Six-membered Janus-type ditopic N-heterocyclic carbene coinage metal complexes

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1. NMR Spectra:

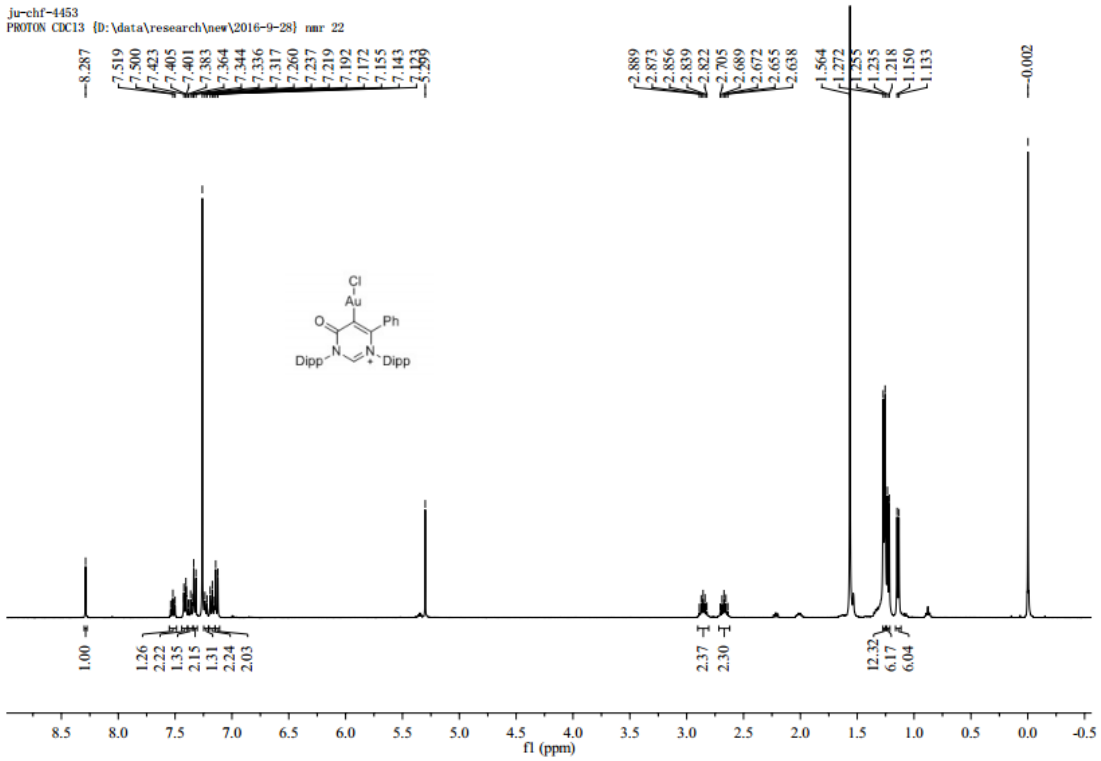

Figure S1. ^{1}H NMR spectrum of **2**

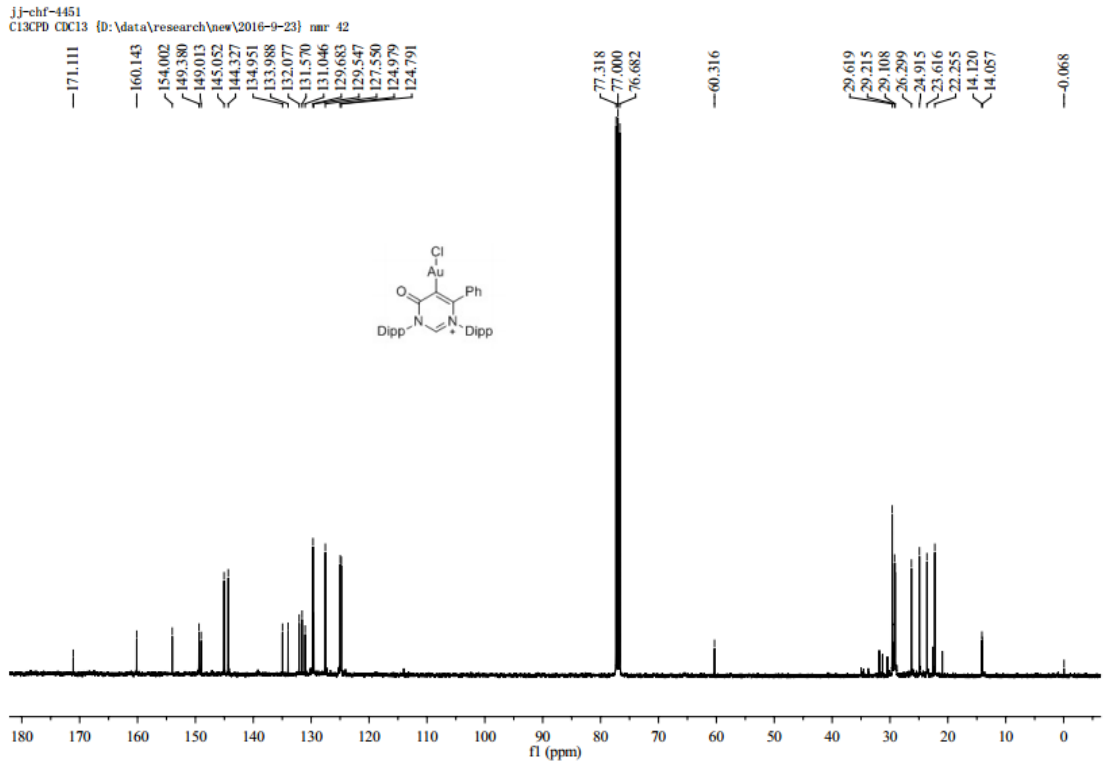

Figure S2. ^{13}C{^{1}H} NMR spectrum of **2**

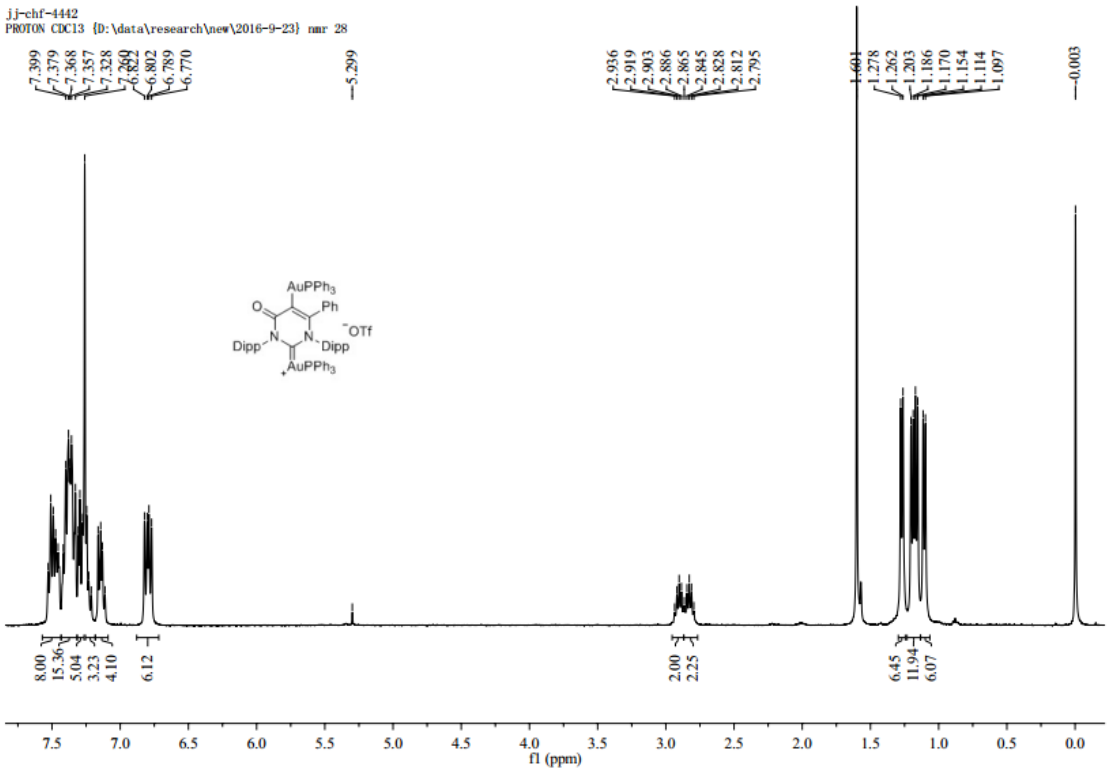

Figure S3. ^{1}H NMR spectrum of **3**

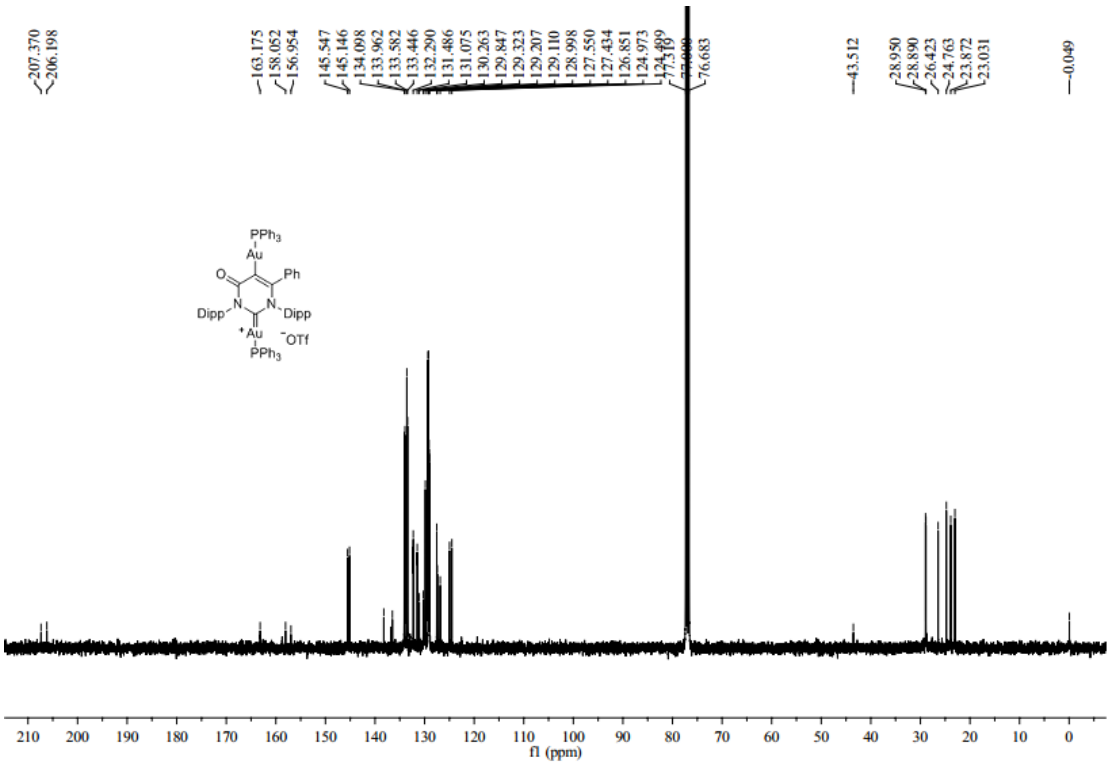

