Supporting Information for

Metal-Phenanthroline Fused Ti_{17} Clusters, a Single Molecular Source for Sensitized Photoconductive Film

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Qin-Yu Zhu,*[ab] and Jie Dai*[ab]

1. Figures

Figure S1. The experimental XRD patterns and the crystal data simulated patterns of compounds **1** (a) and **2** (b).

Figure S2. Solution of compound **1** in a mixture of toluene and methanol.

Figure S3. SEM images of the micro structures of the film of F**1** (prepared at room temperature, except the indicated), showing the hollows (a), bowls (b), surface roughed hollows (c), connected hollows (d), and particle morphologies prepared at higher evaporation rates at temperature 40 ºC (e) and 80 ºC (f).

Figure S4 The experimental XRD pattern of the film F**1**.

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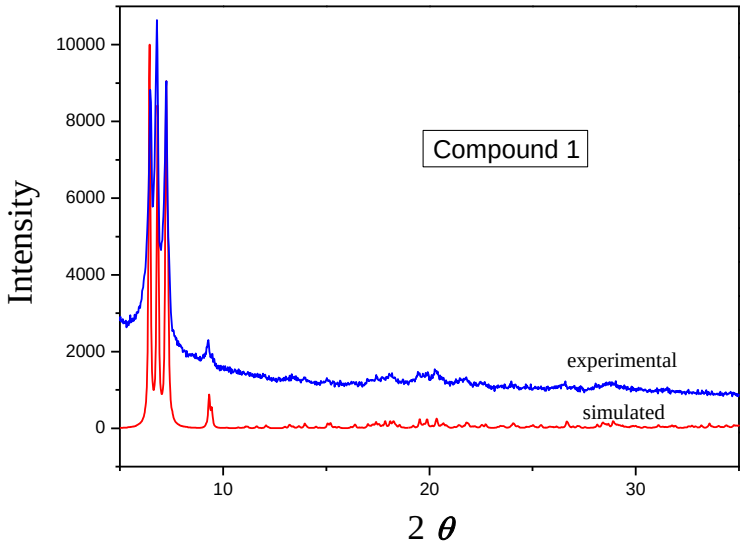
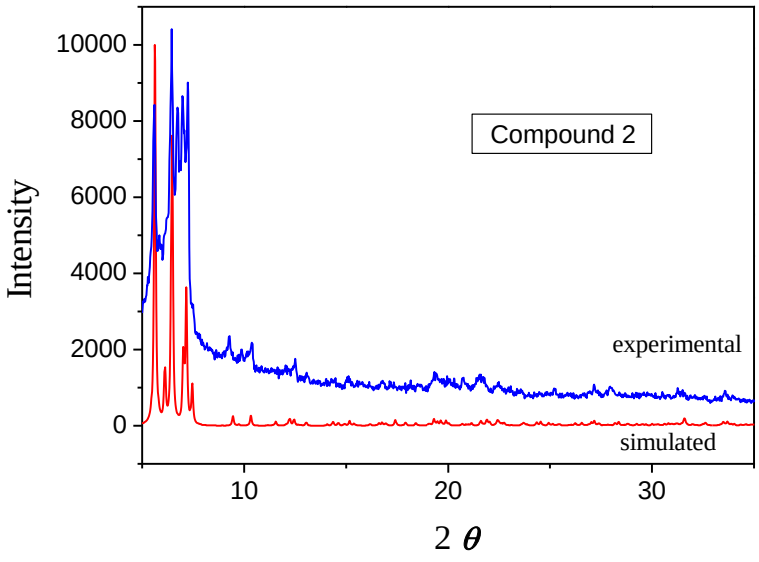
Figure S8. The SEM images showing the thickness of the films, (a) F**1**, (b) F**2**, and (c) FTi_{17}.

2. Table

Table S1. Crystal Data and Structural Refinement Parameters for **1** and **2.**



(a)



(b)

Figure S1. The experimental XRD patterns and the crystal data simulated patterns of compounds **1** (a) and **2** (b).

