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Supporting Information for

Three-coordinate gold(I) *N*-Heterocyclic carbene complexes: a new class of strongly luminescent derivatives

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1. Experimental details

UV-Vis spectra were recorded with a UnicamUV-4 spectrophotometer. Steady-state photoluminescence spectra were recorded with a Jobin-Yvon-Horiba fluorolog FL-3-11 spectrometer using band pathways of 3 nm for both excitation and emission. Phosphorescence lifetimes were recorded with a Fluoromax phosphorimeter accessory containing a UV xenon flash tube at a flash rate between 0.05 and 25 Hz. The lifetime data were fit using the Jobin-Yvon software package and the Origin 5.0 program. Direct quantum yield measurements were performed for solid samples **1**-**7** at room temperature with an integrating sphere from LabSphere that is interfaced to the PTI instrument; in order to verify the reliability and accuracy of our techniques, we determined the direct quantum yield of quinine sulfate solution using this setup and attained the correct value of 0.53.

The monocrystal was mounted in inert oil on glass fibers and transferred to the cold gas stream of a Xcalibur Oxford Diffraction diffractometer equipped with a low-temperature attachment. Data were collected using monochromated Mo Kα radiation (λ= 0.71073 Å). Scan type ω. Absorption correction based on multiple scans was applied with the program SADABS (**5**)[1] or using spherical harmonics implemented in SCALE3 ABSPACK[2] scaling algorithm (**4**). The structures were solved by direct methods and refined on F^2 using the program SHELXL-97.[3] All non-hydrogen atoms were refined anisotropically. In all cases, hydrogen atoms were included in calculated positions and refined using a riding model. Refinements were carried out by full-matrix least-squares on F^2 for all data.

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2. X-ray diffraction analysis data

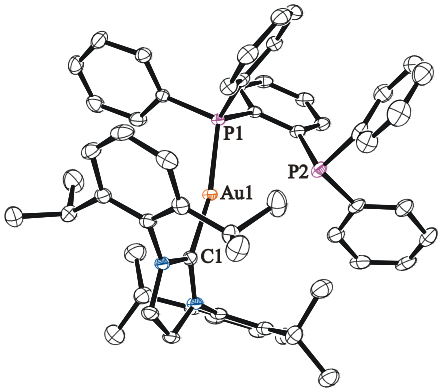

Figure S1.Ortep diagram for **4** with 50 % probability ellipsoids. $CF_3SO_3^-$, $Cl_2CH_2CH_2Cl_2$ molecule and hydrogen atoms are omitted for clarity.

Table S1. X-ray Crystallographic data for **[Au(IPr)(dppbz)]OTf•ClCH$_2$CH$_2$Cl**.

Compound	**4· $C_2H_4Cl_2$**
Formula	$C_{60}H_{64}AuCl_2F_3N_2O_3P_2S$
M_r	1280.00
Habit	pale green tablet
Crystal size (mm)	0.10x0.08x0.08
Crystal system	Triclinic
Space group	P-1
Cell constants:	
a (Å)	11.3839(2)
b (Å)	12.7921(2)
c (Å)	20.0475(3)
α (°)	81.878(2)
β (°)	76.444(2)
γ (°)	89.880(2)
V (Å^3)	2808.14(8)
Z	2
D_X (Mg m^{-3})	1.514
μ(mm^{-1})	2.865
F(000)	1296
T (°C)	-143(2)
$2\theta_{max}$	51
No. of refl.:	
measured	52544
independent	10415
Transmissions	0.8032-0.7626
R_{int}	0.0430
Parameters	667
Restraints	0
Goodness of fit on F^2	1.027
wR(F^2, all Refl.)	0.0548
$R(I>2\sigma(I))$	0.0228
max. Δρ (e Å^{-3})	1.049

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Table S2. Selected bond lengths (Å) and angles (deg) for solid structure of **4**.

