## Electronic supplementary information (ESI)

# The Effect of Doping a Molecular Spin Ladder with Non-Magnetic Impurities

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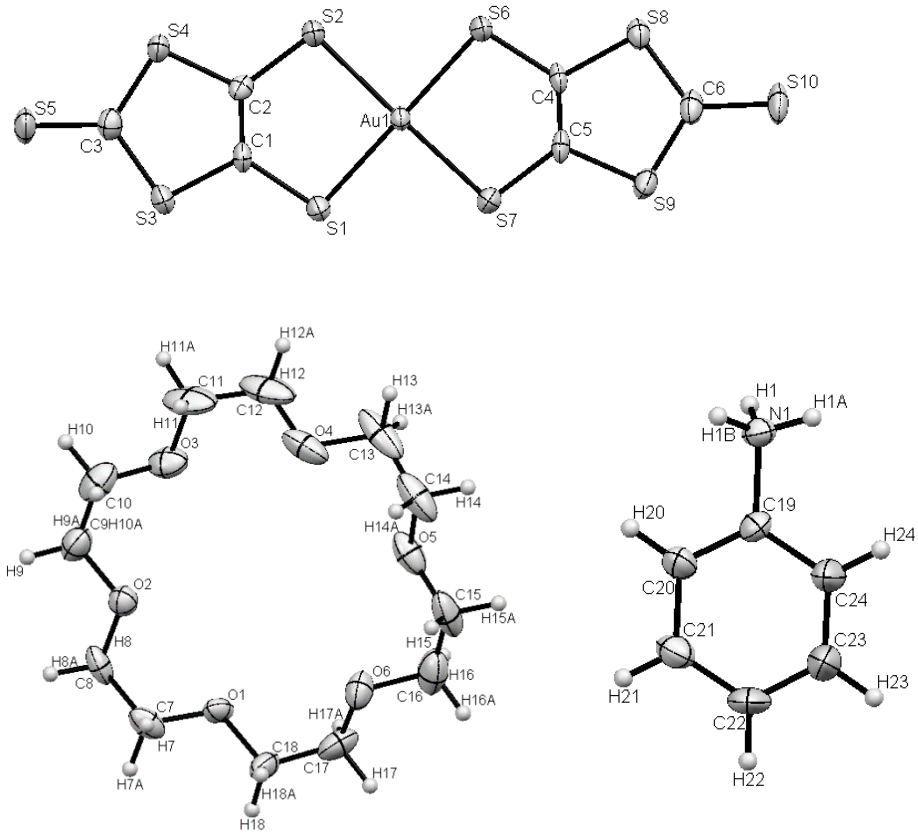


**Figure S1**. Atomic numbering scheme of crystal structure of pure [Au(dmit)$_2$] salt ($x$ = 1) at 173 K.

**Table S1**. Crystallographic data for compounds $[Ni(dmit)_2]^-$ and $[Au(dmit)_2]^-$ salts.

| | $[Ni(dmit)_2]^-$ salt | $[Au(dmit)_2]^-$ salt |
|---|---|---|
| Formula | C24 H32 N Ni O6 S10 | C24 H32 Au N O6 S10 |
| $M_r$ [g mol$^{-1}$] | 809.82 | 948.07 |
| crystal system | triclinic | triclinic |
| space group | $P\bar{1}$ | $P\bar{1}$ |
| $a$ [Å] | 8.0355(10) | 8.1271(5) |
| $b$ [Å] | 14.2216(19) | 14.1157(9) |
| $c$ [Å] | 16.628(2) | 16.6699(10) |
| $\alpha$ [º] | 113.258(2) | 112.6225(16) |
| $\beta$ [º] | 96.998(2) | 95.9764(16) |
| $\gamma$ [º] | 92.858(2) | 94.3523 |
| $D_{calc}$ [g cm$^{-3}$] | 1.561 | 1.808 |
| $V$ [Å$^3$] | 1722.8(4) | 1741.58(19) |
| $Z$ | 2 | 2 |
| $\mu$(Mo$K_\alpha$) [mm$^{-1}$] | 1.207 | 4.861 |
| $T$ [K] | 173 | 173 |
| no. rflns (measd) | 9294 | 18402 |
| no. rflns (unique) | 6976 | 7974 |
| no. params | 380 | 380 |
| $R1$ (I>2σ(I)) | 0.0358 | 0.0564 |
| $wR2$ (all data) | 0.0955 | 0.1462 |

**Table S2**. Crystallographic data for pure $[Ni(dmit)_2]^-$, $[Au(dmit)_2]^-$ and impurity doped compounds with typical $x$, $[Ph(NH_3)]([18]crown-6)[Ni(dmit)_2]_{1-x}[Au(dmit)_2]_x$.