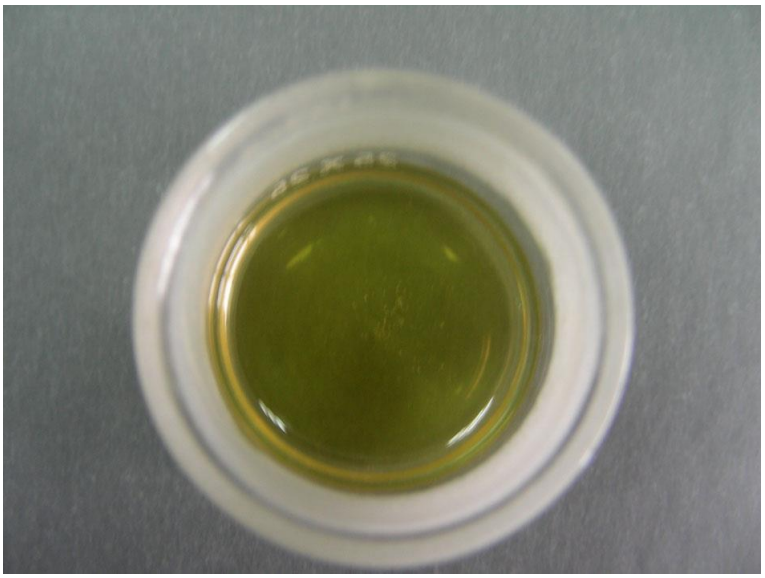


Figure S2. Solution of compound **1** in a mixture of toluene and methanol.