Au(1)-C(1)	2.036(3)	C(1)-Au(1)-P(1)	168.27(7)
Au(1)-P(1)	2.2929(7)	C(40)-P(1)-C(34)	106.32(12)
P(1)-C(40)	1.815(3)	C(40)-P(1)-C(28)	105.04(12)
P(1)-C(34)	1.817(3)	C(34)-P(1)-C(28)	105.69(12)
P(1)-C(28)	1.823(3)	C(40)-P(1)-Au(1)	110.97(9)
P(2)-C(46)	1.828(3)	C(34)-P(1)-Au(1)	109.14(9)
P(2)-C(52)	1.830(3)	C(28)-P(1)-Au(1)	118.90(9)
P(2)-C(33)	1.840(3)	C(46)-P(2)-C(52)	104.28(13)
N(1)-C(1)	1.357(3)	C(46)-P(2)-C(33)	100.45(12)
N(1)-C(2)	1.388(3)	C(52)-P(2)-C(33)	103.40(13)
N(1)-C(4)	1.446(3)	C(1)-N(1)-C(2)	110.8(2)
N(2)-C(1)	1.349(3)	C(1)-N(1)-C(4)	123.0(2)
N(2)-C(3)	1.376(3)	C(2)-N(1)-C(4)	126.2(2)
N(2)-C(16)	1.448(3)	C(1)-N(2)-C(3)	111.1(2)
C(2)-C(3)	1.342(4)	C(1)-N(2)-C(16)	124.0(2)
C(2)-H(2)	0.9500	C(3)-N(2)-C(16)	124.8(2)
C(3)-H(3)	0.9500	N(2)-C(1)-N(1)	104.5(2)
C(4)-C(9)	1.399(4)	N(2)-C(1)-Au(1)	130.56(19)
C(4)-C(5)	1.405(4)	N(1)-C(1)-Au(1)	124.62(19)
C(5)-C(6)	1.395(4)	C(3)-C(2)-N(1)	106.3(2)
C(5)-C(10)	1.513(4)	C(3)-C(2)-H(2)	126.9
C(6)-C(7)	1.376(4)	N(1)-C(2)-H(2)	126.9
C(6)-H(6)	0.9500	C(2)-C(3)-N(2)	107.3(2)
C(7)-C(8)	1.380(4)	C(2)-C(3)-H(3)	126.4
C(7)-H(7)	0.9500	N(2)-C(3)-H(3)	126.4
C(8)-C(9)	1.394(4)	C(9)-C(4)-C(5)	123.6(2)
C(8)-H(8)	0.9500	C(9)-C(4)-N(1)	118.4(2)
C(9)-C(13)	1.522(4)	C(5)-C(4)-N(1)	118.0(2)
C(10)-C(11)	1.531(4)	C(6)-C(5)-C(4)	116.4(3)
C(10)-C(12)	1.531(4)	C(6)-C(5)-C(10)	120.0(3)
C(10)-H(10)	1.0000	C(4)-C(5)-C(10)	123.7(2)
C(11)-H(11A)	0.9800	C(7)-C(6)-C(5)	121.2(3)
C(11)-H(11B)	0.9800	C(7)-C(6)-H(6)	119.4
C(11)-H(11C)	0.9800	C(5)-C(6)-H(6)	119.4
C(12)-H(12A)	0.9800	C(6)-C(7)-C(8)	121.1(3)
C(12)-H(12B)	0.9800	C(6)-C(7)-H(7)	119.4
C(12)-H(12C)	0.9800	C(8)-C(7)-H(7)	119.4
C(13)-C(14)	1.524(4)	C(7)-C(8)-C(9)	120.6(3)
C(13)-C(15)	1.528(4)	C(7)-C(8)-H(8)	119.7
C(13)-H(13)	1.0000	C(9)-C(8)-H(8)	119.7
C(14)-H(14A)	0.9800	C(8)-C(9)-C(4)	117.1(3)
C(14)-H(14B)	0.9800	C(8)-C(9)-C(13)	120.2(3)
C(14)-H(14C)	0.9800	C(4)-C(9)-C(13)	122.7(2)
C(15)-H(15A)	0.9800	C(5)-C(10)-C(11)	111.4(2)
C(15)-H(15B)	0.9800	C(5)-C(10)-C(12)	111.3(2)
C(15)-H(15C)	0.9800	C(11)-C(10)-C(12)	110.3(3)
C(16)-C(17)	1.395(4)	C(5)-C(10)-H(10)	107.9
C(16)-C(21)	1.402(4)	C(20)-C(21)-C(25)	120.9(3)