($x = 0$)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni |
| $M_r$ [g mol$^{-1}$] | 809.87 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.1271(6) |
| $b$ [Å] | 14.217(1) |
| $c$ [Å] | 16.666(2) |
| $\alpha$ [º] | 112.846(2) |
| $\beta$ [º] | 97.120(2) |
| $\gamma$ [º] | 92.599(3) |
| $D_{calc}$ [g cm$^{-3}$] | 1.536 |
| $V$ [Å$^3$] | 1751.6(3) |
| Z | 2 |
| $\mu(Mo_{K\alpha})$ [cm$^{-1}$] | 48.48 |
| $T$ [K] | 300 |
| no. rflns (measd) | 14477 |
| no. rflns (unique) | 7594 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.052 |
| $wR2$ (all data) | 0.122 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | 0.09514(3) | -0.04653(2) | 0.60996(4) | 4.051(9) | 0.3500(7) |
| S(1) | -0.00555(6) | -0.18209(5) | 0.6152(1) | 4.26(2) | 1.0000 |
| S(2) | 0.20038(6) | 0.08865(5) | 0.6202(1) | 4.54(2) | 1.0000 |
| S(3) | 0.18699(6) | -0.08183(5) | 0.4327(1) | 4.29(2) | 1.0000 |
| S(4) | 0.00169(6) | -0.35239(5) | 0.4503(1) | 4.57(2) | 1.0000 |
| S(5) | 0.17660(7) | -0.26111(6) | 0.2817(1) | 5.04(2) | 1.0000 |
| S(6) | -0.00052(6) | -0.01154(5) | 0.7767(1) | 4.43(2) | 1.0000 |
| S(7) | 0.19577(8) | 0.25852(5) | 0.7967(1) | 5.40(2) | 1.0000 |
| S(8) | 0.00992(7) | 0.16553(5) | 0.9390(1) | 4.70(2) | 1.0000 |
| S(9) | 0.08762(8) | -0.45696(6) | 0.2304(2) | 6.40(2) | 1.0000 |
| S(10) | 0.1064(1) | 0.36029(7) | 1.0181(1) | 6.96(3) | 1.0000 |
| O(1) | 0.7096(2) | 0.4217(1) | 0.2353(3) | 5.25(5) | 1.0000 |
| O(2) | 0.7354(2) | 0.2661(2) | 0.2567(3) | 5.33(6) | 1.0000 |
| O(4) | 0.3630(2) | 0.1144(2) | 0.2162(3) | 6.67(7) | 1.0000 |
| O(5) | 0.3527(2) | 0.2782(3) | 0.2131(4) | 7.70(9) | 1.0000 |
| O(7) | 0.5272(2) | 0.4367(2) | 0.2997(3) | 6.69(8) | 1.0000 |
| O(8) | 0.5546(2) | 0.1069(2) | 0.1858(4) | 6.50(7) | 1.0000 |
| N(2) | 0.5459(2) | 0.2745(2) | 0.3473(3) | 3.98(5) | 1.0000 |
| C(3) | 0.0885(2) | -0.3616(2) | 0.3162(4) | 4.44(7) | 1.0000 |
| C(4) | 0.5479(2) | 0.2826(2) | 0.5293(4) | 3.82(6) | 1.0000 |
| C(5) | 0.1449(2) | 0.1443(2) | 0.7457(4) | 3.78(6) | 1.0000 |
| C(6) | 0.0578(2) | 0.1010(2) | 0.8129(4) | 3.73(6) | 1.0000 |
| C(7) | 0.6299(2) | 0.3475(2) | 0.6267(4) | 4.62(7) | 1.0000 |
| C(8) | 0.1040(3) | 0.2665(2) | 0.9216(4) | 4.83(8) | 1.0000 |
