Supporting information of

# Pendant orientation and its influence on the formation of hydrogen-bonded thiacalixarene nanotubes

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Figure S1**.** The propagated chain system of **5** along [101] direction. Hydrogen-bonded interactions are shown as broken lines. The hydrogen atoms connected to carbon atom are omitted for clarity.

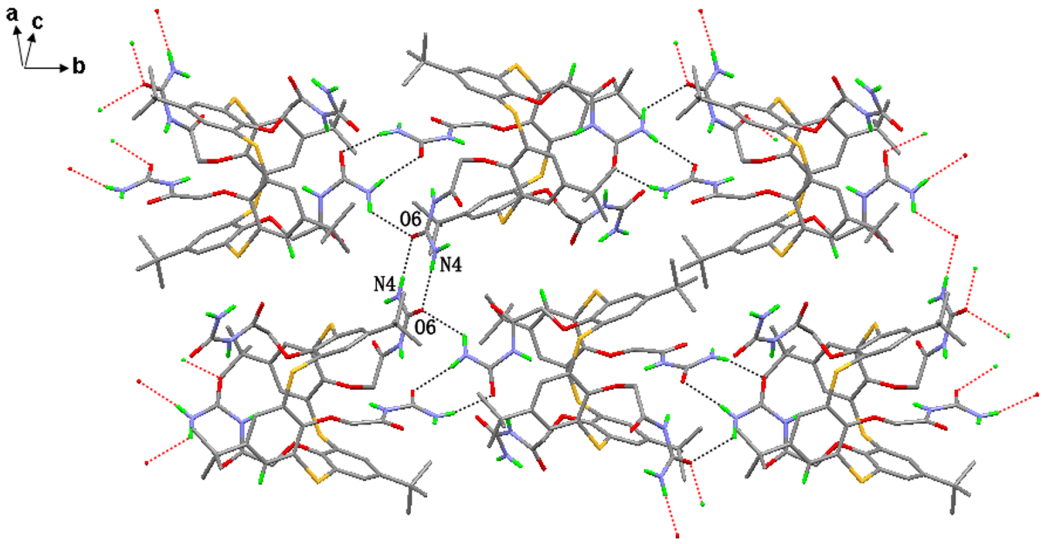


Figure S2**.** The propagated chain system of **5** perpendicular to (101) plane. Hydrogen-bonded interactions are shown as broken lines. The hydrogen atoms connected to carbon atom are omitted for clarity.

