Supporting Information: Synthesis and Thermochromic Luminescence of Ag(I) Complexes Based on 4,6-Bis(diphenylphosphino)pyrimidine

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Table 1. X-Ray crystallographic data for **1**·CH₃CN and **2**·CH₃CN.

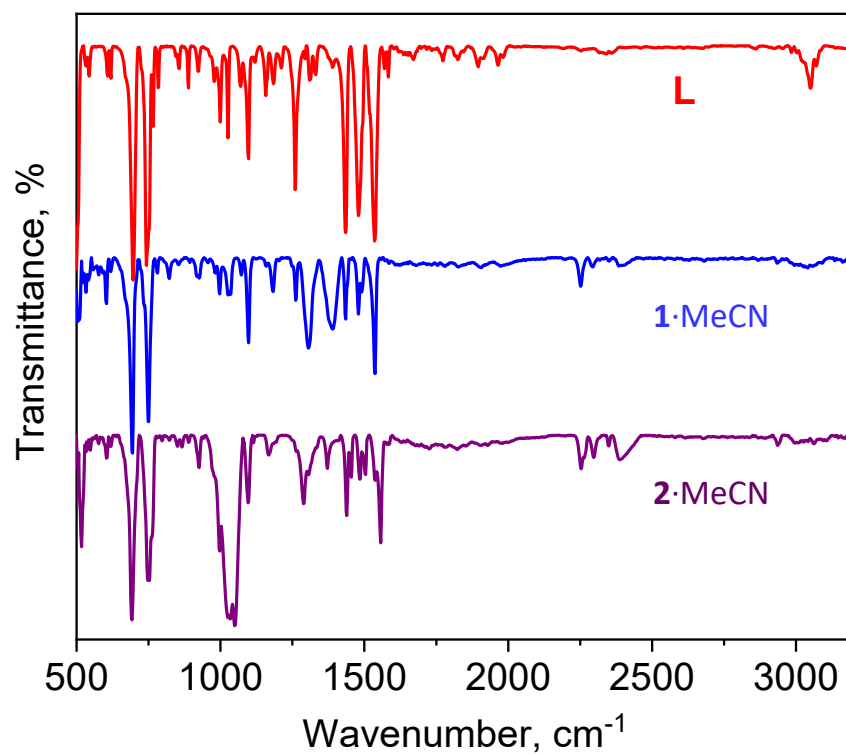|	**1·CH₃CN**	**2·CH₃CN**
Crystal data	2020455	2020456
Chemical formula	$C_{62}H_{53}Ag_2N_9O_6P_4$	$C_{36}H_{34}Ag_2B_2F_8N_6P_2$
M_r	1359.75	1001.99
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, $P2_12_12_1$
Temperature (K)	140	140
a, b, c (Å)	9.2947(2), 18.598(5), 18.314(4)	13.2478(4), 15.6986(4), 19.7010(5)
$\beta(°)$	90.534(2)	-
V (Å³)	3165.78(13)	4097.25(19)
Z	2	4
μ (mm⁻¹)	0.78	1.11
Crystal size (mm)	0.21 × 0.12 × 0.09	0.39 × 0.24 × 0.11
T_{min}, T_{max}	0.993, 1.000	0.922, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14090, 6793, 5449	21537, 9167, 8486
R_{int}	0.018	0.023
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.675	0.682
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.180, 1.06	0.026, 0.056, 1.02
No. of reflections	6793	9167
No. of parameters	565	555
No. of restraints	937	200
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	1.78, −2.30	0.46, −0.38

