Supporting information

Constructions of a series of lanthanide metal-organic frameworks: structure, luminescence and white light emission

Lanlan Shen, Lu Yang, Yong Fan, Li Wang,* and Jianing Xu* a

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Symmetry transformations used to generate equivalent atoms:

#1 -x+3,y-1/2,-z+3/2   #2 x+1,y,z   #3 -x+2,y+1/2,-z+3/2
#4 x-1,y,z   #5 -x+2,y-1/2,-z+3/2   #6 -x+3,y+1/2,-z+3/2
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| O(10)-Tb(1)-O(8)#4 | 122.00(13)   |
| O(2)-Tb(1)-O(8)#4 | 72.07(12)    |
| O(11)-Tb(1)-O(8)#4 | 76.75(12)    |
| O(10)-Tb(1)-O(1) | 75.36(12)    |
| O(2)-Tb(1)-O(1)  | 74.59(13)    |
| O(11)-Tb(1)-O(1) | 123.01(11)   |
| O(8)#4-Tb(1)-O(1) | 137.31(11)   |
| O(10)-Tb(1)-O(6) | 150.40(12)   |
| O(2)-Tb(1)-O(6)  | 88.34(14)    |
| O(11)-Tb(1)-O(6) | 70.65(12)    |
| O(8)#4-Tb(1)-O(6) | 77.53(12)    |
| O(1)-Tb(1)-O(6)  | 75.59(12)    |
| O(10)-Tb(1)-O(15) | 70.90(13)    |
| O(2)-Tb(1)-O(15) | 108.48(15)   |
| O(11)-Tb(1)-O(15) | 75.07(12)    |
| O(8)#4-Tb(1)-O(15) | 72.73(13)    |
| O(1)-Tb(1)-O(15) | 144.52(12)   |
| O(6)-Tb(1)-O(15) | 138.70(12)   |
| O(10)-Tb(1)-O(12) | 72.97(13)    |
| O(2)-Tb(1)-O(12) | 142.82(13)   |
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| O(6)-Tb(1)-O(12) | 104.86(14)   |
| O(15)-Tb(1)-O(12) | 84.45(14)    |
| O(4)-Tb(3)-O(7)#5 | 150.83(11)   |

Table S2: Selected bond length [Å] and bond angle [°] for 1-Tb.
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Symmetry transformations used to generate equivalent atoms:

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#3 -x+1,y+1/2,-z+1/2  #4 -x-1,y-1/2,-z+1/2
#5 -x,y-1/2,-z+1/2   #6 -x+1,y-1/2,-z+1/2
### Table S3

Selected bond length [Å] and bond angle [°] for 2.

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<td>136.67(12)</td>
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<td>121.06(14)</td>
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</table>
Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z    #2 x-1,y,z    #3 -x+1,-y,-z+2
#4 x-1,y-1,z    #5 -x+2,-y+1,-z+1    #6 x+1,y+1,z
<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H) [Å]</th>
<th>d(H...A) [Å]</th>
<th>d(D...A) [Å]</th>
<th>&lt;(DHA) [°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(14)-H(29)...O(9)</td>
<td>0.802(18)</td>
<td>2.30(3)</td>
<td>2.979(2)</td>
<td>143(4)</td>
</tr>
<tr>
<td>O(14)-H(27)...O(21)#7</td>
<td>0.82</td>
<td>1.97</td>
<td>2.662(4)</td>
<td>141.6</td>
</tr>
<tr>
<td>O(6)-H(6)...O(7)#8</td>
<td>0.82</td>
<td>1.83</td>
<td>2.581(2)</td>
<td>150.7</td>
</tr>
<tr>
<td>O(4)-H(4)...O(20)#9</td>
<td>0.82</td>
<td>1.91</td>
<td>2.703(3)</td>
<td>163.0</td>
</tr>
<tr>
<td>O(2)-H(2)...O(8)#10</td>
<td>0.82</td>
<td>1.79</td>
<td>2.593(2)</td>
<td>166.0</td>
</tr>
<tr>
<td>O(21)-H(22)...O(18)#11</td>
<td>0.839(19)</td>
<td>2.47(3)</td>
<td>3.256(5)</td>
<td>157(5)</td>
</tr>
<tr>
<td>O(21)-H(21)...O(8)#9</td>
<td>0.85(2)</td>
<td>2.10(2)</td>
<td>2.943(4)</td>
<td>177(7)</td>
</tr>
<tr>
<td>O(12)-H(28)...O(14)#3</td>
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<td>2.08(4)</td>
<td>2.858(3)</td>
<td>170(4)</td>
</tr>
<tr>
<td>O(12)-H(18)...O(3)</td>
<td>0.84(4)</td>
<td>1.91(4)</td>
<td>2.703(2)</td>
<td>156(3)</td>
</tr>
<tr>
<td>O(20)-H(16)...O(6)#12</td>
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<td>2.820(2)</td>
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<td>2.00(4)</td>
<td>2.774(2)</td>
<td>175(4)</td>
</tr>
<tr>
<td>O(15)-H(26)...O(18)#14</td>
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<td>2.01(4)</td>
<td>2.805(2)</td>
<td>172(4)</td>
</tr>
<tr>
<td>O(15)-H(25)...O(16)</td>
<td>0.82(3)</td>
<td>1.92(4)</td>
<td>2.722(2)</td>
<td>163(3)</td>
</tr>
<tr>
<td>O(11)-H(3)...O(5)#1</td>
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<td>2.13(4)</td>
<td>2.772(2)</td>
<td>154(4)</td>
</tr>
<tr>
<td>O(11)-H(24)...O(20)#2</td>
<td>0.77(3)</td>
<td>2.15(4)</td>
<td>2.906(3)</td>
<td>165(3)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:

1. -x+3, y-1/2, -z+3/2
2. x+1, y, z
3. -x+2, y+1/2, -z+3/2
4. x-1, y, z
5. -x+2, y-1/2, -z+3/2
6. -x+3, y+1/2, -z+3/2
7. -x+1, y-1/2, -z+3/2
8. x, y+1/2, z-1/2
9. -x+1, y+1, -z+2
10. -x+2, y+1, -z+2
11. x, y+3/2, z+1/2
12. x, y+1/2, z+1/2
13. -x, y-1/2, -z+3/2
14. -x+1, -y+1, -z+1
Table S5 Hydrogen bonds for 1-Tb [Å] and [°]

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>&lt;(DHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(20)-H(10)...O(17)#2</td>
<td>0.85(2)</td>
<td>2.57(7)</td>
<td>3.127(8)</td>
<td>124(7)</td>
</tr>
<tr>
<td>O(20)-H(10)...O(16)#7</td>
<td>0.85(2)</td>
<td>2.45(4)</td>
<td>3.219(9)</td>
<td>151(7)</td>
</tr>
<tr>
<td>O(12)-H(7)...O(18)</td>
<td>0.84(2)</td>
<td>2.24(5)</td>
<td>2.973(5)</td>
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</tr>
<tr>
<td>O(20)-H(9)...O(21)#8</td>
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<td>2.12(5)</td>
<td>2.938(9)</td>
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</tr>
<tr>
<td>O(12)-H(8)...O(20)</td>
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<td>1.81(2)</td>
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<td>169(6)</td>
</tr>
<tr>
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<td>2.00(2)</td>
<td>2.842(5)</td>
<td>171(5)</td>
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<td>O(19)-H(11)...O(13)</td>
<td>0.83(2)</td>
<td>1.99(2)</td>
<td>2.816(5)</td>
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<td>O(15)-H(1)...O(7)</td>
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<td>2.751(5)</td>
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<tr>
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<td>2.885(5)</td>
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<tr>
<td>O(6)-H(5)...O(5)#4</td>
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<td>1.88(3)</td>
<td>2.714(5)</td>
<td>166(6)</td>
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<tr>
<td>O(19)-H(12)...O(4)#10</td>
<td>0.84(2)</td>
<td>1.92(3)</td>
<td>2.739(5)</td>
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<tr>
<td>O(17)-H(17A)...O(19)#6</td>
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<td>2.673(6)</td>
<td>163.3</td>
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<td>1.80</td>
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<td>164.7</td>
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Symmetry transformations used to generate equivalent atoms:

#1 -x-1,y+1/2,-z+1/2  #2 -x,y+1/2,-z+1/2  #3 -x+1,y+1/2,-z+1/2
#4 -x-1,y-1/2,-z+1/2  #5 -x,y-1/2,-z+1/2  #6 -x+1,y-1/2,-z+1/2
#7 -x+1,-y,-z+1      #8 x,-y+1/2,z+1/2    #9 x-1,-y+1/2,z-1/2
#10 -x+2,-y,-z+1     #11 x-1,-y+1/2,z+1/2