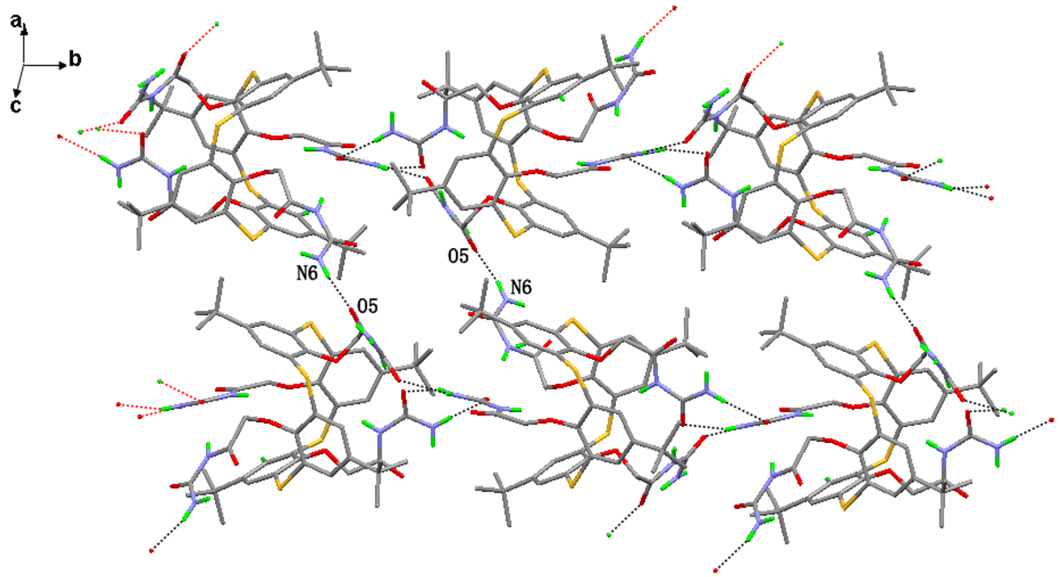

Table S3. Hydrogen bonds of compound **1** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(18)-H(18A)...O(15) | 0.84 | 1.89 | 2.713(7) | 166.3 |
| O(14)-H(14B)...O(4) | 0.82 | 2.36 | 2.909(4) | 124.6 |
| O(14)-H(14A)...O(5) | 0.82 | 1.84 | 2.641(5) | 166.7 |
| O(13)-H(13B)...O(2) | 0.82 | 2.10 | 2.751(4) | 136.7 |
| O(13)-H(13B)...O(1) | 0.82 | 2.25 | 2.948(4) | 142.9 |
| O(13)-H(13A)...O(7) | 0.82 | 2.22 | 2.799(4) | 128.1 |
| O(11)-H(11)...O(14) | 0.84 | 1.87 | 2.641(5) | 152.9 |
| O(9)-H(9)...O(13) | 0.84 | 1.78 | 2.554(4) | 152.9 |
| O(6)-H(6)...O(17) | 0.84 | 1.78 | 2.563(7) | 153.6 |
| O(16)-H(16A)...O(16)#1 | 0.84 | 1.80 | 2.40(3) | 127.8 |
| O(16)-H(16A)...O(12)#1 | 0.84 | 2.10 | 2.728(15) | 131.8 |
| O(15)-H(15)...O(8)#2 | 0.84 | 1.91 | 2.745(6) | 177.7 |
| O(3)-H(3)...O(18)#3 | 0.84 | 1.74 | 2.552(5) | 161.4 |
| C(22)-H(22A)...O(3)#4 | 0.98 | 2.60 | 3.236(6) | 123.1 |

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Hydrogen bonds of compound **2** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1)...S(2) | 0.86 | 2.64 | 3.425(3) | 153.0 |
| N(1)-H(1)...O(7) | 0.86 | 2.27 | 2.712(3) | 112.0 |
| N(2)-H(2)...O(1) | 0.86 | 2.19 | 2.627(3) | 112.0 |
| N(3)-H(3A)...O(12)#1 | 0.86 | 2.20 | 3.013(3) | 158.0 |
| N(3)-H(3B)...O(8) | 0.86 | 2.06 | 2.705(3) | 132.0 |
| N(4)-H(4A)...O(3)#2 | 0.86 | 2.28 | 3.091(4) | 157.0 |
| N(4)-H(4B)...O(2) | 0.86 | 2.06 | 2.705(4) | 132.0 |
| N(4)-H(4B)...O(8)#2 | 0.86 | 2.51 | 2.961(4) | 114.0 |
| O(5)-H(5A)...O(4) | 0.82 | 2.06 | 2.578(3) | 121.0 |
| O(5)-H(5A)...O(10) | 0.82 | 2.45 | 2.923(4) | 118.0 |
| O(11)-H(11)...O(9)#3 | 0.82 | 1.83 | 2.622(3) | 163.0 |
| C(17)-H(17)...O(9) | 0.93 | 2.57 | 3.459(4) | 161.0 |
| C(24)-H(24B)...O(6)#1 | 0.97 | 2.52 | 3.225(4) | 129.0 |
| C(36)-H(36A)...S(3) | 0.97 | 2.64 | 3.139(3) | 112.0 |

| | | | | |
|---|---|---|---|---|
| C(49)-H(49A)...S(3) | 0.97 | 2.67 | 3.350(3) | 127.0 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,1-y,-z #2 -x,2-y,-z #3 x,-1+y,z

Table S5. Hydrogen bonds of compound **3** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1)...O(3)#1 | 0.86 | 2.53 | 3.170(6) | 132.3 |
| N(1)-H(1)...O(4) | 0.86 | 2.17 | 2.634(5) | 113.7 |
| O(3)-H(3A)...O(6)#1 | 0.82 | 1.74 | 2.557(5) | 170.6 |
| N(2)-H(2A)...O(2)#2 | 0.86 | 2.47 | 3.154(6) | 137.2 |
| N(2)-H(2B)...O(5) | 0.86 | 2.03 | 2.679(7) | 131.5 |
| C(5)-H(5)...S(2)#3 | 0.93 | 2.85 | 3.750(5) | 163.0 |
| C(11)-H(11A)...S(1) | 0.97 | 2.85 | 3.429(6) | 119.5 |
| C(23)-H(23B)...S(2) | 0.97 | 2.86 | 3.395(8) | 115.4 |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2 #2 x-1/2,-y+1/2,z+1/2 #3 -x+1,y,-z+3/2

