

A family of Uranyl-aromatic dicarboxylate (pht-, ipa-, tpa-) framework hybrid materials: photoluminescent, surface photovoltage and dye adsorption

Xue Gao,^a Che Wang,^{*a} Zhong-Feng Shi,^c Jian Song,^a Feng-Ying Bai,^b Ji-Xiao Wang^a and Yong-Heng Xing^{*a}

^a*College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian City, 116029, China*

^b*School of Life Science, Liaoning Normal University, Dalian City, 116029, China*

^c*College of Chemistry and Chemical Engineering, Qinzhou University, Qinzhou 535099, PR China*

Fig. S1 The Solid-state IR spectra of complex **1** at a room temperature.

Fig. S2 The Solid-state IR spectra of complex **2** at a room temperature.

Fig. S3 The Solid-state IR spectra of complex **3** at a room temperature.

Fig. S4 The Solid-state IR spectra of complex **4** at a room temperature.

Fig. S5 The TG curve for complex **1**.

Fig. S6 The TG curve for complex **2**.

Fig. S7 The TG curve for complex **3**.

Fig. S8 The TG curve for complex **4**.

Fig. S9 The UV-Vis spectra for complex **1**.

Fig. S10 The UV-Vis spectra for complex **2**.

Fig. S11 The UV-Vis spectra for complex **3**.

Fig. S12 The UV-Vis spectra for complex **4**.

Fig. S13 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **1**, (b) experimental PXRD for coordination polymer **1**.

Fig. S14 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **2**, (b) experimental PXRD for coordination polymer **2**.

Fig. S15 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **3**, (b) experimental PXRD for coordination polymer **3**.

Fig. S16 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **4**, (b) experimental PXRD for coordination polymer **4**.

Table S1 Hydrogen bond lengths (Å) and angles (°) for complexes **1-2***.

* Corresponding author: Associate Professor of Chemistry Che Wang

E-mail address: wangche126@126.com;

* Corresponding author: Professor of Chemistry Yong-Heng Xing

E-mail address: xingyongheng2000@163.com;

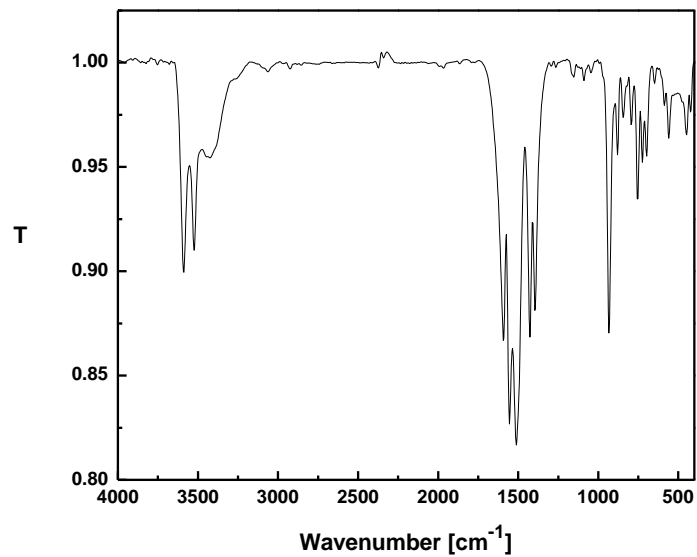


Fig. S1 The Solid-state IR spectra of complex **1** at a room temperature.

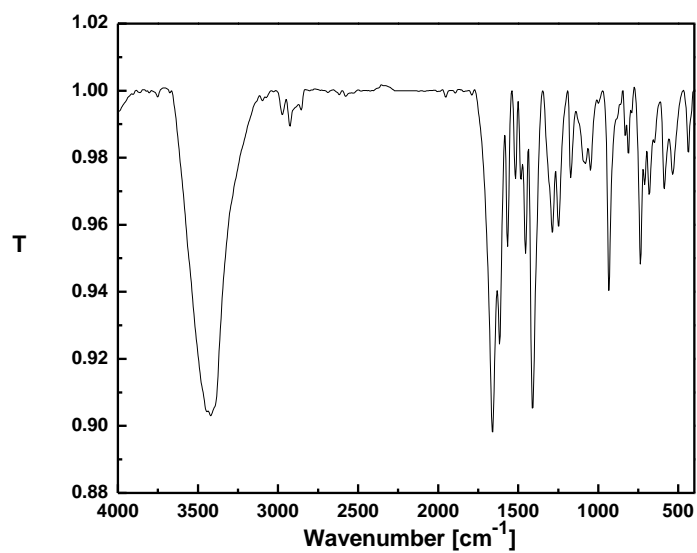


Fig. S2 The Solid-state IR spectra of complex **2** at a room temperature.