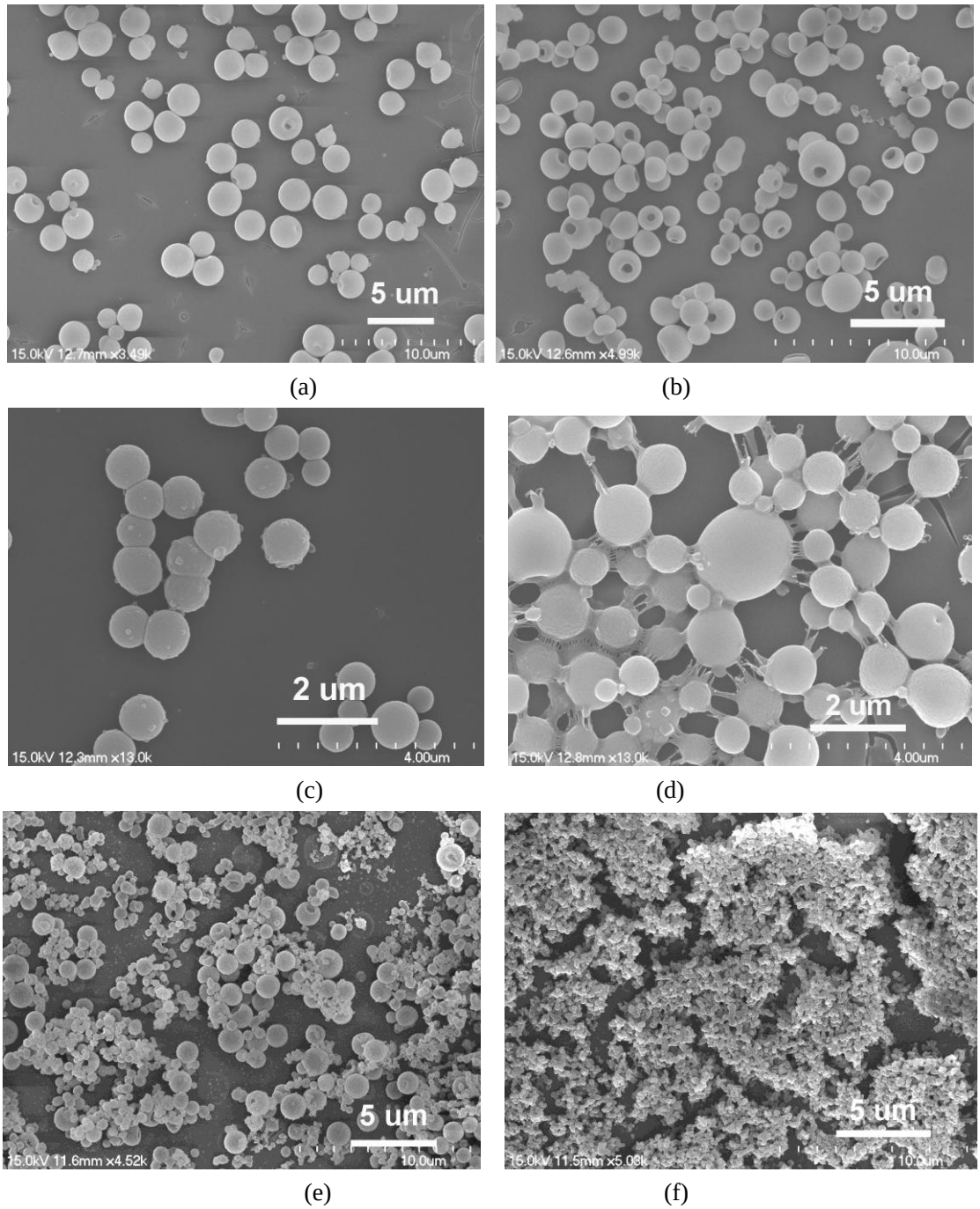


Figure S3. SEM images of the micro structures of the film of F**1** (prepared at room temperature, except the indicated), showing the hollows (a), bowls (b), surface roughed hollows (c), connected hollows (d), and particle morphologies prepared at higher evaporation rates at temperature 40 ºC (e) and 80 ºC (f).

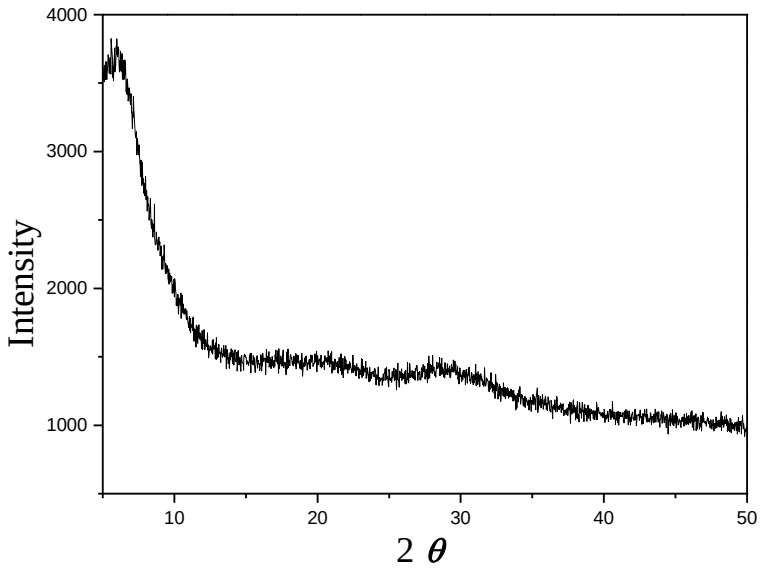


Figure S4. The experimental XRD pattern of the film **F1**.