| C(9) | 0.8049(3) | 0.3344(3) | 0.1796(4) | 5.97(9) | 1.0000 |
| C(10) | 0.6313(3) | 0.3565(3) | 0.7986(4) | 5.59(9) | 1.0000 |
| C(11) | 0.8089(3) | 0.4215(3) | 0.2595(5) | 6.04(9) | 1.0000 |
| C(12) | 0.5506(3) | 0.3028(4) | 0.8692(5) | 7.4(1) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(13) | 0.7349(3) | 0.1835(3) | 0.1920(5) | 6.7(1) | 1.0000 |
| C(14) | 0.2645(3) | 0.2013(5) | 0.2304(7) | 9.5(2) | 1.0000 |
| C(15) | 0.6077(5) | 0.5042(3) | 0.2390(6) | 7.8(1) | 1.0000 |
| C(16) | 0.4680(3) | 0.2283(3) | 0.5978(4) | 7.01(10) | 1.0000 |
| C(17) | 0.7077(4) | 0.5041(2) | 0.2993(5) | 6.9(1) | 1.0000 |
| C(18) | 0.6486(5) | 0.1132(3) | 0.2613(6) | 7.5(1) | 1.0000 |
| C(19) | 0.4679(5) | 0.0363(3) | 0.2262(7) | 8.4(1) | 1.0000 |
| C(20) | 0.3760(4) | 0.0393(4) | 0.1427(6) | 9.2(1) | 1.0000 |
| C(21) | 0.4697(3) | 0.2382(4) | 0.7705(5) | 9.7(1) | 1.0000 |
| C(22) | 0.2774(3) | 0.1231(5) | 0.1415(7) | 10.2(2) | 1.0000 |
| C(23) | 0.4281(5) | 0.4330(4) | 0.2444(8) | 9.4(2) | 1.0000 |
| C(24) | 0.3480(5) | 0.3554(6) | 0.2966(8) | 9.9(2) | 1.0000 |
| C(25) | 0.1312(2) | -0.1943(2) | 0.4080(3) | 3.75(6) | 1.0000 |
| C(26) | 0.0481(2) | -0.2385(2) | 0.4853(4) | 3.61(6) | 1.0000 |
| H(1) | 0.8715 | 0.3329 | 0.1867 | 7.0 | 1.0000 |
| H(2) | 0.7814 | 0.3251 | 0.0619 | 7.0 | 1.0000 |
| H(3) | 0.8582 | 0.4684 | 0.2101 | 7.2 | 1.0000 |
| H(4) | 0.8316 | 0.4307 | 0.3751 | 7.2 | 1.0000 |
| H(5) | 0.7244 | 0.1704 | 0.0739 | 7.8 | 1.0000 |
| H(6) | 0.7987 | 0.1781 | 0.2264 | 7.8 | 1.0000 |
| H(7) | 0.2581 | 0.1927 | 0.3433 | 8.8 | 1.0000 |
| H(8) | 0.2028 | 0.2021 | 0.1824 | 8.8 | 1.0000 |
| H(9) | 0.5977 | 0.4961 | 0.1228 | 9.1 | 1.0000 |
| H(10) | 0.6048 | 0.5603 | 0.2829 | 9.1 | 1.0000 |
| H(11) | 0.7172 | 0.5143 | 0.4166 | 7.5 | 1.0000 |
| H(12) | 0.7614 | 0.5510 | 0.2577 | 7.5 | 1.0000 |
| H(13) | 0.6529 | 0.1282 | 0.3797 | 8.4 | 1.0000 |
| H(14) | 0.6530 | 0.0563 | 0.2390 | 8.4 | 1.0000 |
| H(15) | 0.4728 | -0.0199 | 0.1780 | 8.9 | 1.0000 |
| H(16) | 0.4656 | 0.0364 | 0.3400 | 8.9 | 1.0000 |
| H(17) | 0.3176 | -0.0120 | 0.1622 | 9.1 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.3809 | 0.0389 | 0.0298 | 9.1 | 1.0000 |
