Electronic Supplementary Information (ESI)

belonging to

1,2,4-Triazole-derived Carbene Complexes of Gold: Characterization, Solid-State Aggregation and Ligand Disproportionation

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Table SI-1. Selected X-ray Crystallographic Data for Complexes **2**, **3**, **4'**, **5**·0.25H_2O, **6**, and **7**.

Comp.	**2**	**3**	**4'**	**5**·0.25H_2O	**6**	**7**
Formula	$C_{10}H_{11}AuBr_{0.5}ClN_3$	$C_{10}H_{11}AuBrN_3$	$C_{20}H_{22}Au_2I_2N_6$	$C_{12}H_{14.50}AuN_3$ O2.25	$C_{20}H_{22}AuF_6N_6P$	$C_{10}H_{11}AuI_3N_3$
Formula weight	445.59	450.09	994.17	433.73	688.37	750.88
Crystal size [mm]	0.24 x 0.14 x 0.12	0.46 × 0.36 × 0.12	0.40 × 0.10 × 0.08	0.40 × 0.30 × 0.20	0.50 × 0.16 × 0.10	0.42 × 0.36 × 0.22
Temperature [K]	100(2)	100(2)	223(2)	100(2)	100(2)	100(2)
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P-1	P-1	P-1	P2(1)/n	P2(1)/c	P2(1)/n
a [Å]	6.8063(6)	10.879(2)	6.6322(5)	9.7892(15)	8.0153(6)	8.6366(6)
b [Å]	9.4869(9)	10.971(2)	8.7311(7)	8.7330(14)	11.3120(8)	14.8770(11)
c [Å]	9.6535(9)	12.044(2)	11.7798(9)	16.171(2)	12.4710(9)	12.5813(9)
α [°]	106.0990(10)	77.756(3)	69.501(2)	90	90	90
β [°]	103.6680(10)	96.61(4)	87.692(2)	104.757(2)	90.9850(10)°	96.683(2)
γ [°]	91.5240(10)	60.903(3)	72.119(2)	90	90	90
V [$Å^3$]	579.09(9)	1178.1(4)	606.34(8)	1336.8(4)	1130.57(14)	1605.5(2)
Z	2	4	1	4	2	4
D_c [g·cm^{-3}]	2.785	2.538	2.723	2.155	2.022	3.106
μ [mm^{-1}]	16.356	15.850	14.649	11.005	6.648	14.916
θ range [°]	2.25–27.49	1.803–27.494	1.85–27.50	2.21–27.50	2.43–27.50	2.13–27.46
Reflections Collected	7696	15052	7791	9332	7835	11014
max, min	0.2443, 0.1109	0.7456, 0.3733	0.3870, 0.0673	0.2169, 0.0962	0.5561, 0.1358	0.1379, 0.0620
Final R indices (I > 2σ(I))	R_1 = 0.0179, wR_2 = 0.0448	R_1 = 0.0217, wR_2 = 0.0493	R_1 = 0.0306, wR_2 = 0.0706	R_1 = 0.0255, wR_2 = 0.0652	R_1 = 0.0311, wR_2 = 0.0767	R_1 = 0.0475, wR_2 = 0.1192
R indices (all data)	R_1 = 0.0188, wR_2 = 0.0452	R_1 = 0.0236, wR_2 = 0.0500	R_1 = 0.0342, wR_2 = 0.0721	R_1 = 0.0284, wR_2 = 0.0667	R_1 = 0.0388, wR_2 = 0.0810	R_1 = 0.0519, wR_2 = 0.1216
goodness of fit on	1.069	1.084	1.077	1.071	1.082	1.055
Peak/hole [e·$Å^{-3}$]	1.235 / -0.620	1.046 / -1.673	1.355/ -1.144	1.538 / -1.623	3.260 / -1.759	2.618 / -3.541

Computational details, optimised complex and ligand geometries

Chloride

G = -460.387796 a.u.

Cl	0.000000000	0.000000000	0.000000000

Bromide

G = -2574.334250 a.u.

Br	0.000000000	0.000000000	0.000000000

Iodide

G = -295.998598 a.u.

I	0.000000000	0.000000000	0.000000000

Gold(I) chloride

G = -596.043690 a.u.

Au	0.000000000	0.000000000	0.405758000
Cl	0.000000000	0.000000000	-1.885582000

Au-Cl	2.29134 Å

Gold(I) bromide

G = -2709.992334 a.u.