Figure S1. FT-IR spectra of **1**, **2** and parent ligand **L**.
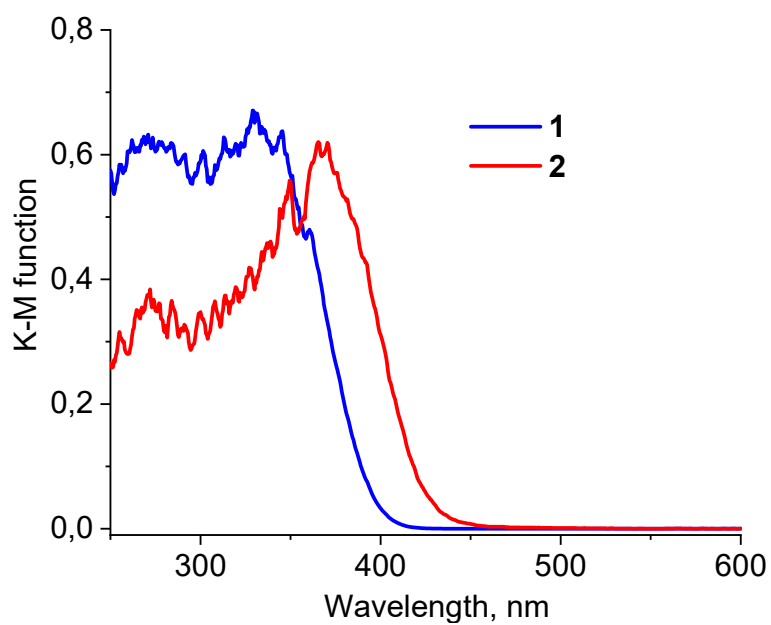

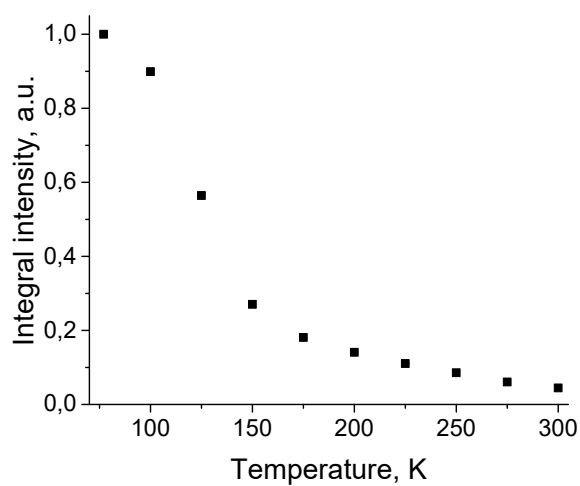**Figure S2.** Solid state absorption spectra of **1** and **2** plotted as a Kubelka-Munk function.

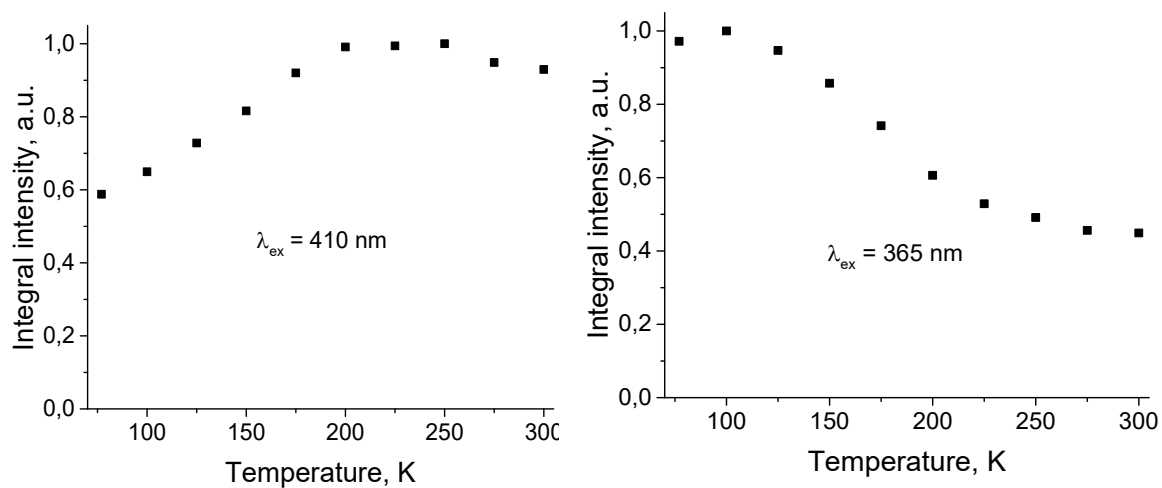**Figure S3.** Temperature dependence of the integral intensity of the emission of **1** (λ_{ex} = 365 nm).

