**Supplementary Information**

A new coordination compound based on 4-amino-3-(tetrazol-5-yl)-furazan (HAFT): Preparation, crystal structure and thermal properties

ZI-MEI DING, WEN-LI CAO, XIAO-JING HANG, XIAO MA, HUI ZHENG, KANG-ZHEN XU and JIE HUANG\*

|  |  |
| --- | --- |
| E:\1205图片\未标题-1D.tif | E:\1205图片\未标题2D-1.tif |
| Figure S1. 1D chain of **1**. | Figure S2. 2D layer of **1**. |

Table S1. Selected hydrogen bonds for **1**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| D−H···A | d(D−H)/(Å) | d(H···A)/(Å) | d(D···A)/(Å) | <(DHA)/(°) |
| N1−H1A···O2#1 | 0.79(3) | 2.37(3) | 3.022(3) | 140(3) |
| N1−HIB···N2#2 | 0.80(3) | 2.25(4) | 3.047(4) | 172(3) |
| N8−H8B···O2#3 | 0.97 | 2.05 | 2.989(3) | 163.0 |
| N9−H9···N4#4 | 0.86 | 2.04 | 2.874(3) | 163.7 |
| N10−H10B···N4#4 | 0.86 | 2.58 | 3.290(4) | 140.5 |
| N10−H10B···N5#4 | 0.86 | 2.41 | 3.263(4) | 171.2 |
| N10−HI0A···O1#5 | 0.86 | 2.56 | 3.393(3) | 162.1 |

Symmetry transformations used to generate equivalent atoms: #1: −1−*x*, 2−*y*, 1−*z*; #2: −2−*x*, 3−*y*, 1−*z*; #3: 1+*x*, *y*, *z*; #4: −*x*, −0.5+*y*, 0.5−*z*; #5: *x*, −1+*y*, *z*.



Figure. S3 Determination results of the continuous specific heat capacity of **1**.