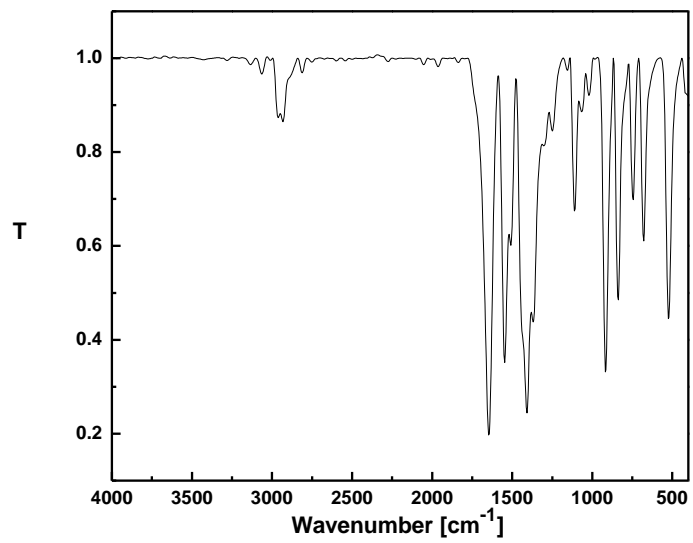


Fig. S3 The Solid-state IR spectra of complex **3** at a room temperature.

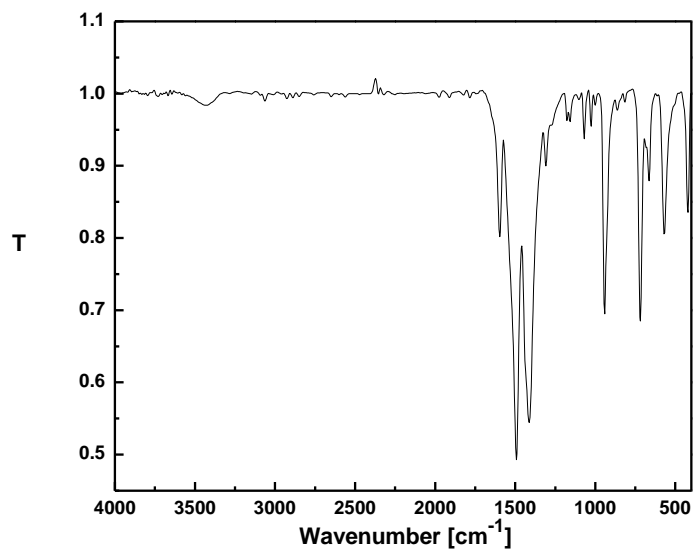


Fig. S4 The Solid-state IR spectra of complex **4** at a room temperature.

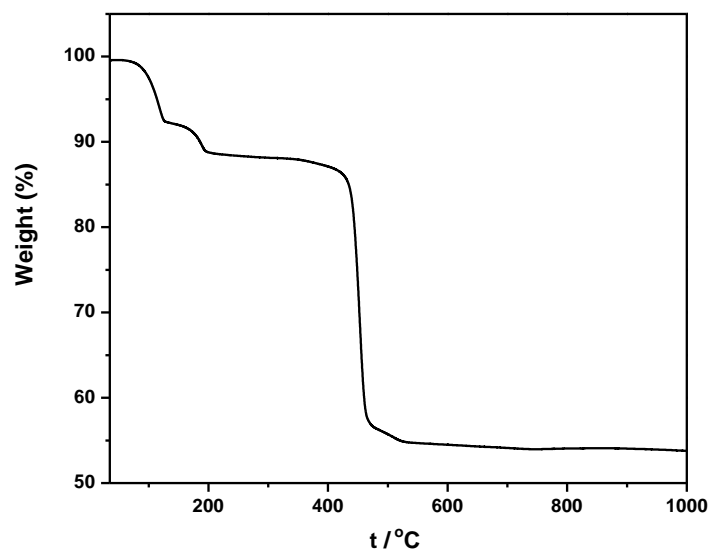


Fig. S5 The TG curve for complex 1.