Figure S4. Temperature dependences of the integral intensity of the emission of **2** recorded at λ_{ex} = 410 nm (***left***) and λ_{ex} = 365 nm (***right***).
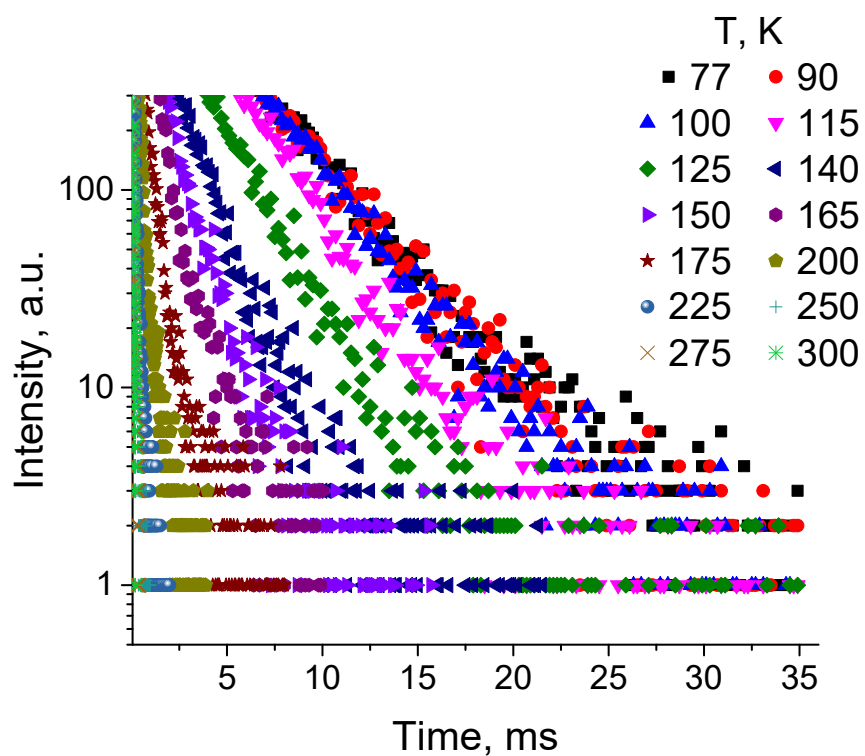
Figure S5. Emission decay profiles of **1** recorded at different temperatures (λ_{ex} = 385 nm, λ_{em} = 550 nm).

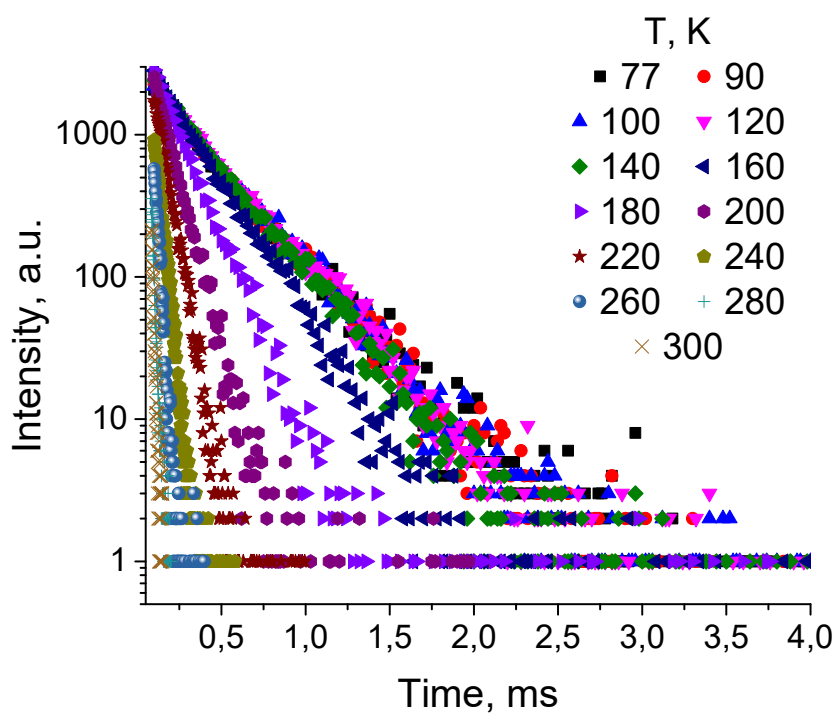**Figure S6.** Emission decay profiles of **2** recorded at different temperatures (λ_{ex} = 410 nm, λ_{em} = 580 nm).