Au	0.000000000	0.000000000	0.738567000
Br	0.000000000	0.000000000	-1.667050000

Au-Br	2.40562 Å

Gold(I) iodide

G = -431.642436 a.u.

Au	0.000000000	0.000000000	1.032135000
I	0.000000000	0.000000000	-1.538465000

Au-I	2.57060 Å

Dichloridoaurate(I)

G = -1056.501435 a.u.

Au	0.000000000	0.000000000	0.000000000
Cl	0.000000000	0.000000000	2.331804000
Cl	0.000000000	0.000000000	-2.331804000

Au-Cl	2.33180 Å
Cl-Au-Cl	180.0°

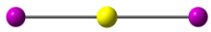
Dibromidoaurate(I)

G = -5284.391993 a.u.

Au	0.000000000	0.000000000	0.000000000
Br	0.000000000	0.000000000	2.456461000
Br	0.000000000	0.000000000	-2.456461000

Au-Br	2.45646 Å
Br-Au-Br	180.0°

Diiodidoaurate(I)

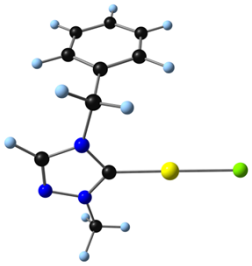


G = -727.683819 a.u.

Au	0.000000000	0.000000000	0.000000000
I	0.000000000	0.000000000	2.634284000
I	0.000000000	0.000000000	-2.634284000

Au-I	2.63428 Å
I-Au-I	180.0°

Chlorido(tazy)gold(I)



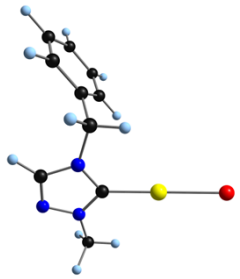
G = -1147.899767 a.u.

Au	-1.368450000	-0.385064000	0.039349000
Cl	-2.600180000	-2.365388000	-0.025481000
N	0.868730000	1.567760000	0.732362000
N	0.304694000	3.487642000	-0.210201000
N	-0.622157000	2.513476000	-0.460723000
C	-0.319438000	1.324910000	0.097893000
C	1.201817000	2.880766000	0.518488000
H	2.095211000	3.352508000	0.918056000
C	-1.794446000	2.854463000	-1.257315000
H	-2.423869000	1.962489000	-1.346608000
H	-2.350451000	3.660253000	-0.759194000
H	-1.472194000	3.189486000	-2.252548000
C	1.675184000	0.587677000	1.487379000
H	2.232389000	1.162220000	2.240104000
H	0.970841000	-0.067034000	2.013683000
C	2.616518000	-0.221596000	0.616182000
C	2.346680000	-1.570624000	0.346266000
H	1.451941000	-2.037570000	0.764077000
C	3.216374000	-2.323427000	-0.450079000
H	2.994365000	-3.373876000	-0.650175000
C	4.364346000	-1.733126000	-0.986020000
H	5.044004000	-2.320017000	-1.607778000
C	4.642890000	-0.387870000	-0.718393000
H	5.542152000	0.077810000	-1.127536000

C	3.776055000	0.361385000	0.080762000
H	4.011458000	1.407857000	0.291530000

Au-Cl	2.33303 Å
Au-C	2.00695 Å
C-Au-Cl	179.64°

Bromido(tazy)gold(I)

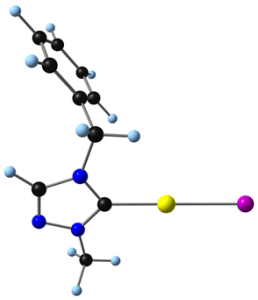


G = -3261.845469 a.u.

