# Electronic Supplementary Information (ESI)

## Anions-Templated Assembly of Three Indium-Organic Frameworks with Diverse Topologies

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**Figure S1**. a) the coordination mode of the In(III) in **JLU-Liu8**; b) a (4,4)-connected framework the channels viewed from the *c* axis; c) space-filling representation of the 3D framework along the *c* axis; d) topological features of **JLU-Liu8** displayed by **ung** tiling.

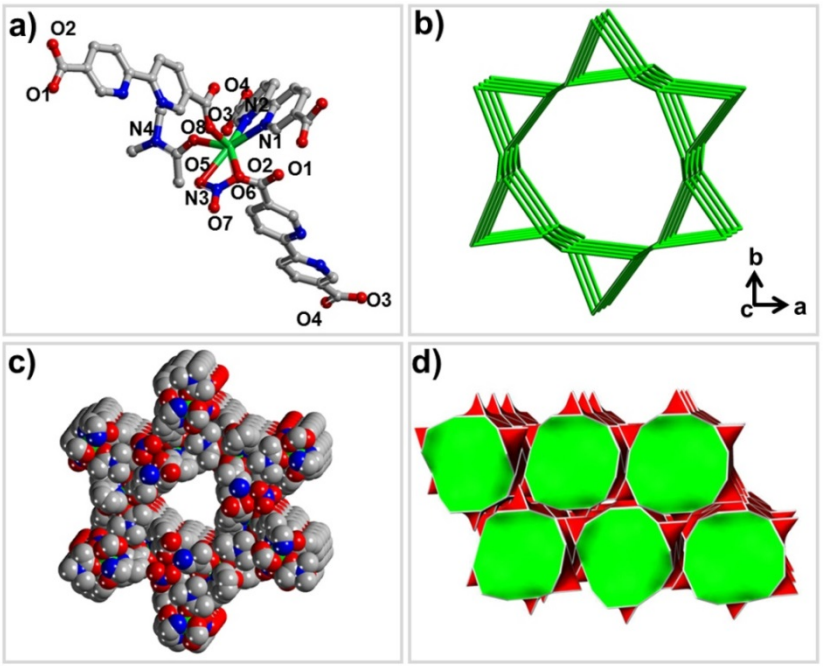



**Figure S2**. a) the coordination mode of the In(III) in **JLU-Liu9**; b) a (4,4)-connected framework; c) the smaller square channel A and the bigger square channel B; d) topological features of **JLU-Liu9** displayed by **crb** tiling.

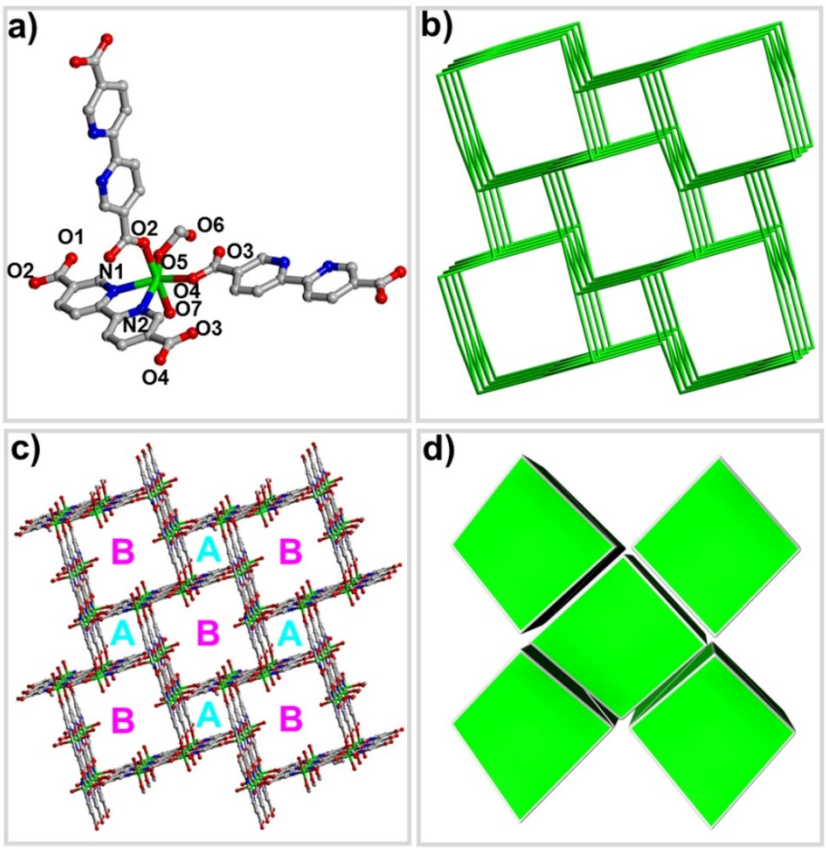


**Figure S3**. a) the coordination mode of the In(III) in **JLU-Liu10**; b) a (4,4)-connected framework; c) space-filling representation of the 3D framework; d) topological features of **JLU-Liu10** displayed by **cbo** tiling.