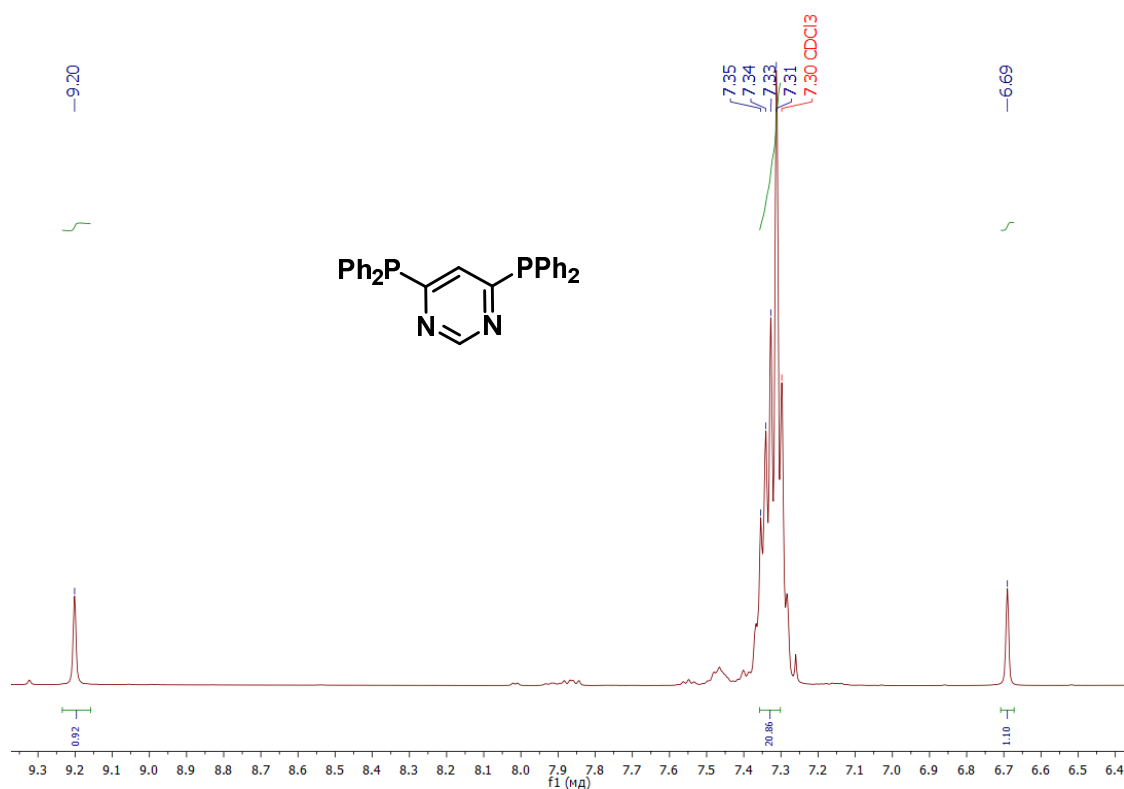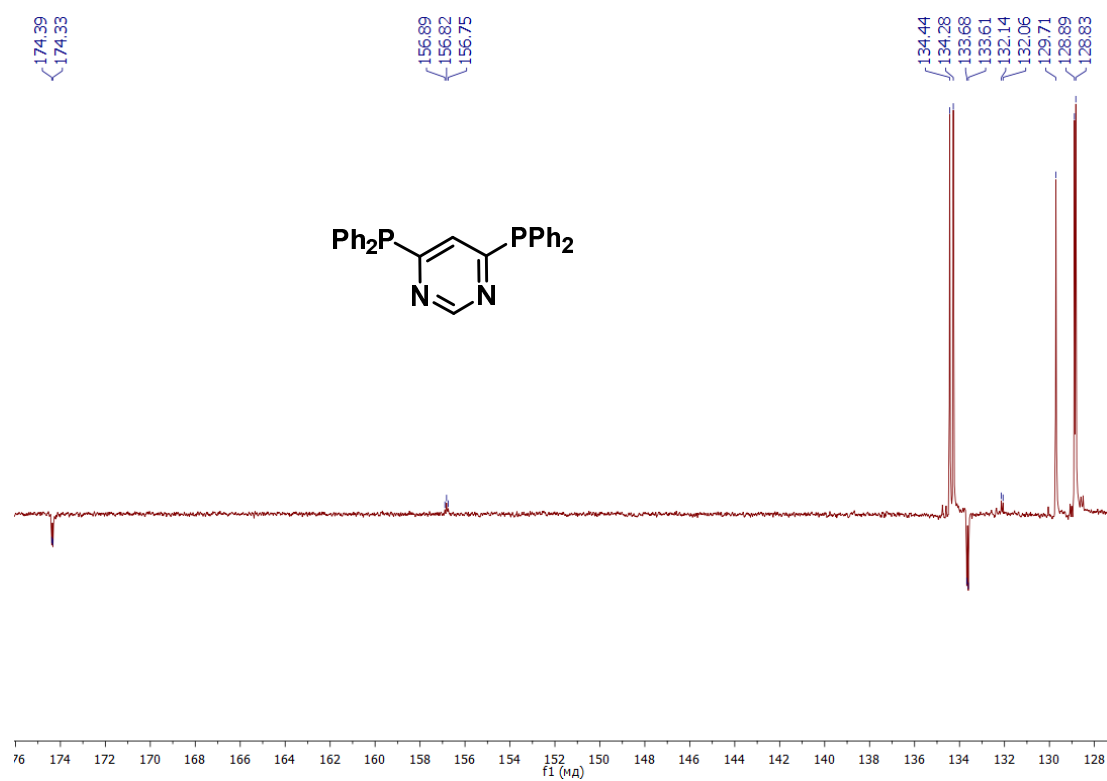**Figure S7.** ^{1}H NMR spectrum of the ligand **L** (CDCl$_3$).

