_4)_3(NH_3)_4$	7.808	8.489	9.871	90.0	95.0	97.8	$P1$ (1)
$NaZn(BH_4)_3(NH_3)_4$	6.205	8.126	8.363	117.5	90.9	90.9	$P1$ (1)
$LiMg(BH_4)_3(NH_3)_4$	7.571	9.761	10.372	113.7	91.8	92.5	$P1$ (1)
$LiCa(BH_4)_3(NH_3)_4$	7.676	8.637	9.398	86.6	81.2	86.9	$P1$ (1)
$LiNi(BH_4)_3(NH_3)_4$	6.778	9.890	10.526	116.3	93.3	91.3	$P1$ (1)
$LiMn(BH_4)_3(NH_3)_4$	6.814	9.266	11.212	98.7	99.5	97.1	$P1$ (1)
$LiSr(BH_4)_3(NH_3)_4$	7.759	8.568	9.311	88.1	87.5	81.3	$P1$ (1)
$LiZn(BH_4)_3(NH_3)_4$	6.108	8.147	8.218	117.8	91.5	90.8	$P1$ (1)
$KMg(BH_4)_3(NH_3)_4$	7.676	9.370	9.892	116.4	90.3	90.9	$P1$ (1)
$KCa(BH_4)_3(NH_3)_4$	9.210	9.389	10.151	87.6	89.0	61.4	$P1$ (1)

$KNi(BH_4)_3(NH_3)_4$	7.567	7.872	7.888	81.6	86.9	89.6	*P1* (1)
$KMn(BH_4)_3(NH_3)_4$	6.483	9.908	11.752	76.1	85.7	72.2	*P1* (1)
$KSr(BH_4)_3(NH_3)_4$	7.808	8.594	10.112	89.7	86.8	81.9	*P1* (1)
$KZn(BH_4)_3(NH_3)_4$	6.185	7.628	8.127	94.5	98.5	96.6	*P1* (1)
$NaMg(BH_4)_3(NH_3)_5$	8.792	8.859	11.333	94.4	93.4	116.3	*P1* (1)
$NaCa(BH_4)_3(NH_3)_5$	7.934	9.220	9.956	89.0	88.0	71.3	*P1* (1)
$NaNi(BH_4)_3(NH_3)_5$	8.341	9.547	9.625	87.2	85.9	74.4	*P1* (1)
$NaMn(BH_4)_3(NH_3)_5$	7.629	9.724	10.665	84.7	72.7	73.9	*P1* (1)
$NaSr(BH_4)_3(NH_3)_5$	8.500	9.137	12.131	82.9	87.4	63.8	*P1* (1)
$NaZn(BH_4)_3(NH_3)_5$	5.859	6.794	10.564	86.4	81.3	88.0	*P1* (1)
$LiMg(BH_4)_3(NH_3)_5$	7.101	8.280	12.672	85.3	80.1	85.9	*P1* (1)
$LiCa(BH_4)_3(NH_3)_5$	7.480	9.226	10.047	86.3	85.4	79.0	*P1* (1)
$LiNi(BH_4)_3(NH_3)_5$	7.213	8.650	8.820	89.7	66.7	86.7	*P1* (1)
$LiMn(BH_4)_3(NH_3)_5$	8.074	9.614	10.009	90.0	88.9	66.5	*P1* (1)
$LiSr(BH_4)_3(NH_3)_5$	8.564	9.029	12.107	98.4	93.1	116.9	*P1* (1)
$LiZn(BH_4)_3(NH_3)_5$	5.910	6.625	10.855	101.2	103.5	96.3	*P1* (1)
$KMg(BH_4)_3(NH_3)_5$	9.005	9.017	11.169	94.3	91.3	115.5	*P1* (1)
$KCa(BH_4)_3(NH_3)_5$	8.060	9.558	9.852	84.7	69.8	89.9	*P1* (1)
$KNi(BH_4)_3(NH_3)_5$	7.218	9.606	9.896	94.9	100.2	92.0	*P1* (1)
$KMn(BH_4)_3(NH_3)_5$	8.222	8.780	10.789	84.2	73.4	76.6	*P1* (1)
$KSr(BH_4)_3(NH_3)_5$	8.131	9.593	10.801	78.4	86.9	78.2	*P1* (1)
$KZn(BH_4)_3(NH_3)_5$	6.823	8.067	8.375	90.8	90.3	112.9	*P1* (1)
$NaMg(BH_4)_3(NH_3)_6$	8.446	8.524	9.767	90.3	91.4	93.2	*P1* (1)
$NaCa(BH_4)_3(NH_3)_6$	8.178	9.194	9.991	93.2	90.5	90.8	*P1* (1)
$NaNi(BH_4)_3(NH_3)_6$	7.523	8.271	9.590	88.7	84.8	74.6	*P1* (1)
$NaMn(BH_4)_3(NH_3)_6$	8.781	8.526	9.914	90.0	96.4	90.0	$P2_1$ (4)
$NaSr(BH_4)_3(NH_3)_6$	7.170	10.014	11.139	99.4	91.7	108.7	*P1* (1)
$NaZn(BH_4)_3(NH_3)_6$	8.236	9.131	9.838	85.7	87.1	86.8	*P1* (1)
$LiMg(BH_4)_3(NH_3)_6$	7.766	9.172	9.869	87.0	88.5	86.2	*P1* (1)
$LiCa(BH_4)_3(NH_3)_6$	7.946	9.684	9.756	87.0	87.4	87.2	*P1* (1)
$LiNi(BH_4)_3(NH_3)_6$	7.512	8.165	9.703	87.0	83.1	73.3	*P1* (1)
$LiMn(BH_4)_3(NH_3)_6$	7.795	8.432	13.340	88.3	87.3	68.4	*P1* (1)
$LiSr(BH_4)_3(NH_3)_6$	7.100	9.508	10.960	99.4	96.9	99.1	*P1* (1)
$LiZn(BH_4)_3(NH_3)_6$	6.980	7.563	9.117	88.2	83.9	74.4	*P1* (1)
$KMg(BH_4)_3(NH_3)_6$	8.563	8.468	12.712	90.0	129.2	90.0	*Pc* (7)
$KCa(BH_4)_3(NH_3)_6$	8.318	9.213	9.883	90.0	92.5	90.0	$P2_1$ (4)
$KNi(BH_4)_3(NH_3)_6$	7.571	8.300	9.673	87.6	85.2	73.0	*P1* (1)
$KMn(BH_4)_3(NH_3)_6$	7.302	9.658	12.888	83.9	82.1	78.1	*P1* (1)
$KSr(BH_4)_3(NH_3)_6$	8.427	9.269	9.873	90.0	93.6	90.0	$P2_1$ (4)
$KZn(BH_4)_3(NH_3)_6$	7.159	7.696	9.015	89.5	84.7	74.9	*P1* (1)