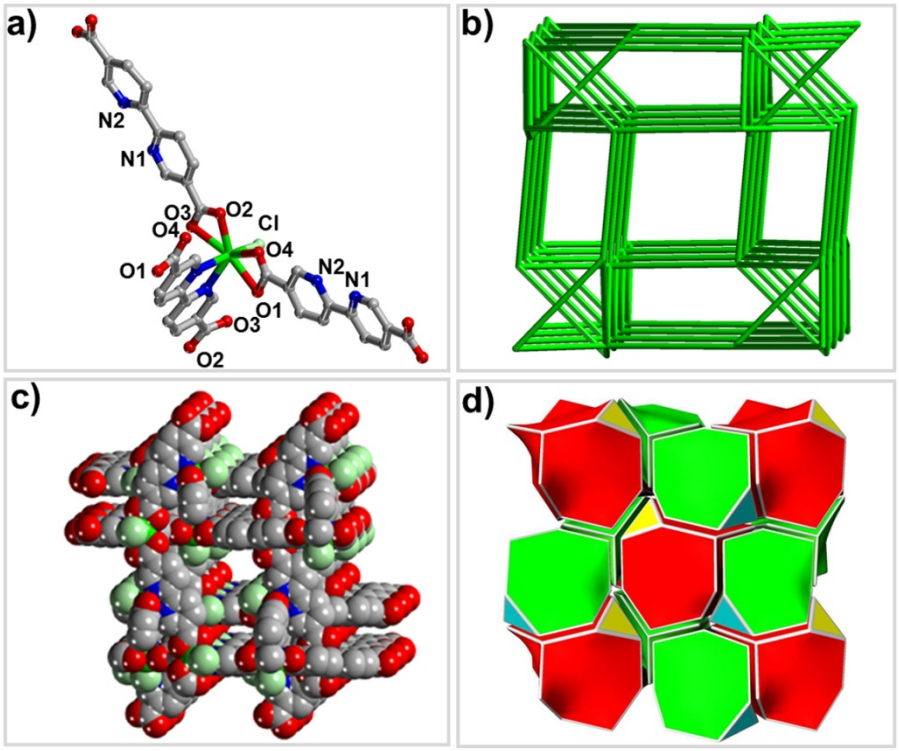
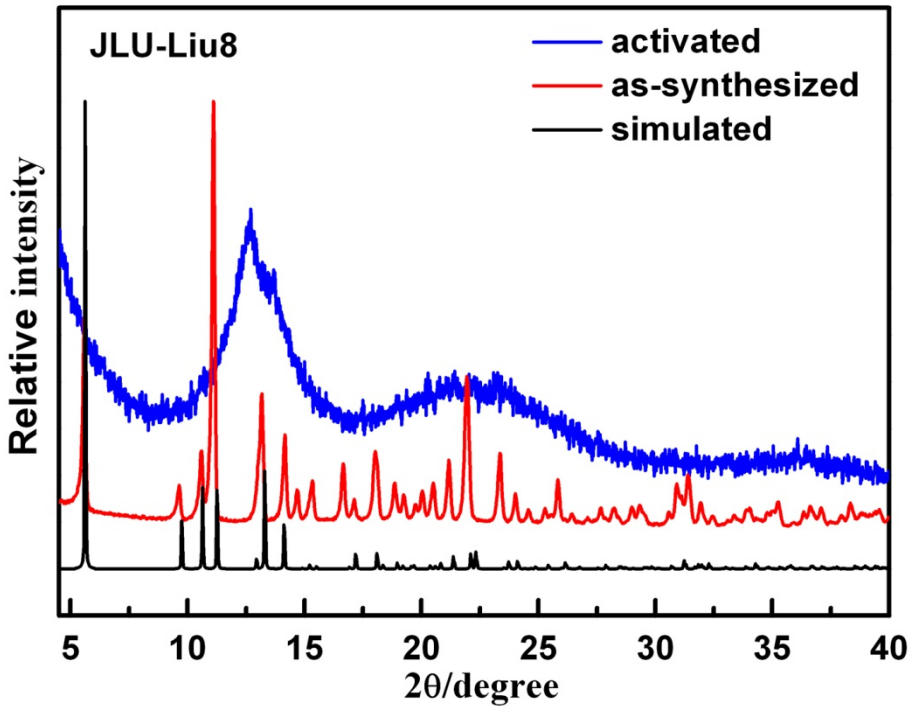
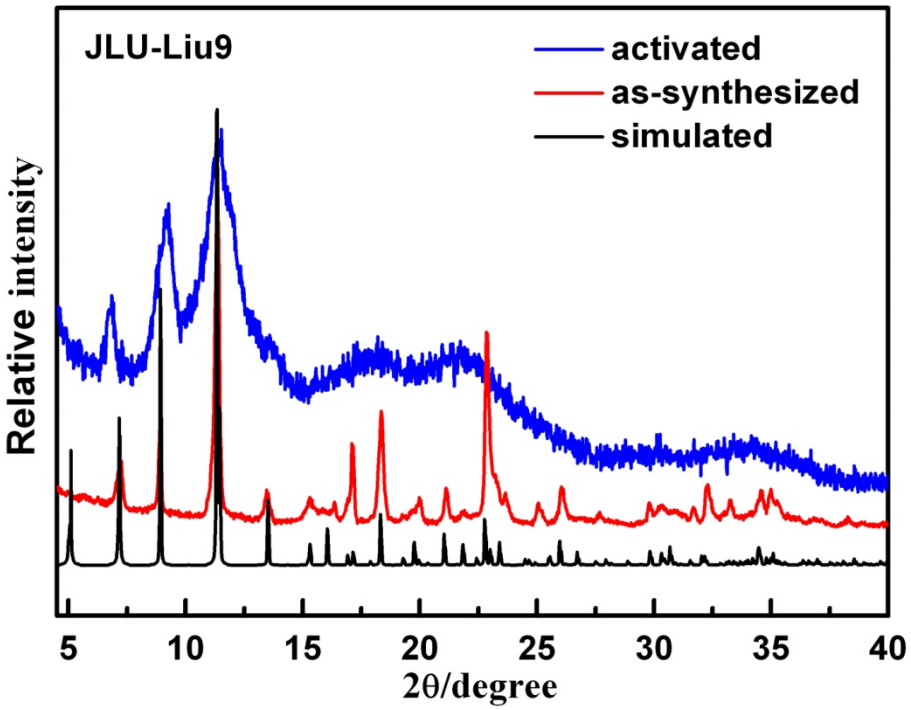



**Figure S4**. PXRD patterns of the activated, as-synthesized and simulated compounds: **JLU-Liu8**, **JLU-Liu9** and **JLU-Liu10**.