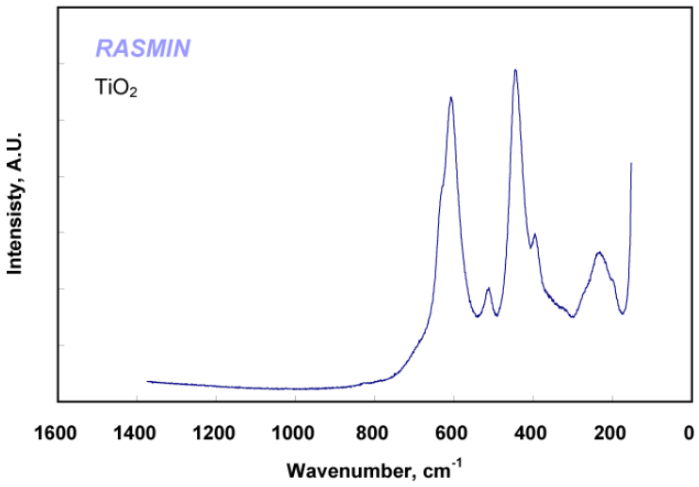
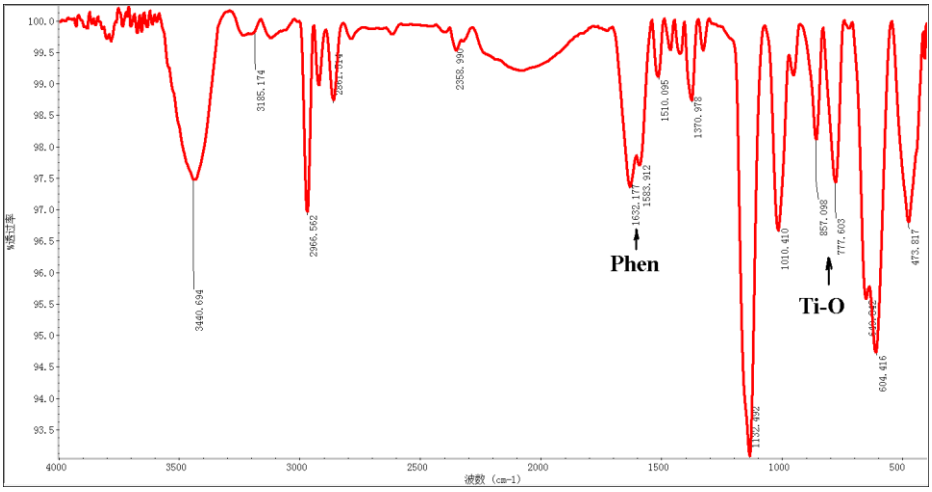
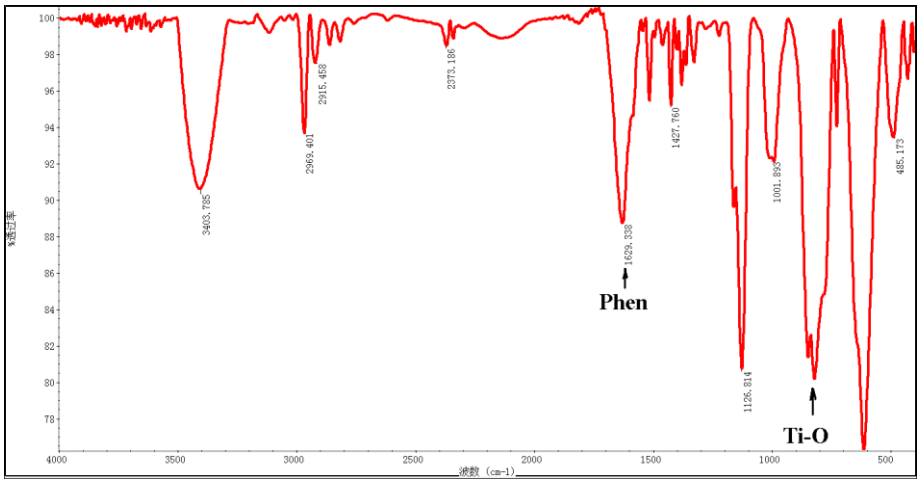


Figure S5. The Raman spectrum of the TiO_2 (AIST data).