| H(19) | 0.2881 | 0.1362 | 0.0307 | 10.2 | 1.0000 |
| H(20) | 0.2170 | 0.0750 | 0.1430 | 10.2 | 1.0000 |
| H(21) | 0.4210 | 0.4841 | 0.2903 | 11.4 | 1.0000 |
| H(22) | 0.4217 | 0.4260 | 0.1261 | 11.4 | 1.0000 |
| H(23) | 0.2809 | 0.3549 | 0.2692 | 10.6 | 1.0000 |
| H(24) | 0.3566 | 0.3562 | 0.4142 | 10.6 | 1.0000 |
| H(25) | 0.4881 | 0.2825 | 0.2995 | 6.7 | 1.0000 |
| H(26) | 0.6069 | 0.3173 | 0.3151 | 6.7 | 1.0000 |
| H(27) | 0.5413 | 0.2170 | 0.3002 | 6.7 | 1.0000 |
| H(28) | 0.6865 | 0.3848 | 0.5724 | 5.5 | 1.0000 |
| H(29) | 0.6877 | 0.4056 | 0.8668 | 6.2 | 1.0000 |
| H(30) | 0.5580 | 0.3076 | 0.9916 | 7.9 | 1.0000 |
| H(31) | 0.4117 | 0.1787 | 0.5275 | 7.7 | 1.0000 |
| H(32) | 0.4093 | 0.2057 | 0.8270 | 10.0 | 1.0000 |

$B_{eq} = 8/3\ PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

($x = 0.01$)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni0.99 Au0.01 |
| $M_r$ [g mol$^{-1}$] | 811.25 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.1411(2) |
| $b$ [Å] | 14.2431(3) |
| $c$ [Å] | 16.6910(4) |
| $\alpha$ [°] | 112.903(1) |
| $\beta$ [°] | 97.076(2) |
| $\gamma$ [°] | 92.609(1) |
| $D_{calc}$ [g cm$^{-3}$] | 1.531 |
| $V$ [Å$^3$] | 1760.0(2) |
| Z | 2 |
| $\mu(Mo_{K\alpha})$ [cm$^{-1}$] | 48.25 |
| $T$ [K] | 300 |
| no. rflns (measd) | 27905 |
| no. rflns (unique) | 7903 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.066 |
| $wR2$ (all data) | 0.120 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | 0.39003(5) | 0.90492(3) | 1.04663(2) | 3.78(1) | 0.3576(7) |
| S(1) | 0.3847(1) | 1.00557(6) | 1.18232(5) | 3.99(2) | 1.0000 |
| S(2) | 0.5675(1) | 0.81324(7) | 1.08192(6) | 3.96(2) | 1.0000 |
| S(3) | 0.5495(1) | 0.99832(7) | 1.35264(6) | 4.26(2) | 1.0000 |
| S(4) | 0.7182(1) | 0.82345(8) | 1.26113(6) | 4.75(2) | 1.0000 |
| S(5) | 0.3797(1) | 0.79973(7) | 0.91133(6) | 4.29(2) | 1.0000 |
| S(6) | 0.2233(1) | 1.00040(7) | 1.01157(5) | 4.12(2) | 1.0000 |
| S(7) | 0.2032(1) | 0.80429(8) | 0.74144(6) | 5.11(3) | 1.0000 |
| S(8) | 0.0609(1) | 0.99011(7) | 0.83434(6) | 4.39(2) | 1.0000 |
| S(9) | 0.7692(2) | 0.91226(8) | 1.45719(7) | 6.08(3) | 1.0000 |
| S(10) | -0.0183(2) | 0.8935(1) | 0.63951(7) | 6.67(3) | 1.0000 |
