# Supporting Information

## Aurophilic interactions in cationic three-coordinate gold(I) bipyridyl/isocyanide complex

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**X-ray crystal structure determination.**

The single-crystal X-ray diffraction data for **4** was collected on a three-circle Bruker D8 Venture (Centre of Joint Equipment of Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences) using ϕ and ω scan mode. The data were indexed and integrated using the SAINT program.[1] Absorption correction based on measurements of equivalent reflections (SADABS) were applied.[2] The structures were determined by direct methods and refined by full-matrix least squares technique on F2 with anisotropic displacement parameters for non-hydrogen atoms. The hydrogen atoms in all compounds were placed in calculated positions and refined within riding model with fixed isotropic displacement parameters [Uiso(H) = 1.5Ueq(C) for the $CH_3$-groups and 1.2Ueq(C) for the other groups]. All calculations were carried out using the SHELXTL program[3] and OLEX2 program package.[4] For details, see Table S2 (Supporting Information).

The crystallographic data were deposited with the Cambridge Crystallographic Data Center, CCDC 2159586. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CHB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

**Table S1**. Cartesian atomic coordinates for model structure **4**.

| Atom | X | Y | Z |
|---|---|---|---|
| Au | 3.558999 | 3.172771 | 4.455413 |
| Au | 6.512407 | 4.440319 | 4.578669 |
| N | 4.403674 | 1.683614 | 5.919137 |
| N | 8.437984 | 2.060440 | 4.589135 |
| N | 5.265109 | 5.886214 | 5.733261 |
| C | 9.299510 | 1.028154 | 4.558457 |
| C | 2.355072 | 4.662468 | 4.444766 |
| N | 4.804102 | 1.726660 | 3.284399 |
| C | 4.701809 | 6.911400 | 5.074577 |
| C | 7.730801 | 2.965430 | 4.630642 |
| N | 1.617558 | 5.571202 | 4.439352 |
| C | 5.366216 | 0.698965 | 3.962934 |
| C | 9.520830 | 0.216338 | 5.677318 |
| C | 10.384052 | -0.898511 | 5.556409 |
| H | 10.595555 | -1.416752 | 6.324850 |
| C | 4.145639 | 1.715388 | 7.229287 |
| H | 3.652086 | 2.446905 | 7.575971 |
| C | 4.335057 | 6.696939 | 7.772476 |
| H | 4.206185 | 6.585437 | 8.707700 |
| C | 0.235249 | 6.982952 | 5.758526 |
| N | 5.659223 | 5.915926 | 3.109351 |
| C | 5.936545 | 5.907982 | 1.804615 |
| H | 6.469026 | 5.199297 | 1.461287 |
| C | -0.589764 | 8.111380 | 5.792814 |
| H | -0.971185 | 8.375358 | 6.621709 |
| C | 5.086866 | 5.791350 | 7.039802 |
| H | 5.500341 | 5.068873 | 7.500881 |
| C | 5.142824 | 0.676746 | 5.401212 |
| C | 9.834556 | 0.626630 | 3.260939 |
| C | 4.996050 | 1.837904 | 1.970639 |
| H | 4.612558 | 2.577911 | 1.511997 |
| C | 5.634475 | -0.324398 | 6.236749 |

| | | | |
|---|---|---|---|
| H | 6.161111 | -1.023766 | 5.872487 |
| C | 4.431456 | 7.948097 | 2.789934 |
| H | 3.893767 | 8.643307 | 3.151038 |
| C | 8.972203 | 0.625765 | 7.012733 |
| H | 9.630868 | 1.169658 | 7.488033 |
| H | 8.763076 | -0.173890 | 7.541882 |
| H | 8.149752 | 1.148863 | 6.882169 |
| C | 6.271403 | -0.152134 | 1.929133 |
| H | 6.766499 | -0.810313 | 1.454953 |
| C | 6.108372 | -0.258849 | 3.284399 |
| H | 6.496737 | -0.983958 | 3.757786 |
| C | 4.924404 | 6.953166 | 3.594793 |
| C | 0.518255 | 6.151509 | 6.991078 |
| H | 0.139653 | 6.598255 | 7.778864 |
| H | 1.484711 | 6.053116 | 7.104462 |
| H | 0.106989 | 5.267403 | 6.890705 |
| C | 10.922946 | -1.236075 | 4.334685 |
| H | 11.482890 | -2.000391 | 4.269520 |
| C | 0.520176 | 7.374230 | 3.336733 |
| C | -0.291346 | 8.484346 | 3.455837 |
| H | -0.470668 | 9.012388 | 2.685772 |
| C | 4.576202 | 0.748076 | 8.097307 |
| H | 4.347605 | 0.785321 | 9.019447 |
| C | 5.360107 | -0.308715 | 7.582991 |
| H | 5.684662 | -0.992891 | 8.154585 |
| C | -0.862033 | 8.852653 | 4.672148 |
| H | -1.432580 | 9.610252 | 4.724806 |
| C | 5.494883 | 6.891921 | 0.923963 |
| H | 5.703931 | 6.855873 | -0.001191 |
| C | 3.960189 | 7.873165 | 5.736870 |
| H | 3.578478 | 8.600854 | 5.258972 |
| C | 10.667381 | -0.489410 | 3.201387 |
| H | 11.056478 | -0.739731 | 2.373249 |
| C | 9.564694 | 1.465030 | 2.051847 |
| H | 8.592569 | 1.544329 | 1.922095 |
| H | 9.962843 | 1.044302 | 1.263718 |
| H | 9.946969 | 2.357381 | 2.178369 |
| C | 5.724388 | 0.916965 | 1.257817 |
| H | 5.841140 | 1.014351 | 0.320987 |
| C | 3.772469 | 7.761305 | 7.099355 |
| H | 3.269045 | 8.412317 | 7.570197 |
| C | 1.127420 | 6.999786 | 2.008536 |
| H | 0.544181 | 6.360000 | 1.549190 |
| H | 2.006898 | 6.591703 | 2.155793 |
| H | 1.229401 | 7.803251 | 1.456721 |
| C | 4.725952 | 7.917968 | 1.443692 |
| H | 4.407952 | 8.605500 | 0.871719 |
| C | 0.816098 | 6.608389 | 4.538606 |

**Table S2.**

| | |
|---|---|
| Identification code | **4** |
| Empirical formula | $C_{21}H_{17}AuF_6N_4O_4S_2$ |
| Formula weight | 764.47 |
| Temperature/K | 100.0 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 8.4150(17) |
| b/Å | 11.939(3) |
| c/Å | 12.767(5) |
| α/° | 94.626(14) |
| β/° | 103.999(14) |
| γ/° | 98.011(9) |
| Volume/Å$^3$ | 1223.7(6) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 2.075 |
| μ/mm$^{-1}$ | 6.265 |
| F(000) | 736.0 |
| Radiation | MoKα (λ = 0.71073) |
| Index ranges | -10 ≤ h ≤ 10<br>-15 ≤ k ≤ 15<br>-16 ≤ l ≤ 16 |
| Reflections collected | 11809 |
| Independent reflections | 5570<br>[$R_{int}$ = 0.0279, $R_{sigma}$ = 0.0409] |
| Data/restraints/parameters | 5570/0/334 |
| Goodness-of-fit on F$^2$ | 1.051 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0333, w$R_2$ = 0.0933 |
| Final R indexes [all data] | $R_1$ = 0.0349, w$R_2$ = 0.0944 |

**References**


1 *Bruker, SAINT, Bruker AXS Inc., Madison, WI, 2018.*

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3 G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.*, 2015, **71**, 3–8.

4 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339–341.