Novel Corrugated 2D In_9 Anionic Layer in $\text{Li}_2\text{Y}_5\text{In}_9$: Square Pyramidal In_5
Clusters Bridged by Unusual Butterfly In_4 Clusters

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Supporting Information

Figure S1. View of the $\text{In}(5)\text{In}(1)_4$ layer in the ab plane. The long In1-In1 separations of 3.567 and 3.670 Å are represented by dotted lines.

Figure S2. Coordination geometries around Y and Li atoms. The thermal ellipsoids for Y and In atoms are drawn at 50% probability. Y, Li and In atoms are represented by red, yellow and cyan circles, respectively.

Figure S3. The coordination geometries around indium atoms. Y, Li and In atoms are represented by red, yellow and cyan circles, respectively.

Table S1. Selected bond angles ($^{\circ}$) for $\text{Li}_2\text{Y}_5\text{In}_9$.

In(3)-Y(1)-In(3)	84.64(3) x4	In(3)-Y(1)-In(3)	144.42(9) x2
In(3)-Y(1)-In(2)	72.21(5) x4	In(3)-Y(1)-In(1)	58.47(2) x4
In(3)-Y(1)-In(1)	101.49(2) x8	In(3)-Y(1)-In(1)	157.10(8) x4
In(2)-Y(1)-In(1)	130.68(3) x4	In(1)-Y(1)-In(1)	64.85(4) x4
In(1)-Y(1)-In(1)	98.63(7) x2	In(2)-Y(2)-In(3)	72.19(3) x2
In(3)-Y(2)-In(3)	82.32(3)	In(2)-Y(2)-In(4)	60.50(3)x2
In(3)-Y(2)-In(4)	132.05(3) x2	In(3)-Y(2)-In(4)	90.16(2) x2

In(4)-Y(2)-In(4)	60.90(3)	In(2)-Y(2)-In(4)	135.85(3) x2
In(3)-Y(2)-In(4)	151.89(3) x2	In(3)-Y(2)-In(4)	102.88(2) x2
In(4)-Y(2)-In(4)	75.93(2) x2	In(4)-Y(2)-In(4)	105.34(2) x2
In(4)-Y(2)-In(4)	60.10(3)	In(2)-Y(2)-In(6)	126.29(3) x2
In(3)-Y(2)-In(6)	55.10(2) x2	In(3)-Y(2)-In(6)	107.14(3) x2
In(4)-Y(2)-In(6)	162.56(3) x2	In(4)-Y(2)-In(6)	106.65(2) x2
In(4)-Y(2)-In(6)	97.47(3) x2	In(4)-Y(2)-In(6)	58.03(2) x2
In(6)-Y(2)-In(6)	82.37(3)	In(5)-Y(3)-In(6)	78.95(3) x2
In(6)-Y(3)-In(6)	85.11(3)	In(5)-Y(3)-In(1)	58.56(3) x2
In(6)-Y(3)-In(1)	137.42(3) x2	In(6)-Y(3)-In(1)	88.96(2) x2
In(1)-Y(3)-In(1)	67.81(3)	In(5)-Y(3)-In(3)	132.02(3) x2
In(6)-Y(3)-In(3)	55.03(2) x2	In(6)-Y(3)-In(3)	106.95(3) x2
In(1)-Y(3)-In(3)	161.82(3) x2	In(1)-Y(3)-In(3)	103.70(2) x2
In(3)-Y(3)-In(3)	79.49(3)	In(5)-Y(3)-In(1)	127.55(3) x2
In(6)-Y(3)-In(1)	153.50(3) x2	In(6)-Y(3)-In(1)	99.13(2)x2
In(1)-Y(3)-In(1)	69.04(3) x2	In(1)-Y(3)-In(1)	104.44(2) x2
In(3)-Y(3)-In(1)	99.10(3) x2	In(3)-Y(3)-In(1)	57.47(2) x2
In(1)-Y(3)-In(1)	65.95(3)	In(6)-Y(4)-In(6)	88.14(2) x4
In(6)-Y(4)-In(6)	159.25(9) x2	In(6)-Y(4)-In(5)	79.62(4) x8
In(6)-Y(4)-In(4)	142.85(7) x4	In(6)-Y(4)-In(4)	57.91(2) x4
In(5)-Y(4)-In(4)	137.53(3) x4	In(6)-Y(4)-In(4)	97.64(3) x4
In(4)-Y(4)-In(4)	57.04(3) x4	In(4)-Y(4)-In(4)	84.94(6) x2
In(1)-Li(1)-In(1)	131(1)	In(1)-Li(1)-In(3)	161(1) x2
In(1)-Li(1)-In(3)	67.4(1) x2	In(3)-Li(1)-In(3)	94.0(9)
In(4)-Li(2)-In(4)	142(1)	In(4)-Li(2)-In(6)	65.5(1) x2
In(4)-Li(2)-In(6)	152.9(8) x2	In(6)-Li(2)-In(6)	87.4(7)
In(5)-In(1)-In(3)	133.49(4)	In(4)-In(2)-In(4)	61.23(3) x4
In(4)-In(2)-In(4)	92.15(5)x2	In(6)-In(3)-In(6)	85.74(3)
In(6)-In(3)-In(1)	106.61(2) x2	In(6)-In(4)-In(2)	147.26(3)
In(6)-In(4)-In(4)	99.39(1) x2	In(2)-In(4)-In(4)	59.38(1) x2