Table S6. Hydrogen bonds of compound **4** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1)...S(2) | 0.86 | 2.68 | 3.485(3) | 156.0 |
| N(1)-H(1)...O(1) | 0.86 | 2.30 | 2.727(4) | 111.0 |
| N(2)-H(2A)...O(9)#1 | 0.86 | 2.07 | 2.928(6) | 174.0 |
| N(2)-H(2B)...O(2) | 0.86 | 2.06 | 2.701(7) | 131.0 |
| N(3)-H(3)...O(4) | 0.86 | 2.24 | 2.668(6) | 111.0 |
| N(3)-H(3)...O(12) | 0.86 | 2.53 | 3.109(8) | 126.0 |
| N(4)-H(4A)...O(11)#2 | 0.86 | 2.27 | 3.053(8) | 151.0 |
| N(4)-H(4B)...O(5) | 0.86 | 2.02 | 2.656(7) | 131.0 |
| N(5)-H(5)...O(7) | 0.86 | 2.16 | 2.618(4) | 113.0 |
| N(6)-H(6A)...O(3)#3 | 0.86 | 2.03 | 2.887(5) | 172.0 |
| N(6)-H(6B)...O(8) | 0.86 | 1.99 | 2.661(6) | 134.0 |
| O(12)-H(12)...O(6) | 0.82 | 1.71 | 2.504(8) | 163.0 |
| C(11)-H(11A)...S(1) | 0.97 | 2.60 | 3.146(4) | 116.0 |
| C(11)- H(11B)...O(9) | 0.97 | 2.56 | 3.093(7) | 115.0 |

| | | | | |
|---|---|---|---|---|
| C(34)-H(34A)...O(6) | 0.96 | 2.49 | 3.438(17) | 173.0 |
| C(50)-H(50B)...S(1) | 0.97 | 2.81 | 3.411(5) | 121.0 |

Symmetry transformations used to generate equivalent atoms:

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

Table S7. Hydrogen bonds of compound **5** [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1A)...O(1) | 0.85 | 2.15 | 2.607(3) | 113.2 |
| N(2)-H(2A)...O(2) | 0.87 | 2.08 | 2.691(4) | 127.3 |
| N(2)-H(2A)...O(6)#1 | 0.87 | 2.38 | 2.974(3) | 125.3 |
| N(2)-H(2B)...O(12)#1 | 0.86 | 2.14 | 2.978(3) | 163.3 |
| N(3)-H(3A)...O(12) | 0.85 | 2.04 | 2.862(3) | 164.3 |
| N(4)-H(4A)...O(5) | 0.85 | 2.07 | 2.737(4) | 134.3 |
| N(4)-H(4B)...O(6)#1 | 0.85 | 2.09 | 2.942(4) | 172.3 |
| N(5)-H(5A)...O(3) | 0.86 | 2.13 | 2.951(4) | 158.3 |
| N(6)-H(6A)...O(5)#2 | 0.88 | 2.14 | 2.976(5) | 159.3 |
| N(6)-H(6B)...O(8) | 0.88 | 1.99 | 2.675(5) | 134.4 |
| N(7)-H(7A)...O(10) | 0.87 | 2.27 | 2.654(3) | 107.2 |
| N(8)-H(8D)...O(3)#3 | 0.88 | 2.15 | 3.012(3) | 166.3 |
| N(8)-H(8E)...O(11) | 0.85 | 1.99 | 2.663(4) | 136.3 |
| C(11)-H(11B)...S(1) | 0.97 | 2.83 | 3.439(3) | 122.0 |
| C(24)-H(24A)...O(12) | 0.97 | 2.44 | 3.082(3) | 123.0 |
| C(24)-H(24B)...S(2) | 0.97 | 2.77 | 3.358(3) | 120.0 |
| C(32)-H(32)...O(6) | 0.93 | 2.57 | 3.479(3) | 165.0 |
| C(37)-H(37A)...S(3) | 0.97 | 2.76 | 3.363(3) | 121.0 |
| C(37)-H(37B)...O(3) | 0.97 | 2.43 | 3.129(4) | 129.0 |

Symmetry transformations used to generate equivalent atoms:

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