**Supplementary Material**

Synthesis and thermal behavior of two Sr(II) compounds derived from isomeric 5‑(n‑pyridyl)tetrazole-2-isopropionic acid (n = 2, 3)

XINYU HAO, YAN LI, XIAOYI LIU, JING’AO REN, CONGHAO SHI, YUANHUI LIU, ZHIKANG WANG, ZIXIANG DU, QIAOYUN LI\* and GAOWEN YANG\*

Table **S**1. Hydrogen bonds (Å and º) for **1** and **2**.

D—H···A D—H H···A D···A D—H···A

Compound **1**

N(5)—H(5A)···O(9)#1 0.86 2.06 2.8581(6) 153

O(5)—H(5B)···N(1)#2 0.86 1.99 2.820(6) 162

O(5)—H(5C)···O(10)#1 0.85 1.96 2.805(7) 164

O(6)—H(6A)···N(6)#3 0.85 2.11 2.883(7) 151

O(6)—H(6B)···O(9)#1 0.85 2.20 2.734(6) 121

O(8)—H(8A)···N(1)#2 0.85 2.59 3.328(6) 146

O(8)—H(8B)···N(2)#2 0.85 2.36 3.169(6) 156

O(8)—H(8B)···N(3)#4 1.04 2.49 3.301(6) 135

O(9)—H(9A)···O(6)#4 1.04 1.79 2.785(7) 159

O(10)—H(10B)···O(7)#5 0.85 2.47 3.322(10) 176

O(12)—H(12A)···N(6)#6 0.85 2.62 3.388(11) 152

O(12)—H(12B)···N(7)#7 0.85 2.33 2.977(11) 133

C(2)—H(2B)···O(4) 0.97 2.42 3.049(6) 122

C(4)—H(4B)···O(2) 0.97 2.34 3.006(7) 125

Compound **2**

O(5)—H(5B)···O(16)#2 0.85 1.95 2.750(8) 155

O(6)—H(6C)···O(7)#5 0.85 2.25 2.797(7) 122

O(6)—H(6D)···N(4) 0.85 2.18 3.009(7) 165

O(7)—H(7A)···N(8)#5 0.85 2.18 2.915(7) 146

O(16)—H(16A)···O(4)#6 0.84 1.87 2.695(7) 164

O(16)—H(16B)···N(7)#5 0.83 2.12 2.940(8) 170

C(2)—H(2A)···N(3)#2 0.97 2.52 3.461(8) 163

C(2)—H(2B)···O(4)#4 0.97 2.47 3.334(7) 148

C(6)—H(6)···O(2)#1 0.93 2.60 3.505(7) 165

C(11)—H(11B)···O(1)#3 0.97 2.59 3.197(8) 121

Symmetry codes for **1**: #1 x, y, -1+z; #2 1-x, 1-y,-z; #3 -x, -y, -z; #4 -1+ x, y,-1+z; #5 1+x,y, 1+z; #6 x, 1+y, z; #7 -x, 1-y, 1-z; for **2**: #1 x, -1+y, z; #2 1-x,1-y, 1-z; #3 2-x,-y,1-z; #4 1- x, -y,1-z; #5 2-x,1-y,1-z; #6 x,1+y,-1+z.



Figure S1. Theoretical and experimental PXRD of compound **1**.



Figure S2. Theoretical and experimental PXRD of compound **1**.



Figure S3. 3D supramolecular structure of compound **1** formed by hydrogen bonds.



Figure S4. 3D supramolecular structure of compound **2** formed by hydrogen bonds.