JLU-Liu9
activated
as-synthesized
simulated
Relative intensity
5
10
15
20
25
30
35
40
2θ/degree

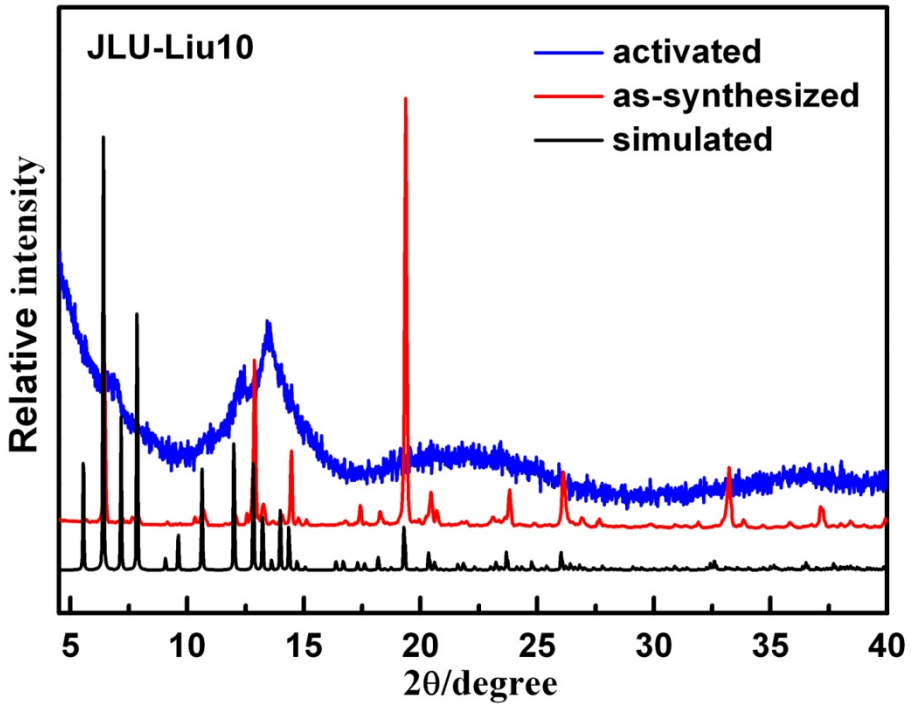

JLU-Liu10
activated
as-synthesized
simulated
Relative intensity
5
10
15
20
25
30
35
40
2θ/degree

**Figure S5**. FT-IR spectra for compounds **JLU-Liu8**, **JLU-Liu9** and **JLU-Liu10**.

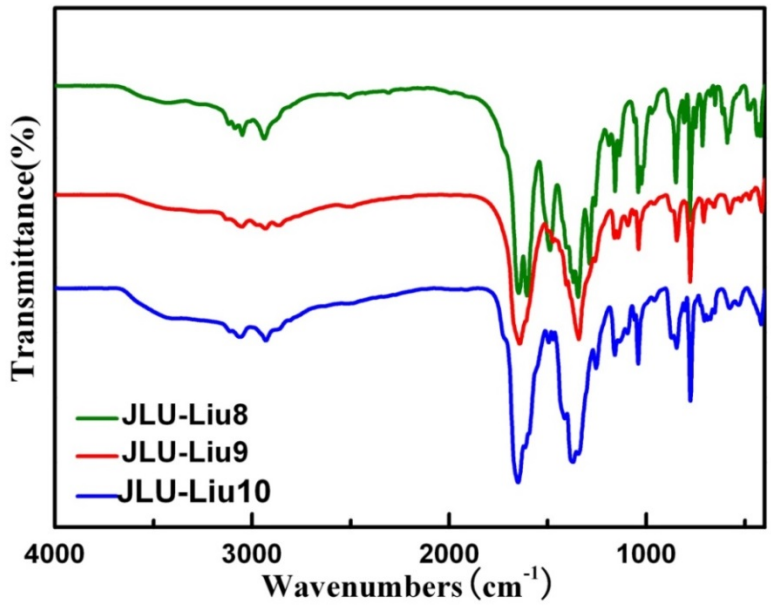
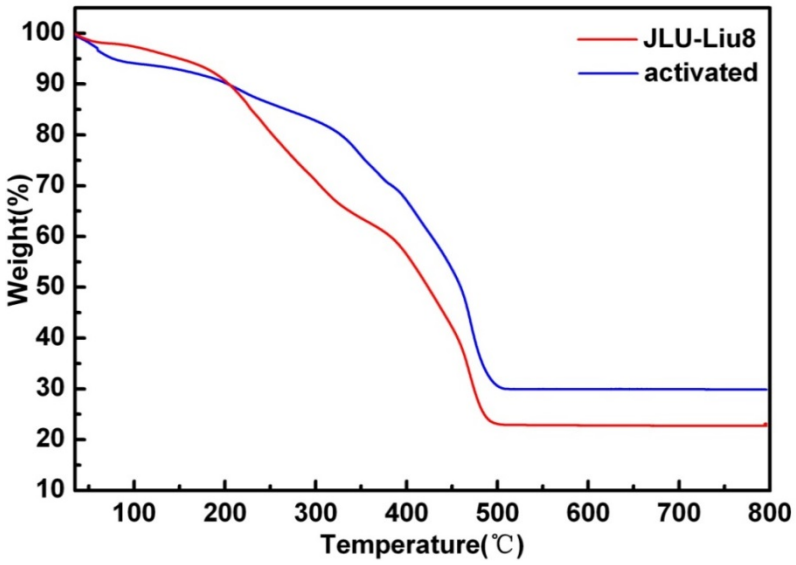