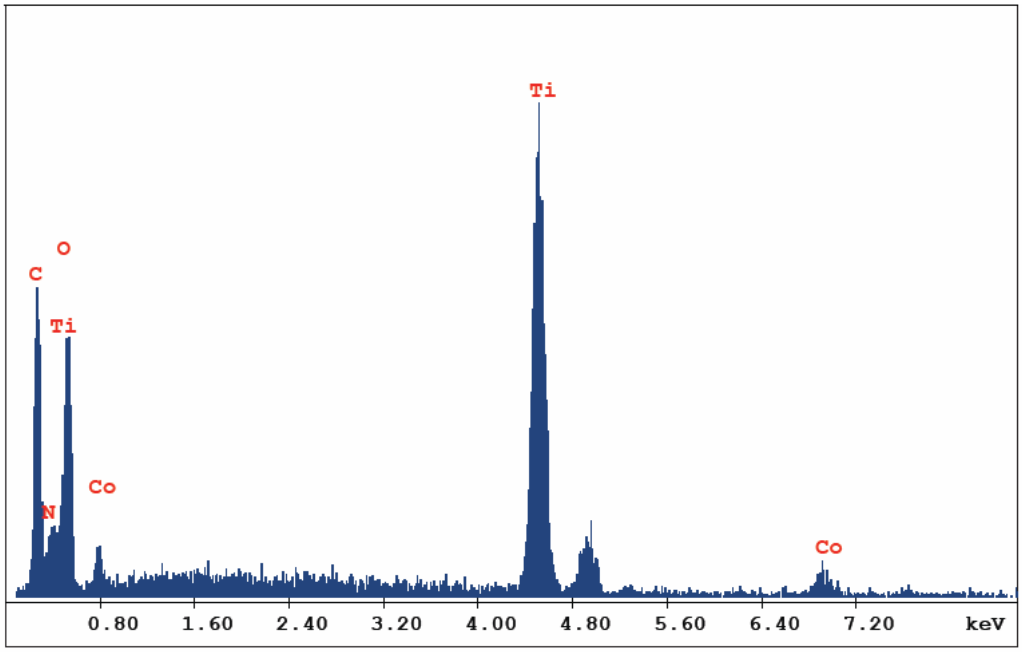


(a)

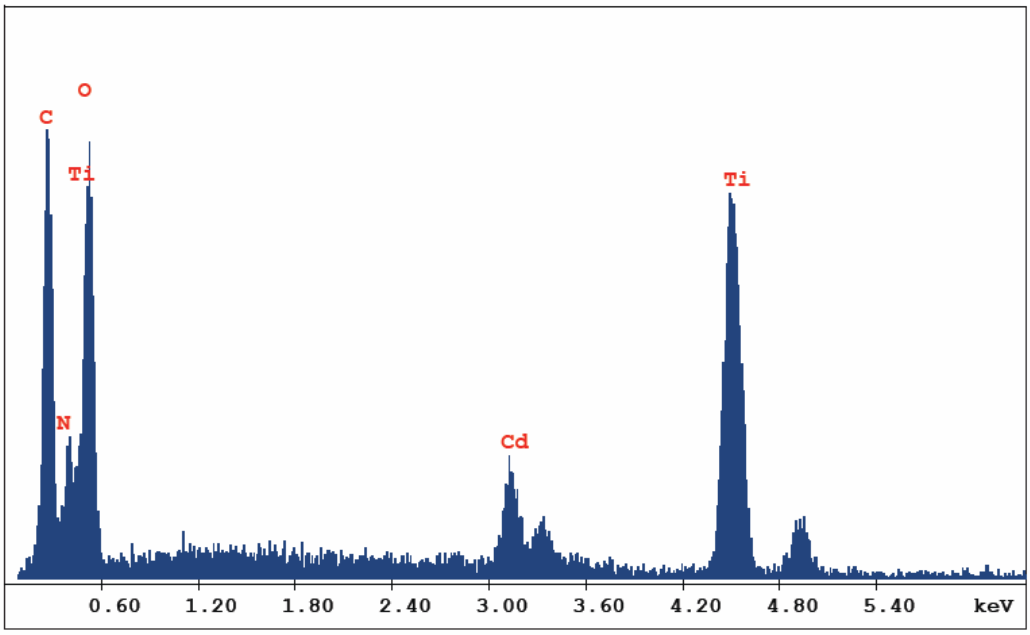


(b)

Figure S6. The IR spectra of the crystal **1** (a) and the film F**1** (b).

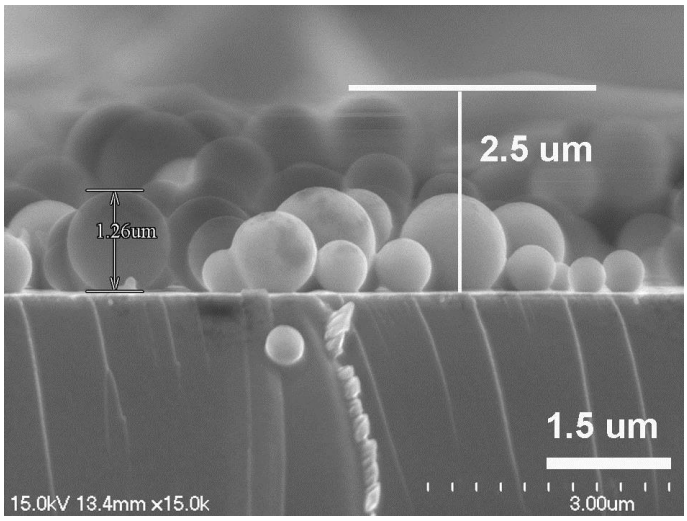


(a)