| O(1) | 0.7649(3) | 0.2905(2) | 0.5783(2) | 4.95(6) | 1.0000 |
| O(2) | 0.7435(3) | 0.2649(2) | 0.7333(2) | 4.87(7) | 1.0000 |
| O(4) | 0.7835(4) | 0.6362(2) | 0.8849(2) | 6.16(8) | 1.0000 |
| O(5) | 0.8139(4) | 0.4451(2) | 0.8930(2) | 6.19(8) | 1.0000 |
| O(6) | 0.7006(4) | 0.4732(2) | 0.5638(2) | 6.37(9) | 1.0000 |
| O(7) | 0.7884(4) | 0.6477(2) | 0.7230(3) | 7.3(1) | 1.0000 |
| N(1) | 0.6526(3) | 0.4535(2) | 0.7251(2) | 3.64(6) | 1.0000 |
| C(1) | 0.5144(4) | 0.9521(2) | 1.2383(2) | 3.16(7) | 1.0000 |
| C(3) | 0.5934(4) | 0.8690(2) | 1.1948(2) | 3.42(7) | 1.0000 |
| C(4) | 0.4714(4) | 0.4520(2) | 0.7176(2) | 3.51(8) | 1.0000 |
| C(5) | 0.1858(4) | 0.9423(2) | 0.8988(2) | 3.38(7) | 1.0000 |
| C(6) | 0.3729(5) | 0.3705(2) | 0.6529(2) | 4.25(8) | 1.0000 |
| C(7) | 0.6834(5) | 0.9120(3) | 1.3623(2) | 4.10(8) | 1.0000 |
| C(8) | 0.0772(5) | 0.8959(3) | 0.7329(2) | 4.50(9) | 1.0000 |
| C(9) | 0.2022(5) | 0.3693(3) | 0.6432(3) | 5.2(1) | 1.0000 |
| C(10) | 0.7396(6) | 0.1924(3) | 0.5787(3) | 5.8(1) | 1.0000 |
| C(11) | 0.8210(5) | 0.1949(3) | 0.6649(3) | 5.7(1) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(12) | 0.8075(6) | 0.2656(3) | 0.8166(3) | 6.3(1) | 1.0000 |
| C(13) | 0.7718(8) | 0.7354(3) | 0.8007(6) | 9.6(2) | 1.0000 |
| C(14) | 0.7003(6) | 0.2928(4) | 0.4960(3) | 6.7(1) | 1.0000 |
| C(15) | 0.4010(5) | 0.5320(3) | 0.7720(3) | 6.9(1) | 1.0000 |
| C(16) | 0.1308(5) | 0.4490(3) | 0.6978(4) | 7.1(1) | 1.0000 |
| C(17) | 0.8573(7) | 0.6255(4) | 0.9607(4) | 8.6(2) | 1.0000 |
| C(18) | 0.8601(7) | 0.7218(4) | 0.8782(5) | 9.4(2) | 1.0000 |
| C(19) | 0.7618(6) | 0.3913(5) | 0.4957(3) | 7.3(2) | 1.0000 |
| C(20) | 0.7394(6) | 0.3503(4) | 0.8860(3) | 6.8(1) | 1.0000 |
| C(21) | 0.7741(7) | 0.5331(5) | 0.9640(3) | 8.0(2) | 1.0000 |
| C(22) | 0.7566(8) | 0.5723(6) | 0.5680(5) | 9.3(2) | 1.0000 |
| C(23) | 0.7047(9) | 0.6523(5) | 0.6458(6) | 9.7(2) | 1.0000 |
| C(24) | 0.2295(6) | 0.5301(4) | 0.7624(4) | 9.4(2) | 1.0000 |
| C(25) | 0.2551(4) | 0.8549(2) | 0.8559(2) | 3.54(7) | 1.0000 |
| H(1) | 0.6242 | 0.1711 | 0.5725 | 6.8 | 1.0000 |
| H(2) | 0.7866 | 0.1420 | 0.5329 | 6.8 | 1.0000 |
| H(3) | 0.9375 | 0.2186 | 0.6743 | 6.6 | 1.0000 |