**Figure S6**. TGA curves for **JLU-Liu8, JLU-Liu9** and **JLU-Liu10**.



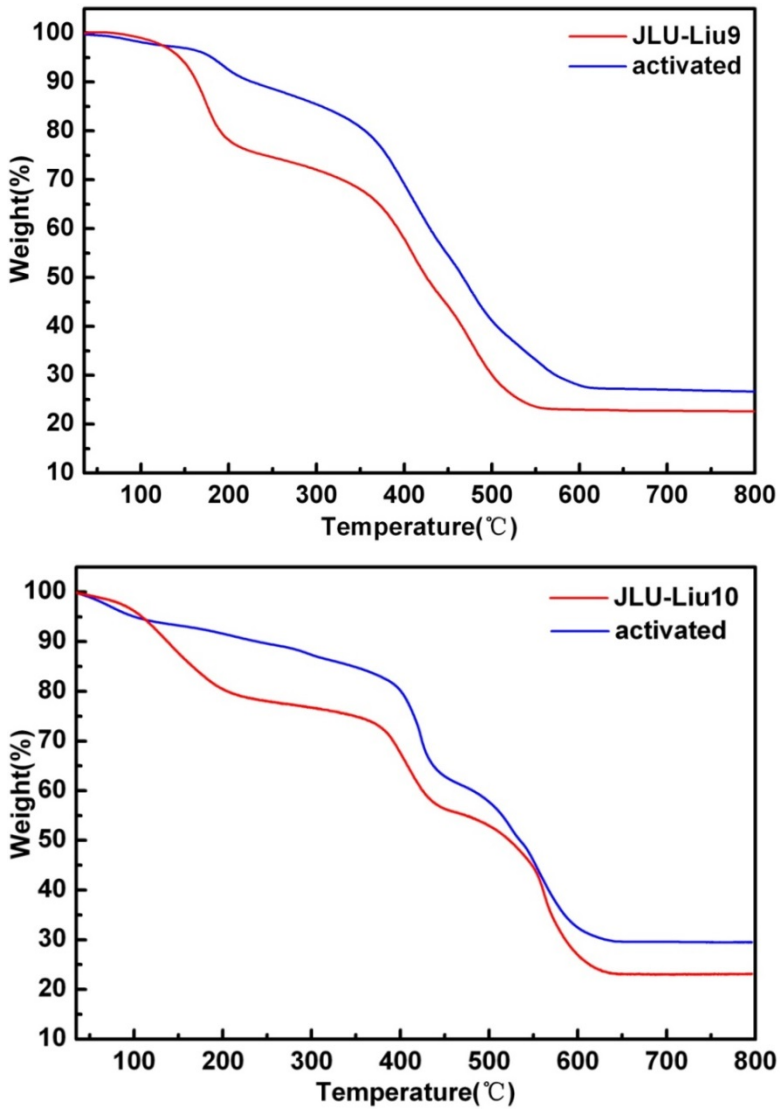



**Figure S7**. Different tetrahedral angles for simplified **JLU-Liu8**, **JLU-Liu9** and **JLU-Liu10**.

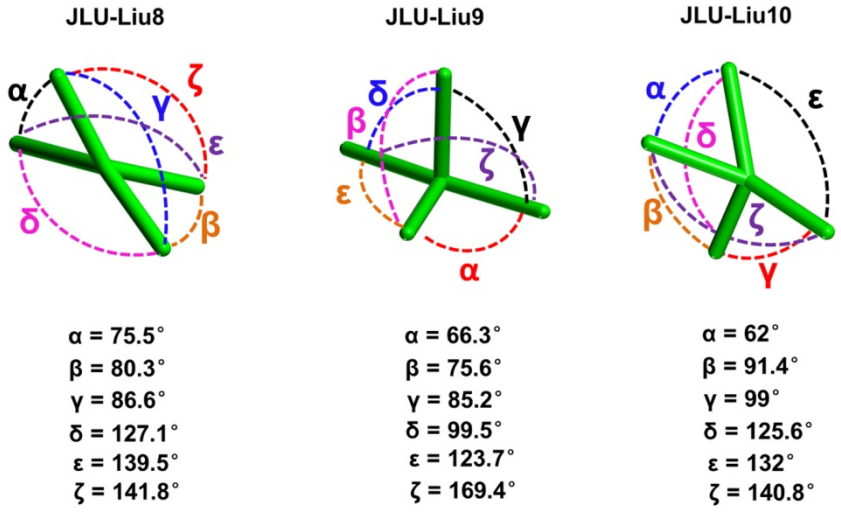


**Figure S8**. Absorption spectra of the $H_2$bpydc ligand and three compounds at room temperature.

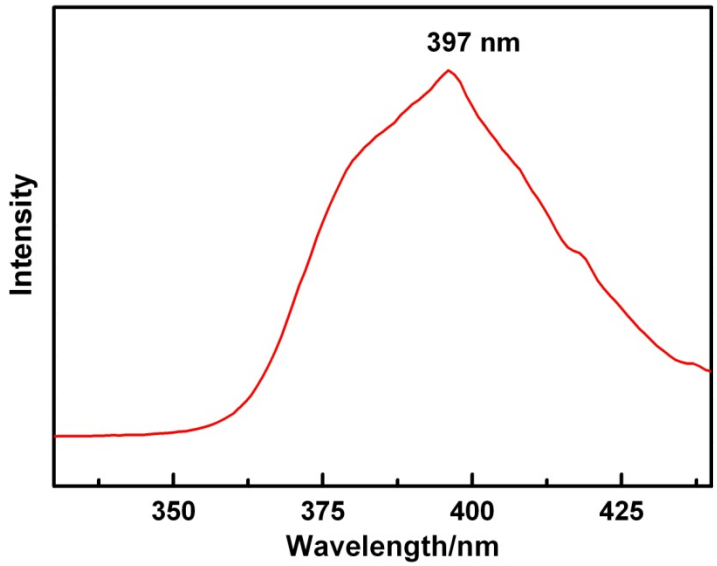



**Table S1**. Selected bond lengths (Å) and angles (°) for **JLU-Liu8**.

| | | | |
|---|---|---|---|
| In(1)-O(3)#1 | 2.095(4) | O(3)#1-In(1)-O(2)#2 | 155.77(19) |
| In(1)-O(2)#2 | 2.100(4) | O(3)#1-In(1)-O(8) | 84.8(2) |
| In(1)-O(8) | 2.151(6) | O(2)#2-In(1)-O(8) | 85.9(2) |
| In(1)-O(6) | 2.258(6) | O(3)#1-In(1)-O(6) | 81.9(2) |
| In(1)-N(1) | 2.276(4) | O(2)#2-In(1)-O(6) | 87.5(2) |
| In(1)-N(2) | 2.284(5) | O(8)-In(1)-O(6) | 130.8(2) |
| In(1)-O(5) | 2.505(8) | O(3)#1-In(1)-N(1) | 83.87(16) |
| O(1)-C(11) | 1.201(9) | O(2)#2-In(1)-N(1) | 116.93(18) |
| O(2)-C(11) | 1.271(8) | O(8)-In(1)-N(1) | 140.14(18) |
| O(2)-In(1)#3 | 2.099(4) | O(6)-In(1)-N(1) | 84.95(18) |
| O(3)-C(12) | 1.254(8) | O(3)#1-In(1)-N(2) | 116.40(17) |
| O(3)-In(1)#4 | 2.095(4) | O(2)#2-In(1)-N(2) | 83.96(18) |
| O(4)-C(12) | 1.205(8) | O(8)-In(1)-N(2) | 80.82(19) |
| O(5)-N(3) | 1.180(11) | O(6)-In(1)-N(2) | 146.52(18) |
| O(6)-N(3) | 1.293(10) | N(1)-In(1)-N(2) | 70.52(15) |
| O(7)-N(3) | 1.245(14) | O(3)#1-In(1)-O(5) | 77.0(2) |
| O(8)-C(13) | 1.226(11) | O(2)#2-In(1)-O(5) | 79.3(2) |
| N(1)-C(5) | 1.322(7) | O(8)-In(1)-O(5) | 78.5(2) |
| N(1)-C(1) | 1.336(6) | O(6)-In(1)-O(5) | 52.4(2) |
| N(2)-C(10) | 1.322(6) | N(1)-In(1)-O(5) | 134.9(2) |
| N(2)-C(6) | 1.324(7) | N(2)-In(1)-O(5) | 154.2(2) |
| N(4)-C(13) | 1.343(13) | C(11)-O(2)-In(1)#3 | 113.2(4) |
| N(4)-C(15) | 1.421(13) | C(12)-O(3)-In(1)#4 | 119.9(4) |
| N(4)-C(14) | 1.573(13) | N(3)-O(5)-In(1) | 90.7(6) |
| C(1)-C(2) | 1.370(8) | N(3)-O(6)-In(1) | 99.6(5) |