Figure S4. ^{13}C{^{1}H} NMR spectrum of **3**

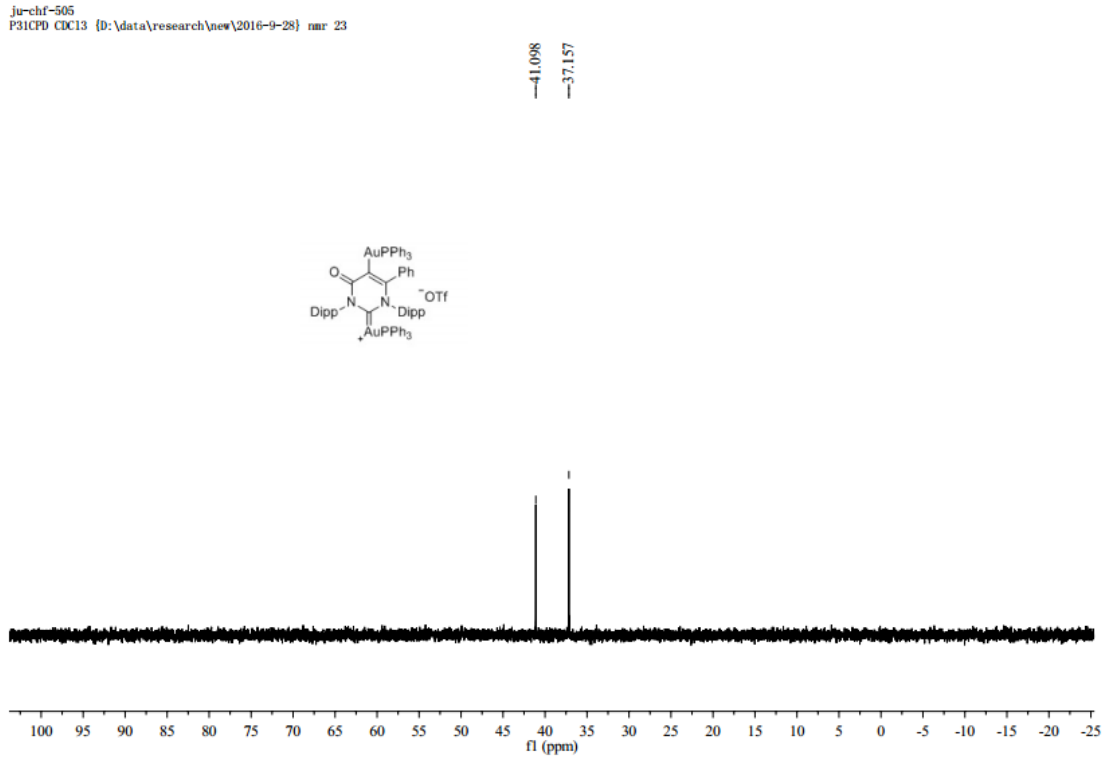

Figure S5. ^{31}P NMR spectrum of **3**

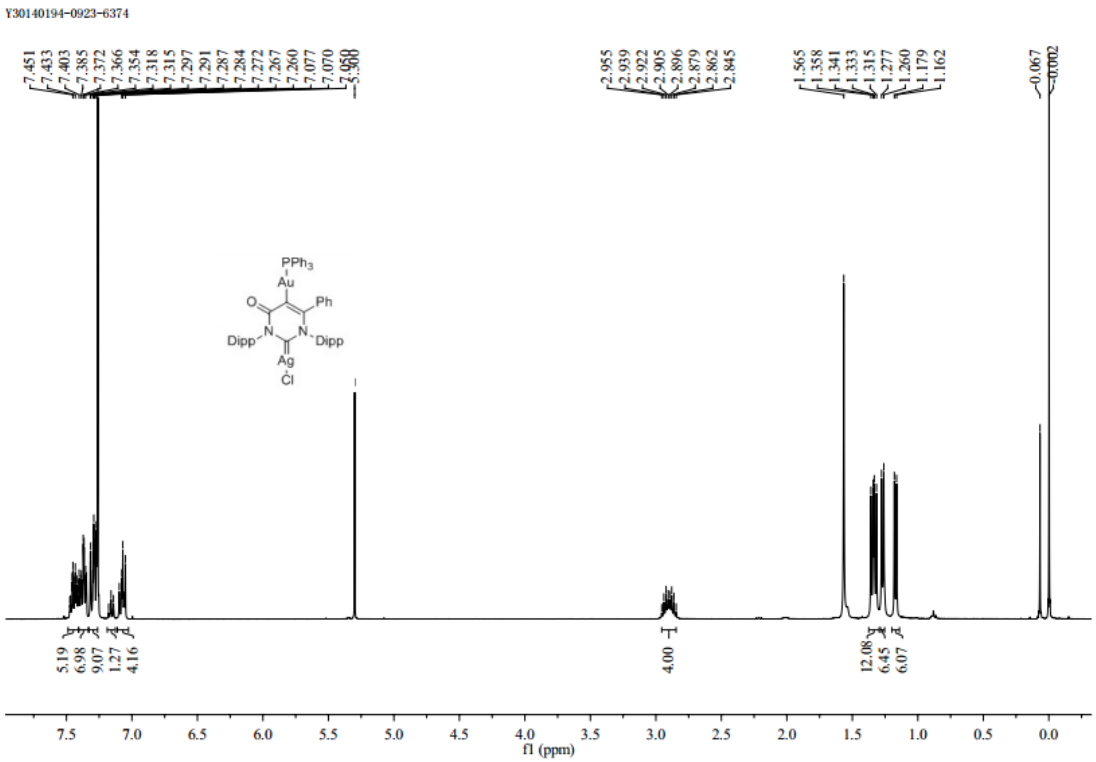

Figure S6. ^{1}H NMR spectrum of **4**

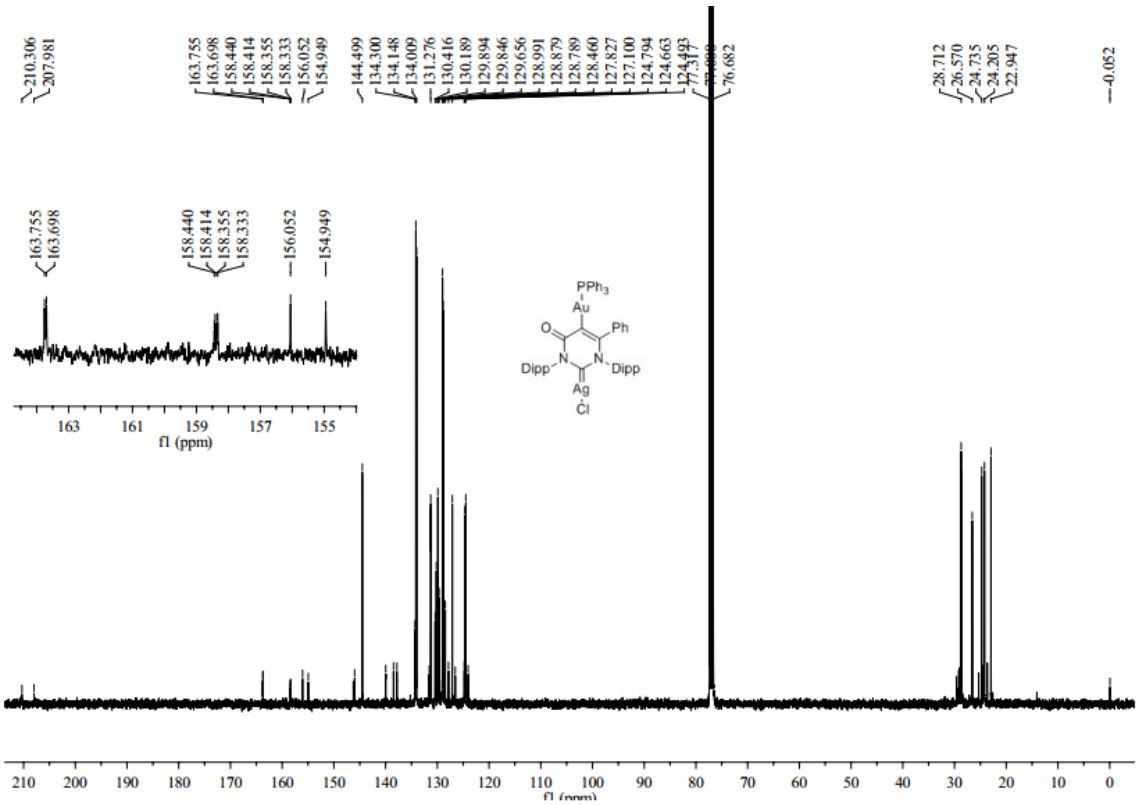

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **4**

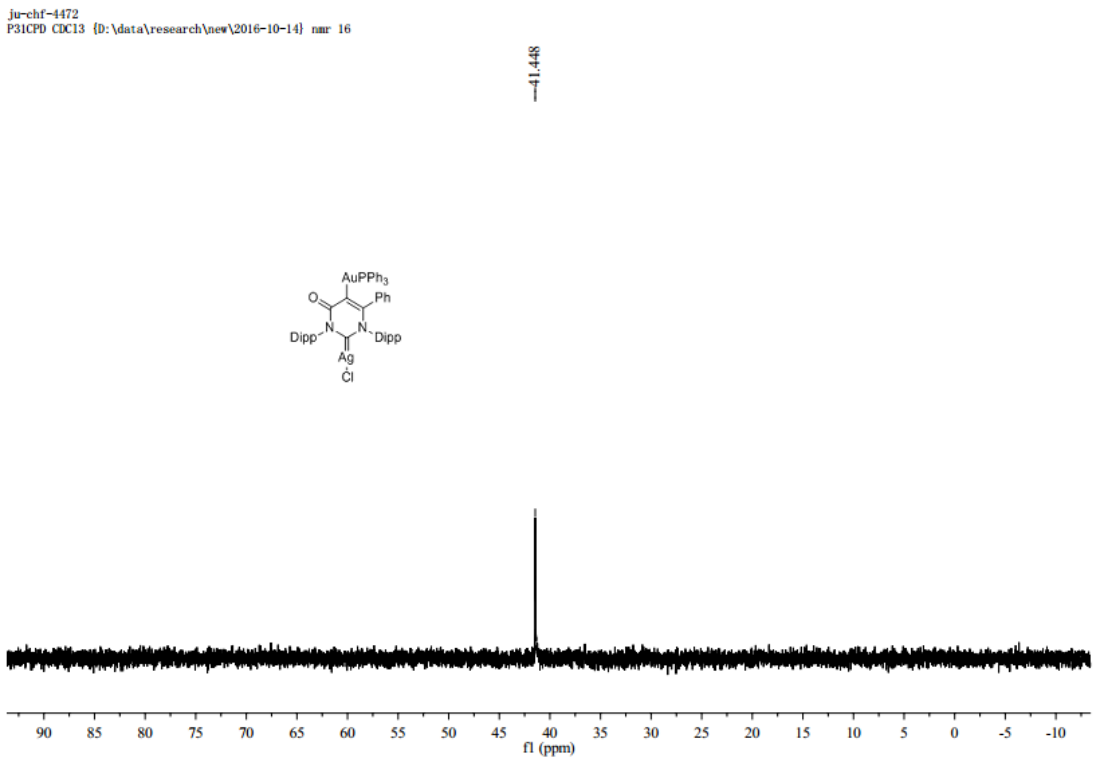

Figure S8. ^{31}P NMR spectrum of **4**

2. **X-Ray Crystallography**.

