Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Material

Synthesis, characterization, biological properties, and molecular docking studies of new phosphoramide-based Ag(I) complexes

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Materials and methods

All chemicals and solvents used in the syntheses were commercially available and were used without further purification. IR spectrum was recorded on a Nicolet 510P spectrophotometer using KBr disks. Elemental analysis was performed using a Heraeus CHN-O-RAPID apparatus.

Methods

X-ray crystallography

colorless crystal of **C*m*** was obtained from the C_2H_5OH/H_2O. The X-ray data for the reported structures were collected at 293(2) K with an Oxford Sapphire CCD diffractometer using Cu Kα radiation λ = 1.54184 Å and ω-2θ method. All structures were solved by direct methods and refined with the full-matrix least-squares method on F^2 with the use of SHELX2014 program packages.[1] The analytical absorption corrections were applied (CrysAlis version 171.38.43 package of programs[2] Rigaku OD., 2015). Positions of hydrogen atoms have been found from the electron density maps and hydrogen atoms were constrained during refinement with the appropriate riding model as implemented in SHELX during refinement. The data collection and refinement processes are summarized in Table S1. The structural data has been deposited at the Cambridge Crystallographic Data Centre: (CCDC No for structure **C*m*** is 2150302)

Table S1 Crystal data and structure refinement parameters for **C*m***

Identification code	**C*m***
Empirical formula	$C_{34}H_{34}Ag_2N_6O_{10}P_2$
Formula weight	964.35
Temperature/K	293.0
Crystal system	monoclinic
Space group	C2/c
a/Å	16.6319(8)
b/Å	9.1023(5)
c/Å	24.8356(16)
α/°	90
β/°	97.289(5)
γ/°	90
Volume/Å^3	3729.5(4)
Z	4
ρ_{calc}g/cm^3	1.718
μ/mm^{-1}	9.794
F(000)	1936.0
Crystal size/mm^3	0.18 × 0.12 × 0.04
2Θ range for data collection/°	7.176 to 136.502
Index ranges	-19 ≤ h ≤ 16, -10 ≤ k ≤ 6, -29 ≤ l ≤ 24
Reflections collected	6341
Independent reflections	3352 [R_{int} = 0.0252, R_{sigma} = 0.0367]
Data/restraints/parameters	3352/0/245
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0397, wR_2 = 0.1081
Final R indexes [all data]	R_1 = 0.0466, wR_2 = 0.1139
Largest diff. peak/hole / e Å^{-3}	1.07/-0.67

Table S2 Selected bond length (Å) and angles (°) around Ag (I) for complex **C*m***

C*m*			
Ag1–O2	2.211(3)Å	Ag1–O4	2.618(4) Å
Ag1–N1	2.185(3) Å	Ag1–O4	2.658(4) Å
N1–Ag1–O2	163.07(13)°	O4– Ag1–O2	83.6(1)°
O4– Ag1–O4	80.4(1)°	O4– Ag1–N1	90.5(1)°

References

1. G. M. Sheldrick, *Acta Cryst*., 2015, C71, 3-8.
2. CrysAlis 171.38.43 package of programs, *Rigaku Oxford Diffraction*, 2015.