| | | | |
|---|---|---|---|
| C(1)-H(1) | 0.9300 | C(13)-O(8)-In(1) | 135.8(7) |
| C(2)-C(3) | 1.365(10) | C(5)-N(1)-C(1) | 119.1(4) |
| C(2)-C(11) | 1.482(7) | C(5)-N(1)-In(1) | 118.3(3) |
| C(3)-C(4) | 1.364(9) | C(1)-N(1)-In(1) | 122.5(4) |
| C(3)-H(3) | 0.9300 | C(10)-N(2)-C(6) | 119.3(5) |
| C(4)-C(5) | 1.365(8) | C(10)-N(2)-In(1) | 122.8(3) |
| C(4)-H(4) | 0.9300 | C(6)-N(2)-In(1) | 117.8(3) |
| C(5)-C(6) | 1.472(6) | O(5)-N(3)-O(7) | 124.1(10) |
| C(6)-C(7) | 1.375(9) | O(5)-N(3)-O(6) | 117.3(9) |
| C(7)-C(8) | 1.392(8) | O(7)-N(3)-O(6) | 118.6(10) |
| C(7)-H(7) | 0.9300 | C(13)-N(4)-C(15) | 131.2(11) |
| C(8)-C(9) | 1.361(9) | C(13)-N(4)-C(14) | 113.1(10) |
| C(8)-H(8) | 0.9300 | C(15)-N(4)-C(14) | 114.6(10) |
| C(9)-C(10) | 1.356(8) | N(1)-C(1)-C(2) | 122.5(5) |
| C(9)-C(12) | 1.507(7) | N(1)-C(1)-H(1) | 118.7 |
| C(10)-H(10) | 0.9300 | C(2)-C(1)-H(1) | 118.7 |
| C(13)-C(16) | 1.454(15) | C(3)-C(2)-C(1) | 118.1(5) |
| C(14)-H(14A) | 0.9600 | C(3)-C(2)-C(11) | 123.0(6) |
| C(14)-H(14B) | 0.9600 | C(1)-C(2)-C(11) | 119.0(5) |
| C(14)-H(14C) | 0.9600 | C(4)-C(3)-C(2) | 119.1(6) |
| C(15)-H(15A) | 0.9600 | C(4)-C(3)-H(3) | 120.4 |
| C(15)-H(15B) | 0.9600 | C(2)-C(3)-H(3) | 120.4 |
| C(15)-H(15C) | 0.9600 | C(3)-C(4)-C(5) | 120.2(6) |
| C(16)-H(16A) | 0.9600 | C(3)-C(4)-H(4) | 119.9 |
| C(16)-H(16B) | 0.9600 | C(5)-C(4)-H(4) | 119.9 |
| C(16)-H(16C) | 0.9600 | N(1)-C(5)-C(4) | 120.9(5) |
| N(1)-C(5)-C(6) | 115.7(5) | C(8)-C(9)-C(12) | 121.4(6) |
| C(4)-C(5)-C(6) | 123.3(5) | N(2)-C(10)-C(9) | 123.2(5) |
| N(2)-C(6)-C(7) | 121.3(5) | N(2)-C(10)-H(10) | 118.4 |
| N(2)-C(6)-C(5) | 116.3(5) | C(9)-C(10)-H(10) | 118.4 |
| C(7)-C(6)-C(5) | 122.4(5) | O(1)-C(11)-O(2) | 123.3(5) |
| C(6)-C(7)-C(8) | 117.9(6) | O(1)-C(11)-C(2) | 121.3(6) |
| C(6)-C(7)-H(7) | 121.1 | O(2)-C(11)-C(2) | 115.4(6) |
| C(8)-C(7)-H(7) | 121.1 | O(4)-C(12)-O(3) | 125.7(6) |
| C(9)-C(8)-C(7) | 119.8(6) | O(4)-C(12)-C(9) | 120.6(6) |
| C(9)-C(8)-H(8) | 120.1 | O(3)-C(12)-C(9) | 113.7(5) |
| C(7)-C(8)-H(8) | 120.1 | O(8)-C(13)-N(4) | 116.5(10) |
| C(10)-C(9)-C(8) | 118.0(5) | O(8)-C(13)-C(16) | 127.3(11) |
| C(10)-C(9)-C(12) | 120.6(5) | N(4)-C(13)-C(16) | 115.1(10) |

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,-x+1,z-1/2 #2 -x+y+5/3,-x+4/3,z+1/3 #3 -y+4/3,x-y-1/3,z-1/3 #4 -y+1,-x+1,z+1/2