Au	-1.309687000	0.046096000	-0.060718000
Br	-3.135136000	-1.593919000	-0.018633000
N	1.438375000	1.255285000	-0.635194000
N	0.206640000	2.644285000	0.410941000
N	1.394591000	3.294957000	0.218150000
C	0.189191000	1.395132000	-0.094832000
C	2.126302000	2.422286000	-0.419583000
H	3.150587000	2.588325000	-0.741247000
C	1.975788000	0.059833000	-1.312155000
H	2.363847000	0.375778000	-2.289886000
H	1.114741000	-0.599049000	-1.485741000
C	3.054884000	-0.638396000	-0.509542000
C	4.363783000	-0.712524000	-1.004114000
H	4.604769000	-0.257968000	-1.968576000
C	5.362182000	-1.369708000	-0.276030000
H	6.378052000	-1.421884000	-0.673696000
C	5.058674000	-1.954987000	0.955860000
H	5.836515000	-2.467586000	1.526093000
C	3.752507000	-1.884877000	1.456159000
H	3.508505000	-2.345005000	2.416176000
C	2.755946000	-1.232770000	0.727337000
H	1.737181000	-1.186318000	1.120514000
C	-0.868720000	3.342498000	1.104271000
H	-1.149510000	4.238360000	0.533832000
H	-0.524658000	3.635733000	2.105255000
H	-1.725456000	2.664605000	1.184630000

Au-Br	2.45432 Å
Au-C	2.01685 Å
C-Au-Br	179.95 °

Iodido(tazy)gold(I)

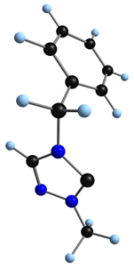


G = -983.488621 a.u.

Au	1.015028000	0.304108000	-0.054494000
N	-1.867939000	1.187613000	-0.623755000
N	-2.054484000	3.232590000	0.196913000
N	-0.799786000	2.724124000	0.395085000
C	-0.641768000	1.477575000	-0.091323000
C	-2.683868000	2.272493000	-0.424492000
H	-3.720897000	2.318257000	-0.745028000
C	0.190743000	3.551349000	1.072932000
H	1.116689000	2.973915000	1.169515000
H	0.373435000	4.459738000	0.482742000
H	-0.186796000	3.827339000	2.066655000
C	-2.261281000	-0.070910000	-1.286618000
H	-2.639426000	0.180382000	-2.286664000
H	-1.333715000	-0.645293000	-1.410271000
C	-3.295729000	-0.852246000	-0.502395000
C	-2.972833000	-1.411327000	0.744918000
H	-1.969383000	-1.277146000	1.156953000
C	-3.925645000	-2.139191000	1.460328000
H	-3.663052000	-2.571304000	2.428407000
C	-5.211606000	-2.320388000	0.936132000
H	-5.955271000	-2.891988000	1.495760000
C	-5.538741000	-1.770442000	-0.305947000
H	-6.538945000	-1.909559000	-0.721989000
C	-4.584243000	-1.038203000	-1.021138000
H	-4.843606000	-0.611142000	-1.993365000
I	3.165642000	-1.209061000	-0.011505000

Au-I	2.62996 Å
Au-C	2.03060 Å
C-Au-I	179.79°

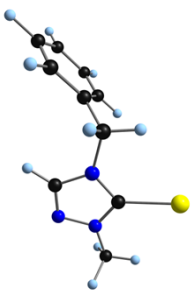
1-methyl-4-benzyl-1,2,4-triazolin-5-ylidene (tazy)



G = -551.768379 a. u.

N	-1.100090000	-0.671498000	0.366379000
N	-2.920506000	0.290540000	-0.050313000
N	-2.664093000	-0.463533000	-1.179305000
C	-1.998561000	0.206421000	0.937054000
C	-1.530596000	-1.039282000	-0.887595000
H	-0.997707000	-1.722088000	-1.544986000
C	0.149766000	-1.103261000	0.993878000
H	0.253608000	-2.190233000	0.865159000
H	0.027916000	-0.903947000	2.067675000
C	1.379165000	-0.392902000	0.454995000
C	1.427184000	1.009171000	0.395190000
H	0.558300000	1.589767000	0.714675000
C	2.571578000	1.659462000	-0.071791000
H	2.595919000	2.750919000	-0.113375000
C	3.685431000	0.917147000	-0.483557000
H	4.579914000	1.426721000	-0.848884000
C	3.645460000	-0.478523000	-0.426808000
H	4.508116000	-1.066055000	-0.749416000
C	2.496201000	-1.128798000	0.037839000
H	2.469121000	-2.221138000	0.076537000
C	-4.137808000	1.082965000	-0.017474000
H	-5.019474000	0.430875000	-0.106178000
H	-4.142700000	1.804751000	-0.847606000
H	-4.167109000	1.617475000	0.938693000

(tazy)gold(I)

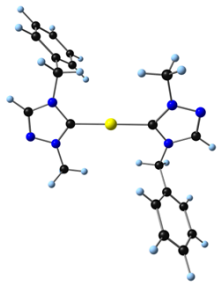


G = -687.429898 a.u.