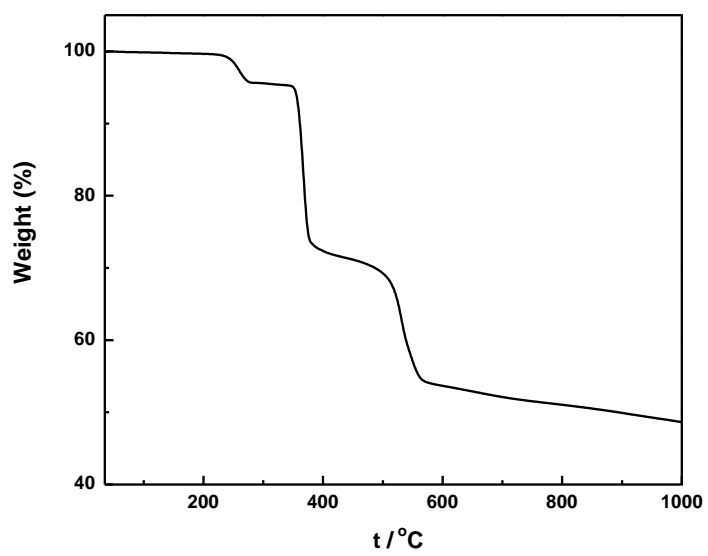


Fig. S6 The TG curve for complex 2.

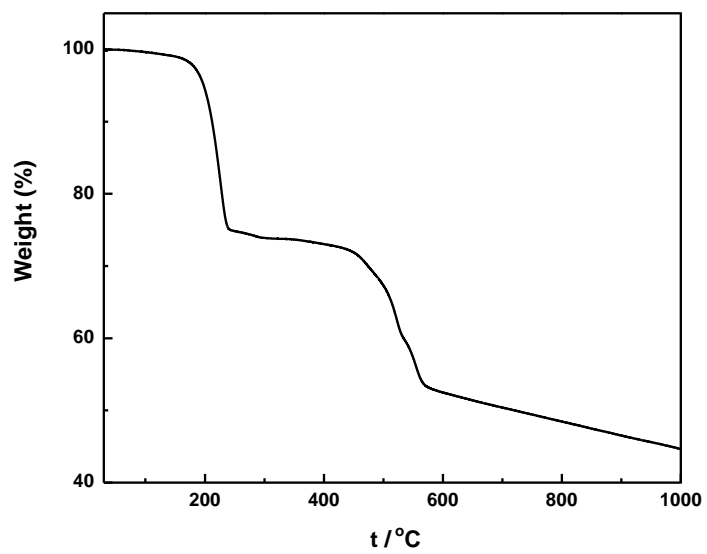


Fig. S7 The TG curve for complex 3.

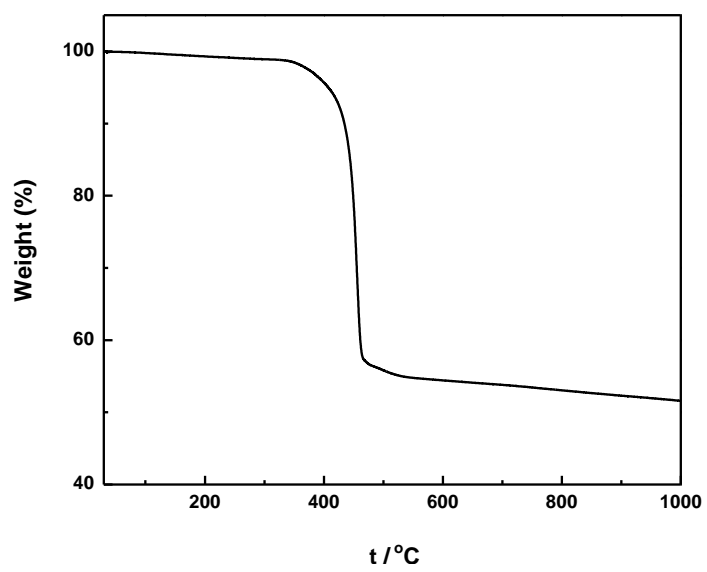


Fig. S8 The TG curve for complex 4.