**Table S2**. Selected bond lengths (Å) and angles (°) for **JLU-Liu9**.

| | | | |
|---|---|---|---|
| In(1)-O(2)#1 | 2.094(9) | O(2)#1-In(1)-O(5) | 83.9(3) |
| In(1)-O(5) | 2.100(8) | O(2)#1-In(1)-O(4)#2 | 90.1(4) |
| In(1)-O(4)#2 | 2.130(9) | O(5)-In(1)-O(4)#2 | 115.3(3) |
| In(1)-O(7) | 2.149(7) | O(2)#1-In(1)-O(7) | 170.2(4) |
| In(1)-N(2) | 2.261(8) | O(5)-In(1)-O(7) | 86.7(4) |
| In(1)-N(1) | 2.286(9) | O(4)#2-In(1)-O(7) | 96.3(4) |
| O(1)-C(11) | 1.259(14) | O(2)#1-In(1)-N(2) | 99.1(4) |
| O(2)-C(11) | 1.270(13) | O(5)-In(1)-N(2) | 160.9(3) |
| O(2)-In(1)#3 | 2.094(9) | O(4)#2-In(1)-N(2) | 83.7(3) |
| O(3)-C(12) | 1.238(14) | O(7)-In(1)-N(2) | 89.0(4) |
| O(4)-C(12) | 1.258(14) | O(2)#1-In(1)-N(1) | 90.9(3) |
| O(4)-In(1)#4 | 2.130(9) | O(5)-In(1)-N(1) | 90.0(3) |
| O(5)-C(13) | 1.536(13) | O(4)#2-In(1)-N(1) | 154.6(3) |
| O(6)-C(13) | 1.224(12) | O(7)-In(1)-N(1) | 86.5(3) |
| O(6')-C(13) | 1.381(14) | N(2)-In(1)-N(1) | 71.1(3) |
| N(1)-C(5) | 1.321(13) | C(11)-O(2)-In(1)#3 | 130.9(8) |
| N(1)-C(1) | 1.334(12) | C(12)-O(4)-In(1)#4 | 126.7(9) |
| N(2)-C(10) | 1.318(12) | C(13)-O(5)-In(1) | 115.6(6) |
| N(2)-C(6) | 1.338(12) | C(5)-N(1)-C(1) | 118.5(9) |
| C(1)-C(2) | 1.375(13) | C(5)-N(1)-In(1) | 117.7(6) |
| C(1)-H(1) | 0.9300 | C(1)-N(1)-In(1) | 123.7(7) |
| C(2)-C(3) | 1.375(15) | C(10)-N(2)-C(6) | 118.8(8) |
| C(2)-C(11) | 1.454(13) | C(10)-N(2)-In(1) | 120.7(7) |
| C(3)-C(4) | 1.421(16) | C(6)-N(2)-In(1) | 120.5(6) |
| C(3)-H(3) | 0.9300 | N(1)-C(1)-C(2) | 124.0(8) |
| C(4)-C(5) | 1.281(16) | N(1)-C(1)-H(1) | 118.0 |
| C(4)-H(4) | 0.9300 | C(2)-C(1)-H(1) | 118.0 |
| C(5)-C(6) | 1.512(13) | C(3)-C(2)-C(1) | 116.8(9) |
| C(6)-C(7) | 1.33(2) | C(3)-C(2)-C(11) | 121.1(9) |
| C(7)-C(8) | 1.31(2) | C(1)-C(2)-C(11) | 122.1(8) |
| C(7)-H(7) | 0.9300 | C(2)-C(3)-C(4) | 116.3(10) |
| C(8)-C(9) | 1.423(17) | C(2)-C(3)-H(3) | 121.9 |
| C(8)-H(8) | 0.9300 | C(4)-C(3)-H(3) | 121.9 |
| C(9)-C(10) | 1.405(14) | C(5)-C(4)-C(3) | 123.1(11) |
| C(9)-C(12) | 1.498(14) | C(5)-C(4)-H(4) | 118.5 |
| C(10)-H(10) | 0.9300 | C(3)-C(4)-H(4) | 118.5 |
| C(13)-H(13) | 0.9300 | C(4)-C(5)-N(1) | 121.3(10) |
| O(1W)-O(1W)#5 | 1.245(18) | C(4)-C(5)-C(6) | 121.1(9) |
| N(1)-C(5)-C(6) | 117.4(8) | N(2)-C(10)-H(10) | 118.7 |
| C(7)-C(6)-N(2) | 119.3(12) | C(9)-C(10)-H(10) | 118.7 |
| C(7)-C(6)-C(5) | 127.7(12) | O(1)-C(11)-O(2) | 123.1(10) |