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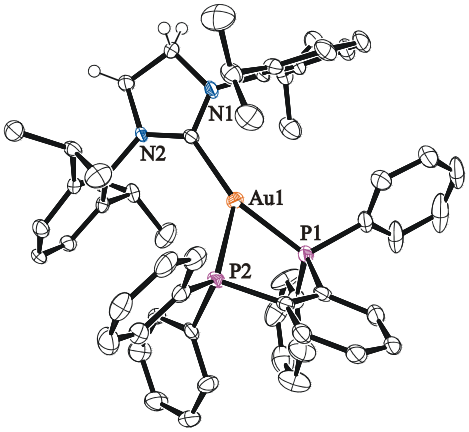

Figure S2.Ortep diagram for **5** with 50 % probability ellipsoids. $CF_3SO_3^-$, CH_2Cl_2 molecule and most of hydrogen atoms are omitted for clarity.

Table S3. X-ray Crystallographic data for **[Au(SIPr)(dppbz)]OTf·CH_2Cl_2**.

Compound	**5· CH_2Cl_2**
Formula	$C_{59}H_{64}AuCl_2F_3N_2O_3P_2S$
M_r	1267.99
Habit	pale green tablet
Crystal size (mm)	0.40x0.24.0.16
Crystal system	Triclinic
Space group	P-1
Cell constants:	
a (Å)	11.4745(10)
b (Å)	12.6486(11)
c (Å)	19.5252(16)
α (°)	85.6100(10)
β (°)	79.8940(10)
γ (°)	89.4190(10)
V (Å^3)	2781.6(4)
Z	2
D_X (Mg m^{-3})	1.514
μ(mm^{-1})	2.892
F(000)	1284
T (°C)	-173(2)
$2\theta_{max}$	51
No. of refl.:	
measured	28157
independent	10289
Transmissions	0.6548-0.3909
R_{int}	0.0313
Parameters	642
Restraints	0
Goodness of fit on F^2	1.174
wR(F^2, all Refl.)	0.1571
R(I >2σ(I))	0.0701
max. Δρ (e Å^{-3})	7.308

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Table S4. Selected bond lengths (Å) and angles (deg) for solid structure of **5**.