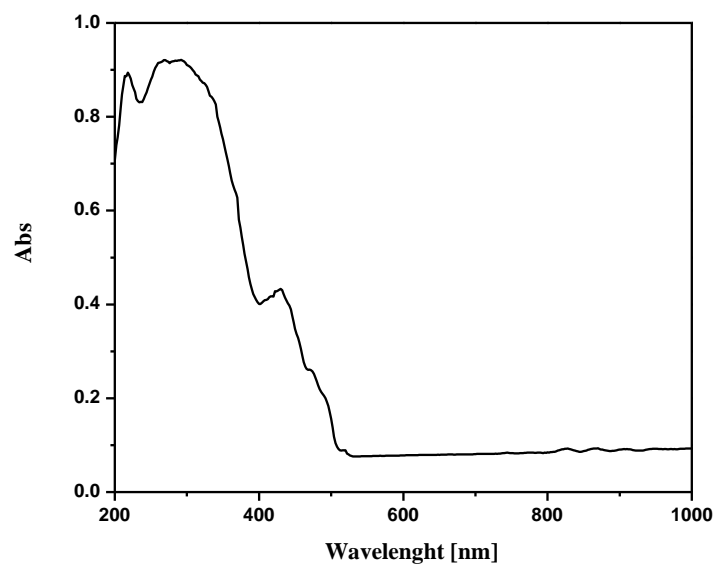


Fig. S9 The UV-Vis spectra for complex 1.

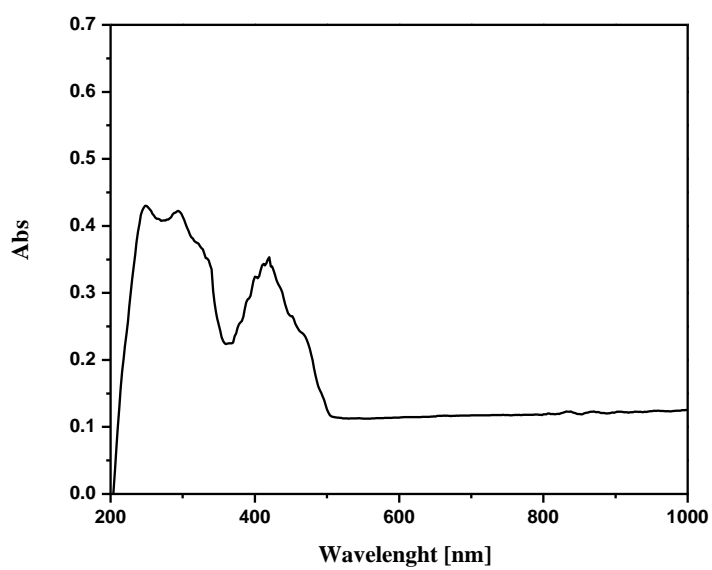


Fig. S10 The UV-Vis spectra for complex 2.

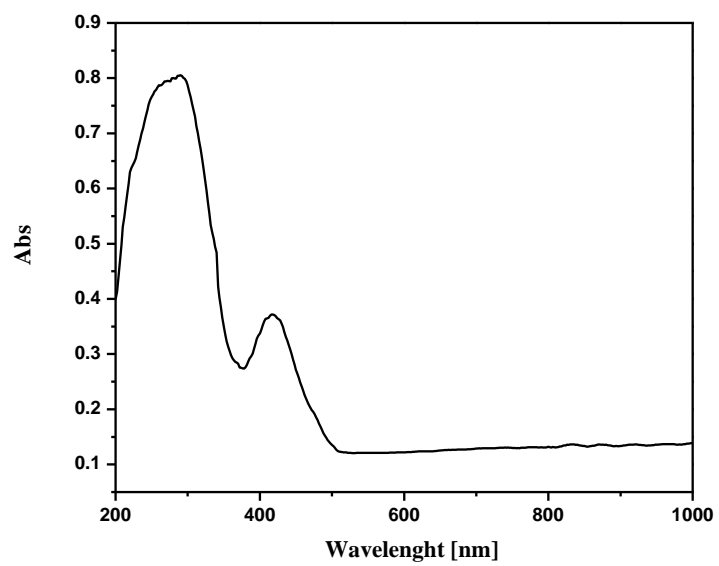


Fig. S11 The UV-Vis spectra for complex 3.