| | | | |
|---|---|---|---|
| N(2)-C(6)-C(5) | 113.0(8) | O(1)-C(11)-C(2) | 117.7(9) |
| C(8)-C(7)-C(6) | 126.9(18) | O(2)-C(11)-C(2) | 119.0(10) |
| C(8)-C(7)-H(7) | 116.5 | O(3)-C(12)-O(4) | 124.9(11) |
| C(6)-C(7)-H(7) | 116.5 | O(3)-C(12)-C(9) | 120.2(9) |
| C(7)-C(8)-C(9) | 115.0(15) | O(4)-C(12)-C(9) | 114.9(10) |
| C(7)-C(8)-H(8) | 122.5 | O(6)-C(13)-O(6') | 73.0(10) |
| C(9)-C(8)-H(8) | 122.5 | O(6)-C(13)-O(5) | 92.7(9) |
| C(10)-C(9)-C(8) | 117.4(9) | O(6')-C(13)-O(5) | 100.9(9) |
| C(10)-C(9)-C(12) | 117.4(9) | O(6)-C(13)-H(13) | 133.6 |
| C(8)-C(9)-C(12) | 125.2(9) | O(6')-C(13)-H(13) | 94.3 |
| N(2)-C(10)-C(9) | 122.6(10) | O(5)-C(13)-H(13) | 133.6 |

Symmetry transformations used to generate equivalent atoms:

#1 y-1/2,-x+3/2,-z+1/2 #2 -x+1/2,-y+3/2,z+1/2 #3 -y+3/2,x+1/2,-z+1/2 #4 -x+1/2,-y+3/2,z-1/2 #5 -x+1,-y+1,z

**Table S3**. Selected bond lengths (Å) and angles (°) for **JLU-Liu10**.

| | | | |
|---|---|---|---|
| In(1)-O(2)#1 | 2.185(3) | O(2)#1-In(1)-O(3)#2 | 81.30(11) |
| In(1)-O(3)#2 | 2.236(3) | O(2)#1-In(1)-N(2) | 88.15(12) |
| In(1)-N(2) | 2.247(4) | O(3)#2-In(1)-N(2) | 87.43(11) |
| In(1)-N(1) | 2.266(3) | O(2)#1-In(1)-N(1) | 136.10(11) |
| In(1)-O(4)#2 | 2.351(3) | O(3)#2-In(1)-N(1) | 134.63(11) |
| In(1)-Cl(1) | 2.3723(14) | N(2)-In(1)-N(1) | 72.62(11) |
| In(1)-O(1)#1 | 2.459(3) | O(2)#1-In(1)-O(4)#2 | 137.37(12) |
| In(1)-C(12)#2 | 2.635(4) | O(3)#2-In(1)-O(4)#2 | 56.13(11) |
| In(1)-C(11)#1 | 2.679(4) | N(2)-In(1)-O(4)#2 | 87.83(11) |
| O(1)-C(11) | 1.248(5) | N(1)-In(1)-O(4)#2 | 82.19(11) |
| O(1)-In(1)#3 | 2.459(3) | O(2)#1-In(1)-Cl(1) | 100.00(10) |
| O(2)-C(11) | 1.291(5) | O(3)#2-In(1)-Cl(1) | 102.53(9) |
| O(2)-In(1)#3 | 2.185(3) | N(2)-In(1)-Cl(1) | 167.92(9) |
| O(3)-C(12) | 1.235(5) | N(1)-In(1)-Cl(1) | 95.39(9) |
| O(3)-In(1)#4 | 2.236(3) | O(4)#2-In(1)-Cl(1) | 92.05(9) |
| O(4)-C(12) | 1.248(5) | O(2)#1-In(1)-O(1)#1 | 56.22(10) |
| O(4)-In(1)#4 | 2.351(3) | O(3)#2-In(1)-O(1)#1 | 137.14(10) |
| N(1)-C(1) | 1.314(5) | N(2)-In(1)-O(1)#1 | 85.88(11) |
| N(1)-C(5) | 1.328(5) | N(1)-In(1)-O(1)#1 | 82.76(10) |
| N(2)-C(6) | 1.331(5) | O(4)#2-In(1)-O(1)#1 | 164.83(12) |
| N(2)-C(10) | 1.356(5) | Cl(1)-In(1)-O(1)#1 | 91.23(8) |
| C(1)-C(2) | 1.402(5) | O(2)#1-In(1)-C(12)#2 | 109.17(13) |
| C(1)-H(1) | 0.9300 | O(3)#2-In(1)-C(12)#2 | 27.87(12) |
| C(2)-C(3) | 1.368(7) | N(2)-In(1)-C(12)#2 | 87.89(13) |
| C(2)-C(11) | 1.463(6) | N(1)-In(1)-C(12)#2 | 109.11(13) |
| C(3)-C(4) | 1.405(7) | O(4)#2-In(1)-C(12)#2 | 28.27(12) |