| H(4) | 0.8132 | 0.1284 | 0.6663 | 6.6 | 1.0000 |
| H(5) | 0.7738 | 0.2003 | 0.8202 | 7.3 | 1.0000 |
| H(6) | 0.9252 | 0.2753 | 0.8282 | 7.3 | 1.0000 |
| H(7) | 0.8128 | 0.7936 | 0.7925 | 8.9 | 1.0000 |
| H(8) | 0.6542 | 0.7376 | 0.8030 | 8.9 | 1.0000 |
| H(9) | 0.7381 | 0.2399 | 0.4486 | 7.4 | 1.0000 |
| H(10) | 0.5830 | 0.2873 | 0.4873 | 7.4 | 1.0000 |
| H(11) | 0.9697 | 0.6175 | 0.9624 | 8.5 | 1.0000 |
| H(12) | 0.8387 | 0.6819 | 1.0133 | 8.5 | 1.0000 |
| H(13) | 0.8495 | 0.7861 | 0.9217 | 9.9 | 1.0000 |
| H(14) | 0.9680 | 0.7171 | 0.8638 | 9.9 | 1.0000 |
| H(15) | 0.7255 | 0.3965 | 0.4400 | 8.2 | 1.0000 |
| H(16) | 0.8810 | 0.4029 | 0.5065 | 8.2 | 1.0000 |
| H(17) | 0.7619 | 0.3436 | 0.9420 | 8.3 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.6207 | 0.3444 | 0.8709 | 8.3 | 1.0000 |
| H(19) | 0.6571 | 0.5358 | 0.9611 | 8.6 | 1.0000 |
| H(20) | 0.8146 | 0.5281 | 1.0200 | 8.6 | 1.0000 |
| H(21) | 0.8719 | 0.5794 | 0.5704 | 10.8 | 1.0000 |
| H(22) | 0.7029 | 0.5820 | 0.5174 | 10.8 | 1.0000 |
| H(23) | 0.5908 | 0.6456 | 0.6489 | 10.3 | 1.0000 |
| H(24) | 0.7378 | 0.7203 | 0.6511 | 10.3 | 1.0000 |
| H(25) | 0.6873 | 0.3941 | 0.6840 | 6.2 | 1.0000 |
| H(26) | 0.7002 | 0.5126 | 0.7177 | 6.2 | 1.0000 |
| H(27) | 0.6994 | 0.4606 | 0.7839 | 6.2 | 1.0000 |
| H(28) | 0.4273 | 0.3131 | 0.6172 | 5.4 | 1.0000 |
| H(29) | 0.1347 | 0.3106 | 0.5940 | 6.1 | 1.0000 |
| H(30) | 0.4716 | 0.5897 | 0.8198 | 7.6 | 1.0000 |
| H(31) | 0.0101 | 0.4449 | 0.6902 | 7.8 | 1.0000 |
| H(32) | 0.1720 | 0.5885 | 0.7941 | 9.6 | 1.0000 |

($x$ = 0.029)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni0.971 Au0.029 |
| $M_r$ [g mol$^{-1}$] | 813.88 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.15(2) |
| $b$ [Å] | 14.23(3) |
| $c$ [Å] | 16.69(3) |
| $\alpha$ [º] | 112.94(6) |
| $\beta$ [º] | 97.07(7) |
| $\gamma$ [º] | 92.62(6) |
| $D_{calc}$ [g cm$^{-3}$] | 1.536 |
| $V$ [Å$^3$] | 1760(20) |
| Z | 2 |
| $\mu$(Mo$_{K\alpha}$) [cm$^{-1}$] | 48.24 |
| $T$ [K] | 300 |
| no. rflns (measd) | 28005 |
| no. rflns (unique) | 7980 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.077 |
| $wR2$ (all data) | 0.129 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | -0.11007(6) | 0.90486(4) | 0.54665(3) | 4.02(1) | 0.3708(9) |