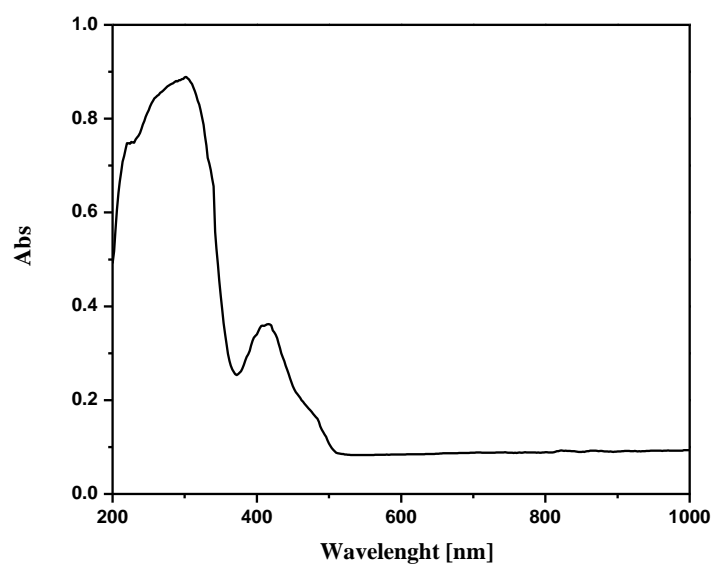


Fig. S12 The UV-Vis spectra for complex 4.

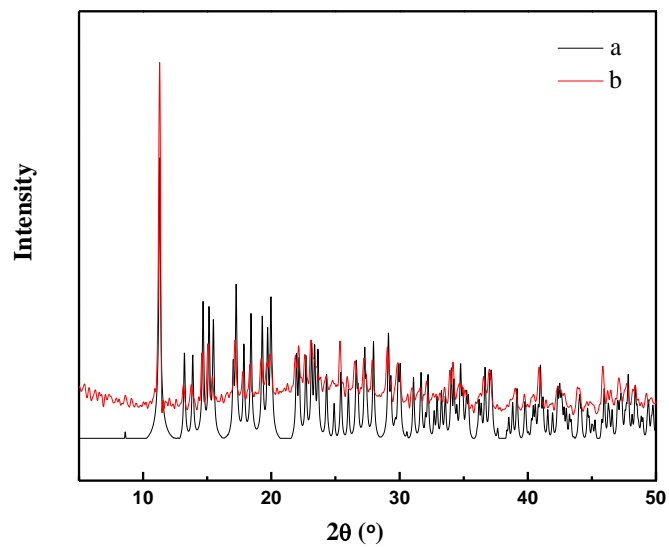


Fig. S13 PXR D powder patterns: (a) the simulated PXR D pattern calculated from single-crystal structure of coordination polymer **1**, (b) experimental PXR D for coordination polymer **1**.

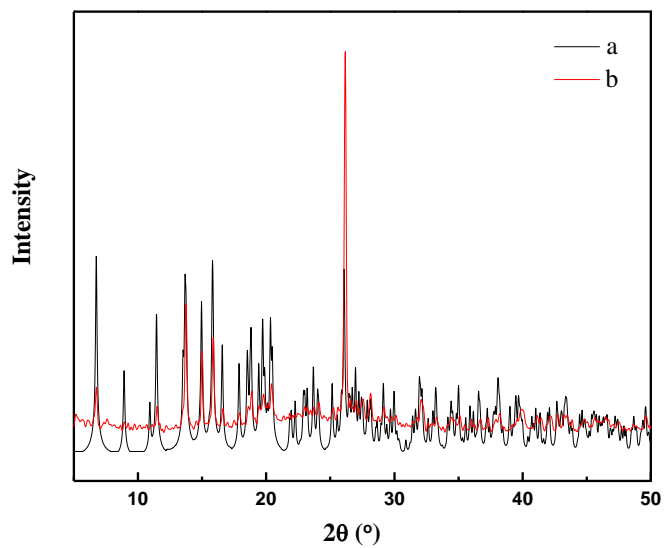


Fig. S14 PXR D powder patterns: (a) the simulated PXR D pattern calculated from single-crystal structure of coordination polymer **2**, (b) experimental PXR D for coordination polymer **2**.