| | | | |
|---|---|---|---|
| C(3)-H(3) | 0.9300 | Cl(1)-In(1)-C(12)#2 | 97.71(11) |
| C(4)-C(5) | 1.364(7) | O(1)#1-In(1)-C(12)#2 | 164.25(12) |
| C(4)-H(4) | 0.9300 | O(2)#1-In(1)-C(11)#1 | 28.54(12) |
| C(5)-C(6) | 1.505(6) | O(3)#2-In(1)-C(11)#1 | 109.70(13) |
| C(6)-C(7) | 1.358(7) | N(2)-In(1)-C(11)#1 | 86.81(12) |
| C(7)-C(8) | 1.357(8) | N(1)-In(1)-C(11)#1 | 109.35(13) |
| C(7)-H(7) | 0.9300 | O(4)#2-In(1)-C(11)#1 | 165.09(14) |
| C(8)-C(9) | 1.409(7) | Cl(1)-In(1)-C(11)#1 | 96.08(10) |
| C(8)-H(8) | 0.9300 | O(1)#1-In(1)-C(11)#1 | 27.69(11) |
| C(9)-C(10) | 1.366(6) | C(12)#2-In(1)-C(11)#1 | 137.48(15) |
| C(9)-C(12) | 1.488(5) | C(11)-O(1)-In(1)#3 | 86.0(2) |
| C(10)-H(10) | 0.9300 | C(11)-O(2)-In(1)#3 | 97.5(3) |
| C(11)-In(1)#3 | 2.679(4) | C(12)-O(3)-In(1)#4 | 94.3(3) |
| C(12)-In(1)#4 | 2.635(4) | C(12)-O(4)-In(1)#4 | 88.6(3) |
| C(1)-N(1)-C(5) | 119.2(4) | C(8)-C(7)-C(6) | 122.8(6) |
| C(1)-N(1)-In(1) | 124.1(3) | C(8)-C(7)-H(7) | 118.6 |
| C(5)-N(1)-In(1) | 116.8(3) | C(6)-C(7)-H(7) | 118.6 |
| C(6)-N(2)-C(10) | 118.0(4) | C(7)-C(8)-C(9) | 116.3(6) |
| C(6)-N(2)-In(1) | 118.4(3) | C(7)-C(8)-H(8) | 121.8 |
| C(10)-N(2)-In(1) | 123.5(3) | C(9)-C(8)-H(8) | 121.8 |
| N(1)-C(1)-C(2) | 123.5(4) | C(10)-C(9)-C(8) | 118.8(4) |
| N(1)-C(1)-H(1) | 118.3 | C(10)-C(9)-C(12) | 119.7(4) |
| C(2)-C(1)-H(1) | 118.3 | C(8)-C(9)-C(12) | 121.5(5) |
| C(3)-C(2)-C(1) | 116.9(4) | N(2)-C(10)-C(9) | 122.8(4) |
| C(3)-C(2)-C(11) | 121.4(4) | N(2)-C(10)-H(10) | 118.6 |
| C(1)-C(2)-C(11) | 121.7(4) | C(9)-C(10)-H(10) | 118.6 |
| C(2)-C(3)-C(4) | 119.6(5) | O(1)-C(11)-O(2) | 120.3(4) |
| C(2)-C(3)-H(3) | 120.2 | O(1)-C(11)-C(2) | 122.3(4) |
| C(4)-C(3)-H(3) | 120.2 | O(2)-C(11)-C(2) | 117.4(4) |
| C(5)-C(4)-C(3) | 118.7(5) | O(1)-C(11)-In(1)#3 | 66.3(2) |
| C(5)-C(4)-H(4) | 120.7 | O(2)-C(11)-In(1)#3 | 53.97(19) |
| C(3)-C(4)-H(4) | 120.7 | C(2)-C(11)-In(1)#3 | 171.3(3) |
| N(1)-C(5)-C(4) | 122.2(4) | O(3)-C(12)-O(4) | 120.9(4) |
| N(1)-C(5)-C(6) | 117.0(4) | O(3)-C(12)-C(9) | 120.5(4) |
| C(4)-C(5)-C(6) | 120.7(5) | O(4)-C(12)-C(9) | 118.6(4) |
| N(2)-C(6)-C(7) | 121.1(5) | O(3)-C(12)-In(1)#4 | 57.8(2) |
| N(2)-C(6)-C(5) | 115.0(4) | O(4)-C(12)-In(1)#4 | 63.1(2) |
| C(7)-C(6)-C(5) | 123.9(5) | C(9)-C(12)-In(1)#4 | 177.5(4) |

Symmetry transformations used to generate equivalent atoms:

#1 -z+1,-x+1,-y+1 #2 -z+1,x-1/2,-y+1/2 #3 -y+1,-z+1,-x+1 #4 y+1/2,-z+1/2,-x+1