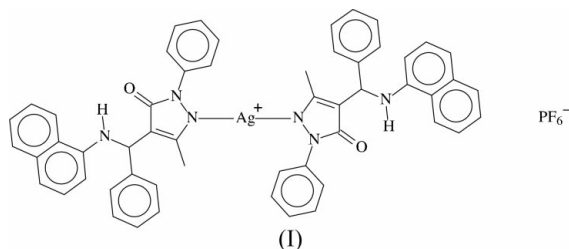


**Bis{5-methyl-4-[(Z)-(1-naphthylamino)phenyl-methylene]-2-phenyl-3H-pyrazol-3-one- $\kappa^2$ N,N'}-silver(I) hexafluorophosphate**Xing-Qiang Lü,<sup>a</sup> Feng Bao,<sup>a</sup> Qing Wu,<sup>a</sup> Bei-Sheng Kang<sup>a</sup> and Seik Weng Ng<sup>a,b\*</sup><sup>a</sup>School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

**Key indicators**Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.097  
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title complex,  $[\text{Ag}(\text{C}_{27}\text{H}_{21}\text{N}_3\text{O})_2]\text{PF}_6$ , the Ag atom occupies a centre of symmetry, resulting in linear N—Ag—N coordination [ $\text{Ag}-\text{N} = 2.124(2)$  Å]. The P atom of the counter-anion has  $\bar{1}$  site symmetry.**Comment**The reaction of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone with primary amines affords Schiff bases that can function as N- and O-donor ligands, *e.g.* 4-[(2-tolylamino)phenylmethylene]pyrazol-5-methyl-2-phenyl-3(2*H*)-one (Bao *et al.*, 2004; Wang *et al.*, 2002) and 4-[(2-hydroxyphenylamino)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3(4*H*)-one (Wang *et al.*, 2002), to a range of metal ions. The 1-naphthyl analogue, whose crystal structure has been reported (Wang *et al.*, 2003), coordinates to the Ag atom of silver hexafluorophosphate, giving rise to linear coordination at the metal atom. In the cationic entity of the title compound, (I), the ligand is bonded through the tertiary pyrazolyl N atom (Fig. 1); as the Ag atom lies on an inversion centre, there is only one unique Ag—N bond [ $2.124(2)$  Å] and the N—Ag—N coordination is linear. The counter-anion has  $\bar{1}$  site symmetry. An intramolecular N—H...O hydrogen bond (Table 1) is observed for the ligand.A search of the November 2002 version of the Cambridge Structural Database (Allen, 2002) yields only two examples of *N*-coordinated pyrazolone complexes, *viz.* a molybdenum complex of 1-acetimido-4-phenyl-3-pyrazolone and a manganese complex of 5-phenyl-3-pyrazolone (Aromi *et al.*, 2002). The class of pyrazolones, as represented by the organic moiety in the present compound, is also known to interact through the carbonyl O atom. The Schiff base derivative with 1,3-diaminopropane binds to the Ni atom through the two carbonyl O atoms as well as the deprotonated imine N atoms (la Cour *et al.*, 1996).**Experimental**4-[(1-Naphthylamino)phenylmethylene]pyrazole-5-methyl-2-phenyl-3(2*H*)-one was synthesized from the reaction of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone and 1-naphthylamine (Wang *et al.*, 2003). The

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compound (0.41 g, 0.1 mmol) was dissolved in dichloromethane (5 ml) along with silver hexafluorophosphate (0.26 g, 0.1 mmol). Yellow prismatic crystals of (I) separated from the solution in about 70% yield. Analysis calculated for  $C_{54}H_{42}AgN_6O_2P$ : C 61.20, H 3.99, N 7.93%; found: C 60.71, H 4.02, N 7.82%.

#### Crystal data

$[Ag(C_{27}H_{21}N_3O)_2]PF_6$   
 $M_r = 1059.78$   
 Triclinic,  $P\bar{1}$   
 $a = 9.655$  (1) Å  
 $b = 10.859$  (1) Å  
 $c = 11.384$  (1) Å  
 $\alpha = 88.695$  (2)°  
 $\beta = 79.453$  (2)°  
 $\gamma = 88.840$  (2)°  
 $V = 1172.9$  (2) Å<sup>3</sup>

$Z = 1$   
 $D_x = 1.500$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 974 reflections  
 $\theta = 2.6$ – $26.8$ °  
 $\mu = 0.54$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Prism, yellow  
 $0.43 \times 0.36 \times 0.30$  mm

#### Data collection

Bruker SMART area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\min} = 0.693$ ,  $T_{\max} = 0.837$   
 10 053 measured reflections

5042 independent reflections  
 3499 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\text{max}} = 27.0$ °  
 $h = -12 \rightarrow 12$   
 $k = -13 \rightarrow 13$   
 $l = -14 \rightarrow 14$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.097$   
 $S = 0.91$   
 5042 reflections  
 320 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0582P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.55$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>

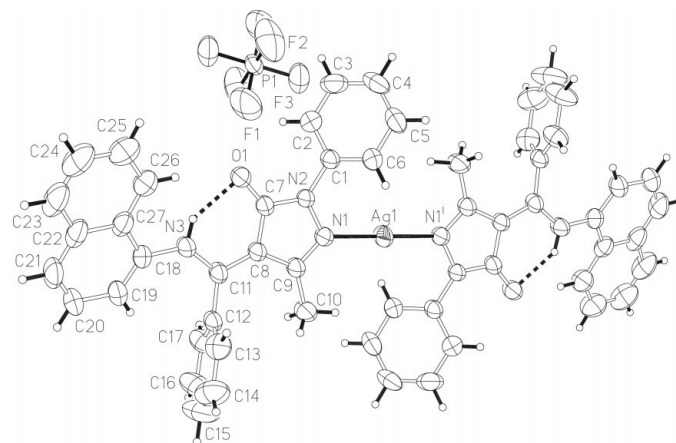
**Table 1**

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3-H3n \cdots O1$	0.86	1.92	2.669 (2)	145

H atoms were placed in idealized positions and included in the refinement in the riding-model approximation [ $C-H_{\text{aromatic}} = 0.93$  Å and  $U(H_{\text{aromatic}}) = 1.2U_{\text{eq}}(C)$ ,  $C-H_{\text{methyl}} = 0.97$  Å and  $U_{\text{iso}}(H_{\text{methyl}}) = 1.5U_{\text{eq}}(C)$ , and  $N-H = 0.86$  Å and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(N)$ ].

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97; molecular graphics: ORTEPII (Johnson,



**Figure 1**

ORTEPII (Johnson, 1976) plot of (I) (50% probability displacement ellipsoids). H atoms are drawn as spheres of arbitrary radii and the N–H···O hydrogen bonds are indicated by dashed lines. [Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ ].

1976); software used to prepare material for publication: SHELXL97.

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