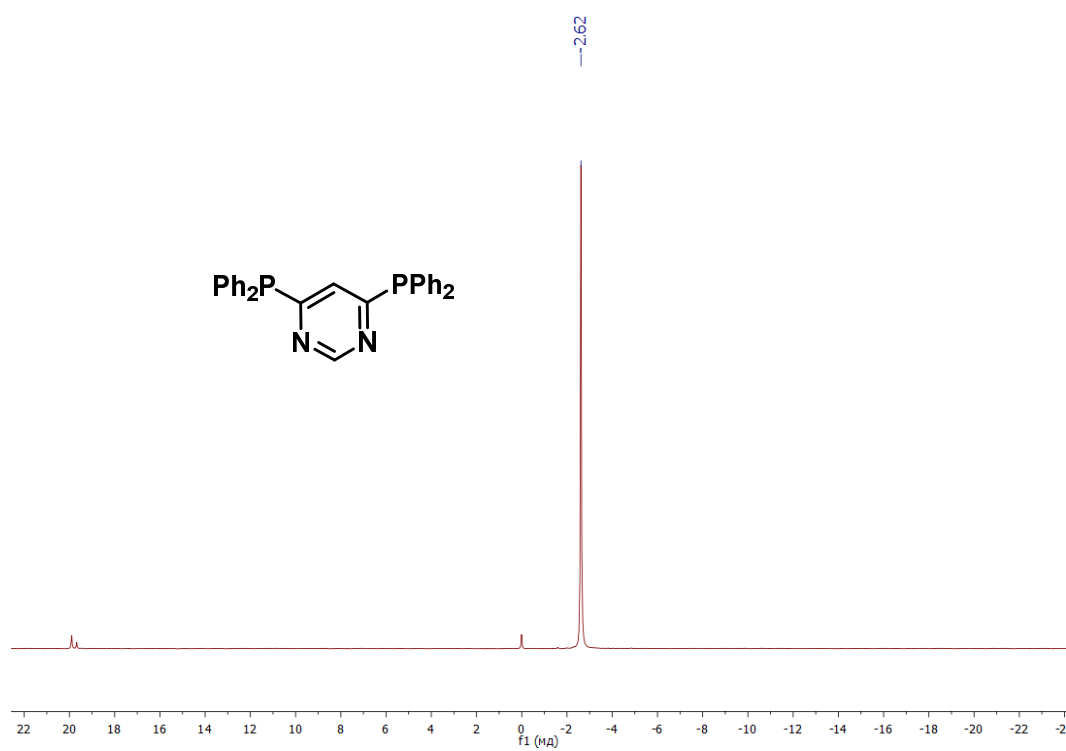**Figure S8.** J-modulated ^{13}C NMR spectrum of the ligand **L** (CDCl$_3$).

