Electronic Supplementary Information for Dalton Transactions

Supplementary Information

for

Exploring the Coordination Modes of Pyrrolyl Ligands in Bis(imido) Uranium(VI) Complexes

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Table S1. X-ray Crystallographic Data for Complexes **3** and **4**.

Crystal Data	**3-2 CH_2Cl_2**	**4**
Empirical formula	$C_{58}H_{68}Cl_4N_4O_2P_2U$	$C_{27}H_{46}N_4O_2U$
Crystal habit, color	Block, dark red	Block, dark red
Crystal size (mm)	0.14 x 0.14 x 0.10	0.32 x 0.08 x 0.06
Crystal system	Monoclinic	Orthorhombic
Space group	C 2/c	P nma
Volume ($Å^3$)	5369.4(13)	2816(2)
a(Å)	17.705(2)	17.189(8)
b(Å)	19.068(3)	14.566(7)
c(Å)	16.984(2)	11.246(5)
α(°)	90	90
β(°)	110.5310(10)	90
γ(°)	90	90
Z	4	4
Formula weight (g/mol)	1294.93	696.71
Density (calculated)(Mg/m^3)	1.602	1.644
Absorption coefficient (cm^{-1})	3.329	5.794
F_{000}	2600	1376
Radiation	MoKα, 0.71073 Å	MoKα, 0.71073 Å
Data Refinement		
Final R indices[a]	$R_1 = 0.0396$, $wR_2 = 0.0725$	R1 = 0.0442, wR2 = 0.0884
Largest diff. peak and hole ($eÅ^{-3}$)	0.732 and -0.543	0.871 and -1.205

[a]Number of observed reflections: **3**, 5550 ($I_o > 2\sigma I_o$), $R_1 = \Sigma \mid (|F_o| - |F_c|) \mid / \Sigma |F_o|$, $wR_2 = [\ \Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma wF_o^4\ ]^{1/2}$, $w = [\ \sigma^2 F_o^2 + (0.0315 \cdot p)^2\ ]^{-1}$, $p = [F_o^2 + 2 \cdot F_c^2]/3$. **4**, 2793 ($I_o > 2\sigma I_o$), $R_1 = \Sigma \mid (|F_o| - |F_c|) \mid / \Sigma |F_o|$, $wR_2 = [\ \Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma wF_o^4\ ]^{1/2}$, $w = [\ \sigma^2 F_o^2 + (0.0415 \cdot p)^2\ ]^{-1}$, $p = [F_o^2 + 2 \cdot F_c^2]/3$.

Table S2. X-ray Crystallographic Data for Complexes **5** and **6**.

Crystal Data	**5**	**6**
Empirical formula	$C_{37}H_{50}N_4U$	$C_{46}H_{73}N_4P_2U$
Crystal habit, color	Needle, black	Needle, black
Crystal size (mm)	0.14 x 0.11 x 0.08	0.20 x 0.18 x 0.02
Crystal system	Triclinic	Monoclinic
Space group	P $\bar{1}$	P 2_1/c
Volume (Å^3)	1696.1(2)	4540.9(17)
a(Å)	11.1415(9)	11.649(3)
b(Å)	12.5846(11)	17.676(4)
c(Å)	12.7942(11)	22.136(5)
α(^{o})	87.3010(1)	90
β(^{o})	80.7680(1)	94.986(3)
γ(^{o})	73.3150(1)	90
Z	2	4
Formula weight (g/mol)	788.84	982.05
Density (calculated)(Mg/m^3)	1.545	1.436
Absorption coefficient (cm-^{1})	4.815	3.680
F_{000}	784	1996
Radiation	MoKα, 0.71073 Å	MoKα, 0.71073 Å
Data Refinement		
Final R indices[a]	R1 = 0.0411, wR2 = 0.0852	R1 = 0.0779, wR2 = 0.1472
Largest diff. peak and hole (eÅ^{-3})	1.345 and -0.851	1.864 and -1.467

[a]Number of observed reflections: **2**, 7516 ($I_o > 2\sigma I_o$), $R_1 = \Sigma \mid (|F_o| - |F_c|) \mid / \Sigma |F_o|$, $wR_2 = [\ \Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma wF_o^4\ ]^{1/2}$, $w = [\ \sigma^2 F_o^2 + (0.0534 \cdot p)^2\ ]^{-1}$, $p = [F_o^2 + 2 \cdot F_c^2]/3$. **6**, 8079 ($I_o > 2\sigma I_o$), $R_1 = \Sigma \mid (|F_o| - |F_c|) \mid / \Sigma |F_o|$, $wR_2 = [\ \Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma wF_o^4\ ]^{1/2}$, $w = [\ \sigma^2 F_o^2 + (0.0354 \cdot p)^2\ ]^{-1}$, $p = [F_o^2 + 2 \cdot F_c^2]/3$.