Au(1)-C(1)	2.055(8)	C(1)-Au(1)-P(1)	154.5(2)
Au(1)-P(1)	2.333(2)	C(1)-Au(1)-P(2)	127.7(2)
Au(1)-P(2)	2.764(2)	P(1)-Au(1)-P(2)	77.79(7)
P(1)-C(34)	1.816(10)	C(34)-P(1)-C(28)	106.2(4)
P(1)-C(28)	1.820(8)	C(34)-P(1)-C(40)	106.1(5)
P(1)-C(40)	1.823(9)	C(28)-P(1)-C(40)	102.7(4)
P(2)-C(46)	1.830(8)	C(34)-P(1)-Au(1)	114.0(3)
P(2)-C(33)	1.834(9)	C(28)-P(1)-Au(1)	111.8(3)
P(2)-C(52)	1.836(10)	C(40)-P(1)-Au(1)	115.0(3)
N(1)-C(1)	1.340(10)	C(46)-P(2)-C(33)	101.3(4)
N(1)-C(4)	1.443(10)	C(46)-P(2)-C(52)	104.5(4)
N(1)-C(2)	1.489(10)	C(33)-P(2)-C(52)	102.5(4)
N(2)-C(1)	1.341(10)	C(46)-P(2)-Au(1)	101.3(3)
N(2)-C(16)	1.437(10)	C(33)-P(2)-Au(1)	100.7(3)
N(2)-C(3)	1.484(10)	C(52)-P(2)-Au(1)	140.9(3)
C(2)-C(3)	1.527(11)	C(1)-N(1)-C(4)	124.4(7)
C(4)-C(5)	1.398(12)	C(1)-N(1)-C(2)	112.3(6)
C(4)-C(9)	1.406(12)	C(4)-N(1)-C(2)	120.2(7)
C(5)-C(6)	1.379(12)	C(1)-N(2)-C(16)	126.5(7)
C(5)-C(10)	1.527(13)	C(1)-N(2)-C(3)	112.6(6)
C(6)-C(7)	1.384(14)	C(16)-N(2)-C(3)	120.7(6)
C(7)-C(8)	1.371(14)	N(1)-C(1)-N(2)	108.4(7)
C(8)-C(9)	1.397(12)	N(1)-C(1)-Au(1)	122.5(6)
C(9)-C(13)	1.500(13)	N(2)-C(1)-Au(1)	129.0(6)
C(10)-C(12)	1.522(14)	N(1)-C(2)-C(3)	101.7(6)
C(10)-C(11)	1.537(13)	N(2)-C(3)-C(2)	101.8(6)
C(13)-C(15)	1.527(14)	C(5)-C(4)-C(9)	122.4(8)
C(13)-C(14)	1.528(14)	C(5)-C(4)-N(1)	118.3(7)
C(16)-C(17)	1.390(12)	C(9)-C(4)-N(1)	119.2(7)
C(16)-C(21)	1.415(12)	C(6)-C(5)-C(4)	117.9(8)
C(17)-C(18)	1.396(11)	C(6)-C(5)-C(10)	121.1(8)
C(17)-C(22)	1.525(12)	C(4)-C(5)-C(10)	121.0(7)
C(18)-C(19)	1.392(12)	C(5)-C(6)-C(7)	121.2(9)
C(19)-C(20)	1.366(13)	C(8)-C(7)-C(6)	120.1(8)
C(20)-C(21)	1.405(11)	C(7)-C(8)-C(9)	121.5(9)
C(21)-C(25)	1.502(12)	C(8)-C(9)-C(4)	116.8(9)
C(22)-C(23)	1.516(13)	C(8)-C(9)-C(13)	119.8(8)
C(22)-C(24)	1.534(12)	C(4)-C(9)-C(13)	123.4(8)
C(25)-C(27)	1.535(12)	C(12)-C(10)-C(5)	110.8(8)
C(25)-C(26)	1.537(13)	C(12)-C(10)-C(11)	111.3(8)
C(28)-C(33)	1.390(13)	C(5)-C(10)-C(11)	112.4(7)
C(28)-C(29)	1.422(12)	C(9)-C(13)-C(15)	111.6(8)
C(29)-C(30)	1.387(13)	C(9)-C(13)-C(14)	111.3(8)
C(39)-C(34)	1.372(15)	C(15)-C(13)-C(14)	110.9(9)
C(39)-C(38)	1.384(16)	C(17)-C(16)-C(21)	122.4(7)
C(30)-C(31)	1.369(14)	C(17)-C(16)-N(2)	118.7(7)
C(31)-C(32)	1.386(13)	C(21)-C(16)-N(2)	118.9(7)
C(32)-C(33)	1.401(12)	C(16)-C(17)-C(18)	118.4(8)

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Optical properties

Table S5. Optical properties for complexes **1-7**.

Complex	Electronic Absorption[a] λ_{max} [nm] (ε [$M^{-1}cm^{-1}$])	Medium (T [K])	Excitation λ_{max} [nm]	Emission λ_{max} [nm]	τ_o [µs]	Φ_{em} [%][b]
1	260 (102200)	Solid (298)	345	490	12.8	18
		Solid (77)	325	480	21.7	-----
		CH_2Cl_2 (298)	-----	-----	-----	-----
2	260 (102400)	Solid (298)	390	520	13.2	73
		Solid (77)	390	530	15.6	-----
		CH_2Cl_2 (298)	-----	-----	-----	-----
3	----- -----	Solid (298)	-----	-----	-----	-----
		Solid (77)	-----	-----	-----	-----
		CH_2Cl_2 (298)	-----	-----	-----	-----
4	310 (15600)	Solid (298)	370	505	14.3	80
		Solid (77)	370	510	23.9	-----
		CH_2Cl_2 (298)	370	525	14.6	1.2
5	310 (15800)	Solid (298)	370	490	17.9	98
		Solid (77)	370	500	30.7	-----
		CH_2Cl_2 (298)	370	540	13.6	1.9
6	310 (15200)	Solid (298)	370	530	17.2	99
		Solid (77)	370	530	21.0	-----
		CH_2Cl_2 (298)	390	550	11.7	1.4
7	310 (14500)	Solid (298)	370	545	10.2	59
		Solid (77)	390	525	78.0	-----
		CH_2Cl_2 (298)	370	550	13.4	1.4

[a] Electronic Absorption measured in degassed CH_2Cl_2. [b] Quantum yields measured at room temperature.