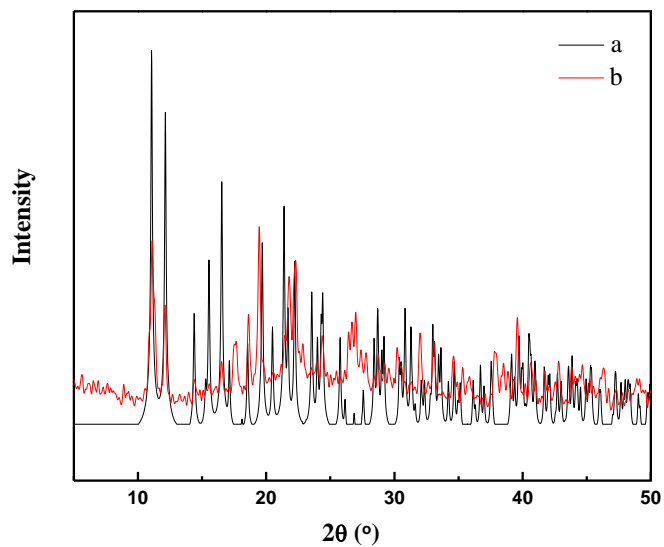


Fig. S15 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **3**, (b) experimental PXRD for coordination polymer **3**.

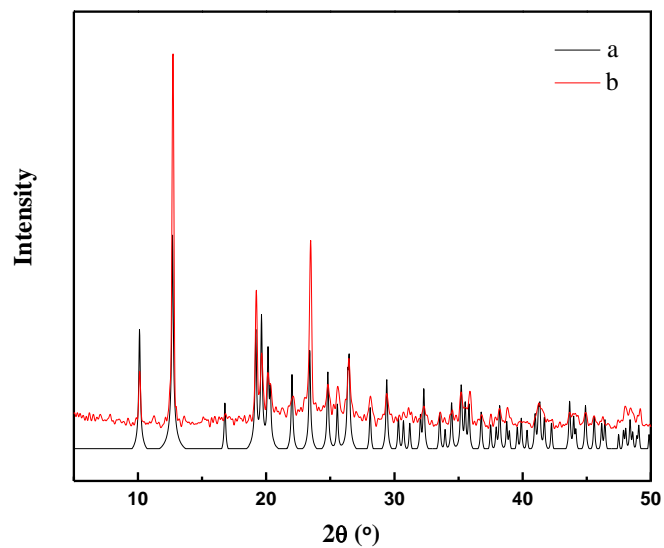


Fig. S16 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of coordination polymer **4**, (b) experimental PXRD for coordination polymer **4**.

Table S1 Hydrogen bond lengths (Å) and angles (°) for complexes **1-2***

D–H···A	d(D–H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
Complex 1				
O(1W)-H(1WB)···O(1) ^{#4}	0.85	2.07	2.866(8)	154.6
O(7)-H(7A)···O(1W) ^{#5}	0.85	1.98	2.687(7)	140.7
Complex 2				
O(7)-H(7C)···O(11) ^{#2}	0.85	2.25	2.818(5)	124.4
O(8)-H(8)···O(3) ^{#3}	0.82	1.86	2.673(4)	168.3
O(10)-H(10)···O(11) ^{#4}	0.82	1.85	2.671(4)	175.1
C(3)-H(3)···O(4) ^{#1}	0.93	2.45	3.369(4)	168.8
C(13)-H(13)···O(1) ^{#5}	0.93	2.60	3.360(5)	139.6
C(15)-H(15)···O(8) ^{#3}	0.93	2.47	3.358(5)	159.3

*Symmetry transformation used to generate equivalent atoms: complex **1**: #4: x, y+1, z,

#5: -x+1, -y+1, -z+1; complex **2**: #1: -x, -y+1, -z+2, #2: x-1, y+1, z, #3: -x, -y+1, -z+1, #4:

-x+1, -y-1, -z+1, #5: x+1, y-1, z.