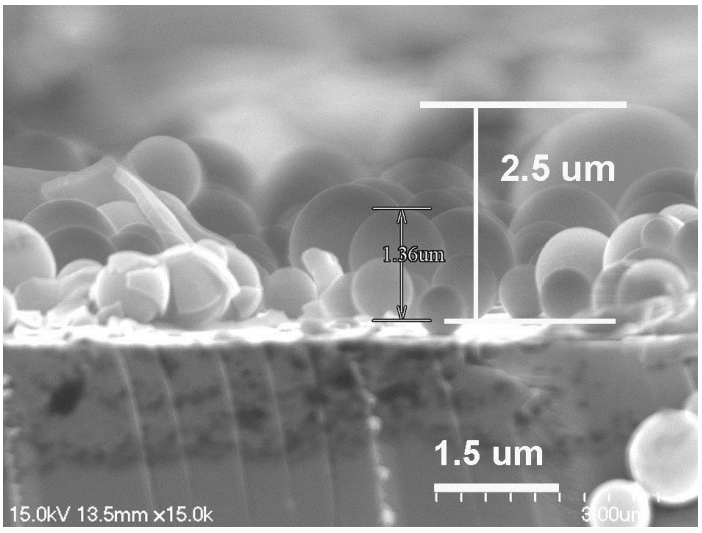


(b)

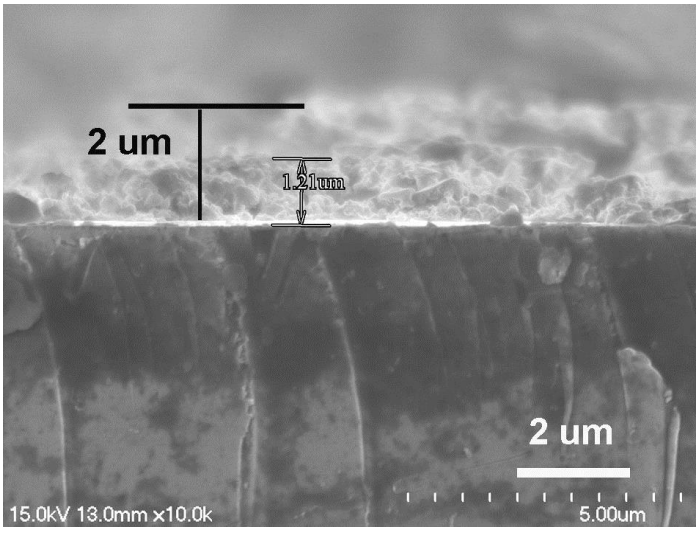
Figure S7. The EDX spectra of the F**1** (a) and F**2** (b).



(a)



(b)



(c)

Figure S8. The SEM images showing the thickness of the films, (a) F1, (b) F2, and (c) FTi_{17}.

Table S1. Crystal Data and Structural Refinement Parameters for **1** and **2.**

	1	**2**
formula	$C_{72}H_{128}Co_2N_4O_{44}Ti_{17}$	$C_{78}H_{142}Cd_2N_4O_{46}Ti_{17}$
Fw	2685.64	2910.76
cryst size (mm^3)	0.60 × 0.20 × 0.15	0.20 × 0.20 × 0.20
cryst syst	monoclinic	monoclinic
space group	$P2_1/n$	$C2/c$
a (Å)	15.800(3)	18.802(5)
b (Å)	27.683(6)	28.875(6)
c (Å)	25.877(5)	23.835(6)
α (deg)	90.0	90.00
β (deg)	90.90(3)	96.129(5)
γ (deg)	90.0	90.00
V ($Å^3$)	11317(4)	12866(5)
Z	4	4
ρ_{calcd} (g cm^{-3})	1.576	1.575
F(000)	5472	6232
μ (mm^{-1})	1.486	1.390
T (K)	293.2(2)	223(2)
R_{int}	0.0880	0.0675
reflns collected	54537	51830
unique reflns	19740	11255
observed reflns	10392	8914
no. params	1259	693
GOF on F^2	1.014	1.022
$R_1[I>2\sigma(I)]$ / $R_1{}^a$	0.1099/0.1899	0.0818/0.1051
${}_wR_2[I>2\sigma(I)]$ / ${}_wR_2{}^b$	0.2165/0.2549	0.1749/0.1853