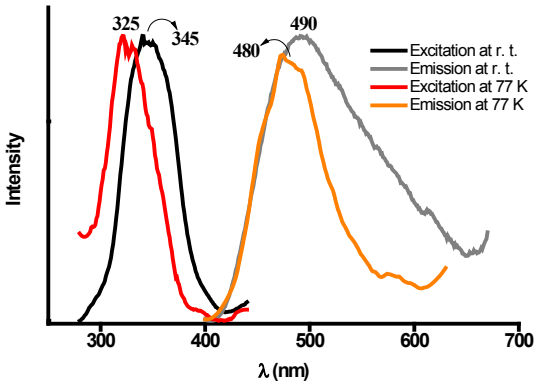

Figure S3. Excitation and emission spectra of **1** in the solid state.

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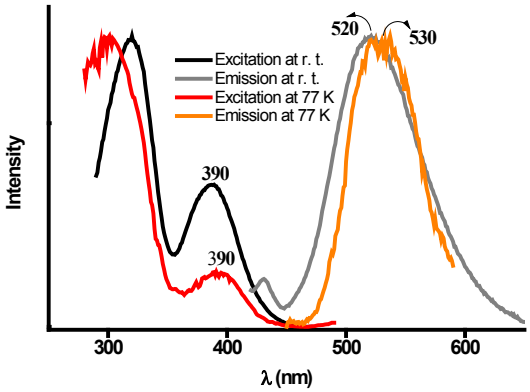

Figure S4. Excitation and emission spectra of **2** in the solid state.

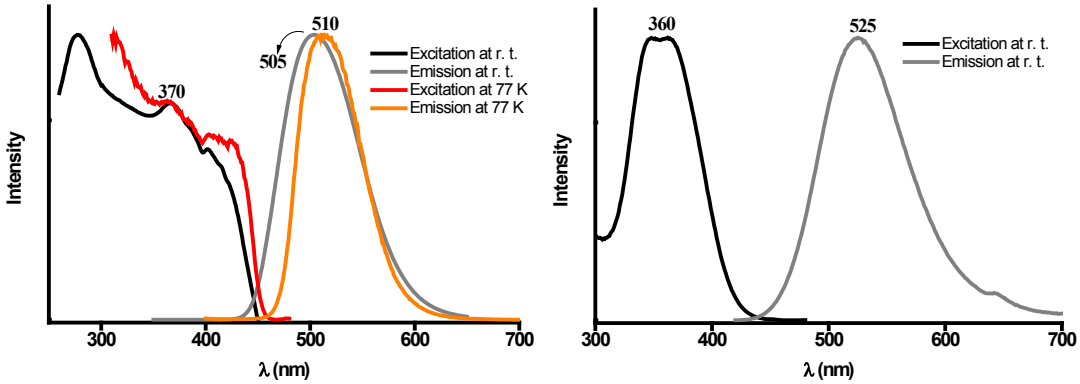

Figure S5. Excitation and emission spectra of **4** in the solid state (left) and in dichloromethane (10^{-4} M) (right).