Figure S9. $^{31}P\{^1H\}$ NMR spectrum of the ligand **L** (CDCl3).

HOMO+3

HOMO+2

HOMO+1
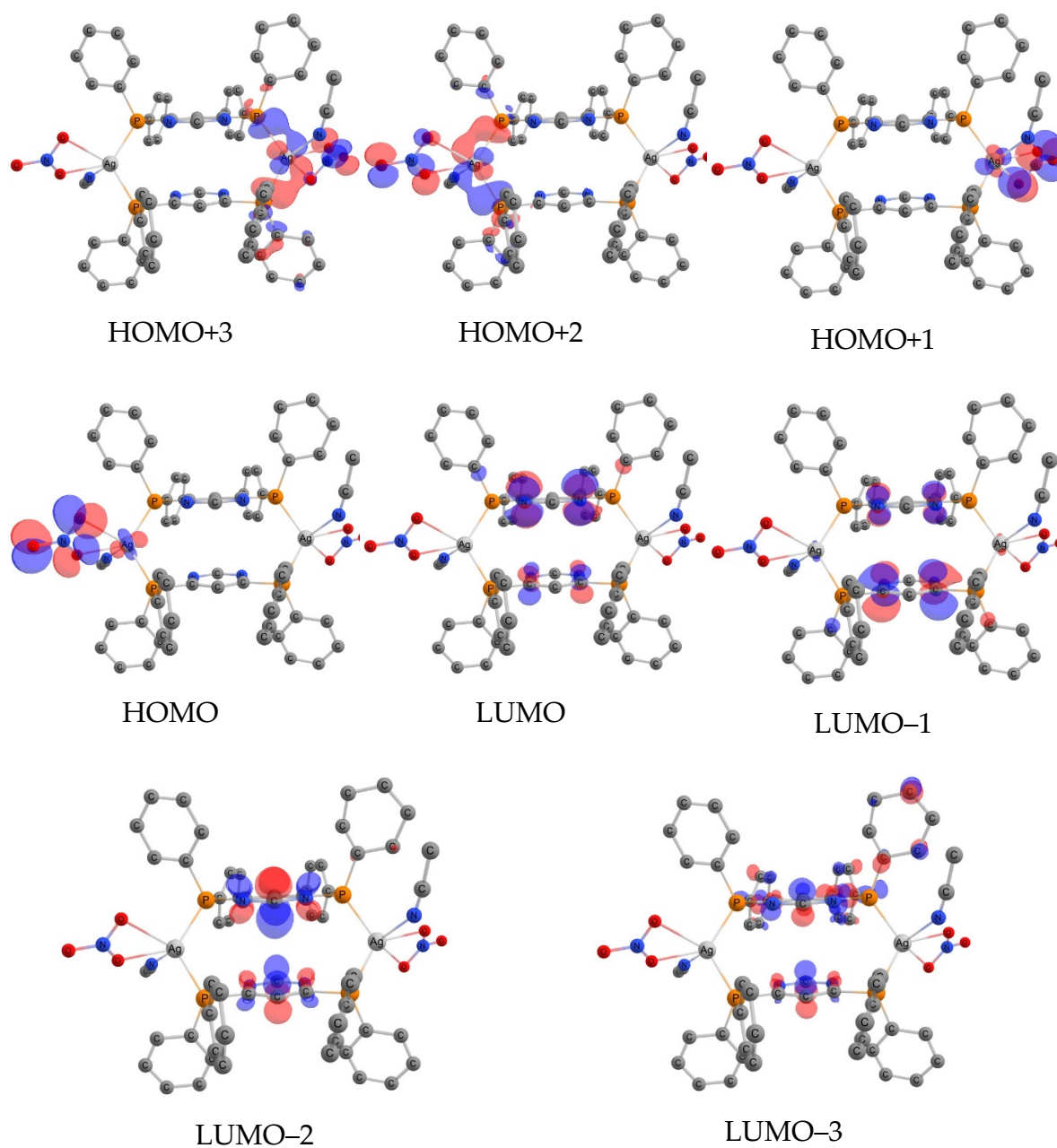
HOMO

LUMO

LUMO–1

LUMO–2

LUMO–3

Figure 10. Four lowest unoccupied and 4 highest occupied MOs (iso-value = 0.045) for the S_0 state of the complex **1** calculated at the B3LYP/def2TZVP level. .