N	0.511052000	0.885733000	-0.544050000
N	-1.101692000	2.043518000	0.260954000
N	-0.080525000	2.928546000	0.069876000
C	-0.774377000	0.793087000	-0.103042000
C	0.886413000	2.199461000	-0.420309000
H	1.868324000	2.575245000	-0.693350000
C	1.349418000	-0.204455000	-1.095550000
H	1.461263000	-0.024863000	-2.173404000
H	0.766468000	-1.125473000	-0.963822000
C	2.700376000	-0.300107000	-0.420684000
C	2.802606000	-0.681408000	0.927385000
H	1.900138000	-0.902351000	1.503081000
C	4.053641000	-0.781691000	1.538568000
H	4.122684000	-1.080215000	2.586729000
C	5.216868000	-0.507404000	0.808680000
H	6.194900000	-0.589087000	1.287613000
C	5.122764000	-0.132537000	-0.533852000
H	6.025815000	0.080533000	-1.109582000
C	3.868572000	-0.027895000	-1.145493000
H	3.799532000	0.263956000	-2.196372000
C	-2.361605000	2.531027000	0.814627000
H	-2.767838000	3.304196000	0.149698000
H	-2.175343000	2.956379000	1.809332000
H	-3.060331000	1.690692000	0.887723000
Au	-1.906652000	-0.828887000	-0.023001000

Au-C 1.97971 Å

Bis(tazy)gold(I)



G = -1239.276469

N	2.636180000	-1.477763000	0.558592000
N	1.448333000	-2.710258000	-0.707934000
N	2.573752000	-3.442315000	-0.452392000
C	1.444178000	-1.503503000	-0.109667000
C	3.281830000	-2.664305000	0.320733000
H	4.257472000	-2.915178000	0.727277000

C	3.163243000	-0.371862000	1.383092000
H	3.395401000	-0.778045000	2.376786000
H	2.336065000	0.340943000	1.495386000
C	4.385073000	0.286781000	0.775895000
C	4.289553000	1.002692000	-0.428723000
H	3.327259000	1.081748000	-0.941486000
C	5.418109000	1.614700000	-0.977779000
H	5.332782000	2.169648000	-1.914540000
C	6.654780000	1.522150000	-0.327295000
H	7.536309000	2.002919000	-0.756824000
C	6.756510000	0.814942000	0.873305000
H	7.717319000	0.739823000	1.386894000
C	5.625821000	0.198684000	1.421276000
H	5.709264000	-0.352647000	2.361350000
C	0.418507000	-3.295154000	-1.559148000
H	0.026082000	-4.204619000	-1.084443000
H	0.857221000	-3.548630000	-2.533315000
H	-0.385652000	-2.562966000	-1.689461000
N	-2.726858000	1.307178000	-0.679139000
N	-1.303273000	2.728768000	0.018485000
N	-2.455704000	3.439837000	-0.165035000
C	-1.423492000	1.421747000	-0.283898000
C	-3.307932000	2.546618000	-0.589747000
H	-4.345225000	2.749208000	-0.840806000
C	-3.410645000	0.075235000	-1.121481000
H	-3.789181000	0.248226000	-2.137949000
H	-2.631728000	-0.696668000	-1.177862000
C	-4.534590000	-0.339844000	-0.194512000
C	-4.263839000	-0.732810000	1.126367000
H	-3.234755000	-0.730139000	1.494962000
C	-5.301948000	-1.127193000	1.972602000
H	-5.080413000	-1.431740000	2.997766000
C	-6.622844000	-1.137500000	1.507421000
H	-7.433848000	-1.447843000	2.169744000
C	-6.899234000	-0.751170000	0.193592000
H	-7.926699000	-0.757698000	-0.176335000
C	-5.858670000	-0.352272000	-0.653041000
H	-6.079389000	-0.051883000	-1.680475000
C	-0.121165000	3.433104000	0.501632000
H	0.135555000	4.235660000	-0.202632000
H	-0.332912000	3.864245000	1.489330000
H	0.705968000	2.718563000	0.573572000
Au	0.006793000	-0.043510000	-0.188971000

Au-C	2.04981 Å
Au-C	2.05035 Å
C-Au-I	179.50°