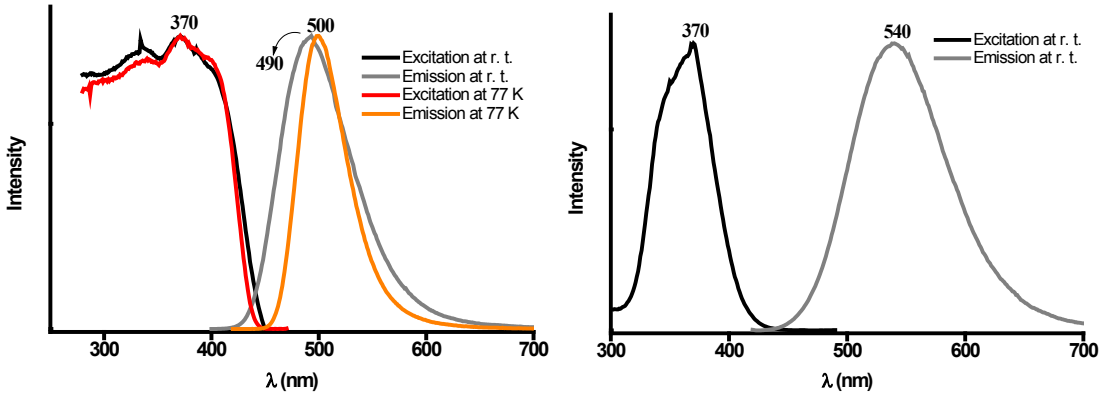

Figure S6. Excitation and emission spectra of **5** in the solid state (left) and in dichloromethane (10^{-4} M) (right).

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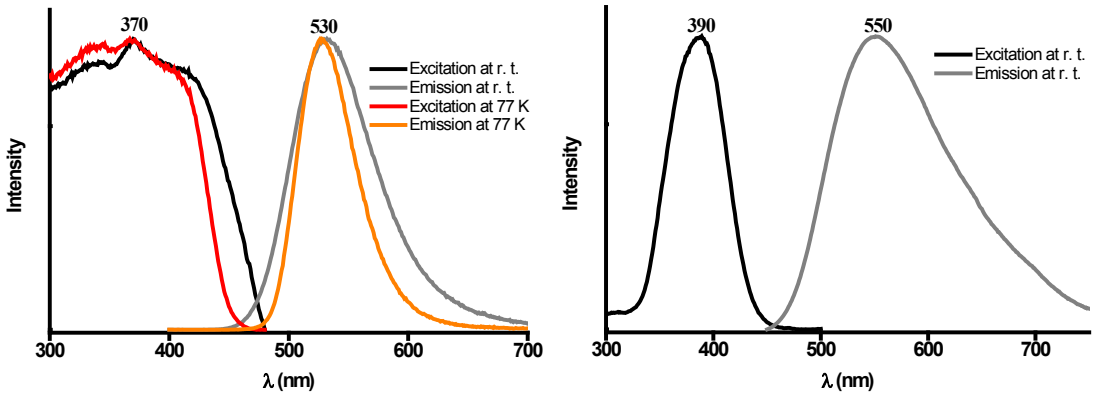

Figure S7. Excitation and emission spectra of **6** in the solid state (left) and in dichloromethane (10^{-4} M) (right).

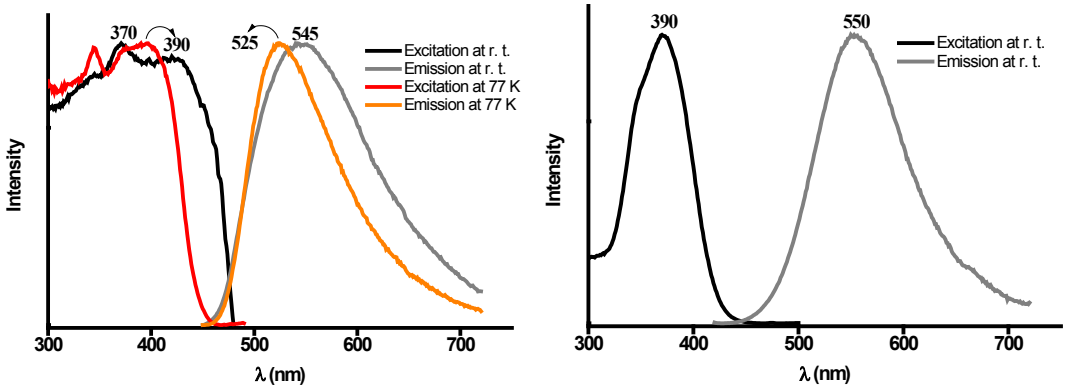

Figure S8. Excitation and emission spectra of **7** in the solid state (left) and in dichloromethane (10^{-4} M) (right).

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