In(4)-In(4)-In(4)	90.0	In(1)-In(5)-In(1)	70.20(3) x4
In(1)-In(5)-In(1)	108.82(6) x2	In(3)-In(6)-In(3)	90.10(3)
In(3)-In(6)-In(4)	110.01(2) x2		

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Li}_2\text{Y}_5\text{In}_9$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\text{h}^2\text{a}^{*2}\text{U}^{11} + \dots + 2\text{hka}^*\text{b}^*\text{U}^{12} \dots]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Y(1)	12(1)	12(1)	40(1)	0	0	0
Y(2)	8(1)	8(1)	8(1)	-1(1)	1(1)	0(1)
Y(3)	8(1)	8(1)	7(1)	0(1)	0(1)	-1(1)
Y(4)	11(1)	11(1)	25(1)	0	0	0
Li(1)	8(13)	35(17)	40(16)	0	0	0
Li(2)	37(18)	36(18)	12(12)	0	0	0
In(1)	22(1)	11(1)	9(1)	0	-4(1)	0
In(2)	9(1)	9(1)	32(1)	0	0	0
In(3)	12(1)	7(1)	10(1)	0	0(1)	0
In(4)	17(1)	9(1)	9(1)	0	-3(1)	0
In(5)	9(1)	9(1)	35(1)	0	0	0
In(6)	7(1)	12(1)	10(1)	0(1)	0	0

Table S3. Selected Bond Distances ($\text{\AA}$) and Mulliken Overlap Populations (MOP) in $\text{Li}_2\text{Y}_5\text{In}_9$.

contact	bond	MOP	contact	bond	MOP
Y1-In6	3.087	0.387	Y4-In3	3.104	0.362
Y3-In2	3.137	0.339	Y2-In5	3.145	0.320
Y3-In3	3.174	0.365	Y2-In6	3.175	0.377
Y1-In5	3.187	0.314	Y2-In1	3.199	0.382
Y4-In2	3.206	0.271	Y3-In4	3.219	0.380
Y3-In6	3.261	0.308	Y2-In3	3.268	0.301
Y2-In1	3.277	0.331	Y4-In1	3.327	0.250
Y1-In4	3.417	0.224	Y1-In4	2.7-3.0	0.023
In3-In6	2.978	0.436	In1-In5	3.102	0.268
In1-In3	3.147	0.341	In4-In6	3.162	0.328
In2-In4	3.204	0.171	In4-In4	3.263	0.241
In1-In1	3.568	0.062	In1-In1	3.670	0.044
Li-In	2.7-3.0	0.03			