Each crystal was mounted on a glass fiber. Crystallographic measurements were made on a Bruker Smart Apex 100 CCD area detector using graphite monochromated Mo-Kα radiation ($\lambda_{\text{Mo-K}\alpha}$ = 0.71073 Å). The structures were solved by direct methods (SHELXS-97) and refined on F^2 by full-matrix least squares (SHELX-97) using all unique data. All the calculations were carried out with the SHELXTL18 program.

Key details of the crystal and structure refinement data are summarized in Table S1. Further crystallographic details may be found in the respective CIF files, which were deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK [1514557 (**3**), 1514558 (**4**)].

Table S1. Crystal Data, Data Collection, and Structure Refinement for **3** and **4**.

	3	**4**
Identification code	mo_60927a	mo_dm16636_0m
CCDC	1514557	1514558
Formula	C71 H69 Au2 F3 N2 O4 P2 S	C_{52} H_{54} Ag Au Cl N_2 O P
Formula weight	1559.21	1094.23
T, K	296(2)	296
crystal system	Monoclinic	Monoclinic
space group	$P2_1/n$	P 1 21/n 1
a, Å	11.428(5) Å	12.8674(13)
b, Å	18.633(8)	16.5479(16)
c, Å	30.513(14)	25.510(3)
, deg	90	90
, deg	91.687(9)	103.277(2)
, deg	90	90
Volume, $Å^3$	6495(5)	5286.7(9)
Z	4	4
D_{calc}, Mg / m^3	1.595	1.375
absorption coefficient, mm^{-1}	4.652	3.257
F(000)	3088	2184
crystal size, mm	0.420 x 0.150 x 0.110	? x ? x ?
2θ range, deg	1.726 to 26.999	1.640 to 27.664
reflections collected /unique	45401/14139 [R(int) = 0.1036]	44065/12263 [R(int) = 0.0438]
data / restraints/ parameters	14139 / 56 / 774	12263 / 0 / 540
goodness of fit on F^2	0.930	1.014
final R indices [$I > 2(I)$][a]	R1 = 0.0513, wR2 = 0.1147	R1 = 0.0345, wR2 = 0.0697
R indices (all data)	R1 = 0.1165, wR2 = 0.1437	R1 = 0.0647, wR2 = 0.0795
lgst diff peak and hole, e/$Å^3$	0.979 and -0.804	0.790 and -1.152