| S(1) | -0.1152(1) | 1.00569(8) | 0.68241(7) | 4.25(3) | 1.0000 |
| S(2) | 0.2186(2) | 0.8234(1) | 0.76103(8) | 4.98(3) | 1.0000 |
| S(3) | 0.0675(1) | 0.81302(9) | 0.58203(7) | 4.27(3) | 1.0000 |
| S(4) | 0.0499(2) | 0.99825(9) | 0.85255(7) | 4.55(3) | 1.0000 |
| S(5) | -0.1202(2) | 0.79941(9) | 0.41124(7) | 4.49(3) | 1.0000 |
| S(6) | -0.2771(2) | 1.00032(9) | 0.51147(7) | 4.38(3) | 1.0000 |
| S(7) | -0.2968(2) | 0.8042(1) | 0.24155(7) | 5.34(3) | 1.0000 |
| S(8) | -0.4393(2) | 0.98993(10) | 0.33436(8) | 4.61(3) | 1.0000 |
| S(9) | 0.2695(2) | 0.9123(1) | 0.95714(9) | 6.33(4) | 1.0000 |
| S(10) | -0.5179(2) | 0.8933(1) | 0.13964(9) | 6.92(4) | 1.0000 |
| O(1) | 0.2654(4) | 0.2899(2) | 0.0784(2) | 5.34(8) | 1.0000 |
| O(2) | 0.2436(4) | 0.2648(2) | 0.2336(2) | 5.25(8) | 1.0000 |
| O(4) | 0.2845(4) | 0.6362(3) | 0.3845(3) | 6.56(10) | 1.0000 |
| O(6) | 0.3142(5) | 0.4446(3) | 0.3928(2) | 6.5(1) | 1.0000 |
| O(7) | 0.2003(4) | 0.4742(3) | 0.0636(3) | 6.7(1) | 1.0000 |
| N(1) | 0.1531(4) | 0.4541(2) | 0.2256(2) | 3.90(8) | 1.0000 |
| C(1) | 0.0159(5) | 0.9522(3) | 0.7391(3) | 3.58(9) | 1.0000 |
| C(2) | 0.2904(7) | 0.6476(4) | 0.2267(4) | 4.4(1) | 1.0000 |
| C(3) | -0.2465(5) | 0.8551(3) | 0.3556(3) | 3.76(10) | 1.0000 |
| C(4) | -0.0303(5) | 0.4521(3) | 0.2173(3) | 3.89(10) | 1.0000 |
| C(5) | -0.1274(6) | 0.3699(3) | 0.1524(3) | 4.5(1) | 1.0000 |
| C(6) | -0.3139(5) | 0.9425(3) | 0.3993(3) | 3.63(9) | 1.0000 |
| C(7) | 0.1834(6) | 0.9117(3) | 0.8624(3) | 4.3(1) | 1.0000 |
| C(8) | -0.4224(6) | 0.8953(4) | 0.2328(3) | 4.7(1) | 1.0000 |
| C(9) | -0.2987(6) | 0.3696(4) | 0.1436(4) | 5.4(1) | 1.0000 |
| C(10) | 0.2411(7) | 0.1910(4) | 0.0794(4) | 6.0(1) | 1.0000 |
| C(11) | 0.3216(6) | 0.1946(4) | 0.1653(4) | 5.9(1) | 1.0000 |

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|---|---|---|---|---|---|
| C(12) | 0.2011(8) | 0.2931(5) | -0.0039(3) | 7.1(2) | 1.0000 |
| C(13) | 0.3065(7) | 0.2664(4) | 0.3167(5) | 6.6(2) | 1.0000 |
| C(14) | -0.3691(6) | 0.4488(5) | 0.1983(5) | 7.6(2) | 1.0000 |
| C(15) | 0.2372(8) | 0.3509(6) | 0.3864(4) | 7.3(2) | 1.0000 |
| C(16) | 0.2738(8) | 0.5319(6) | 0.4637(4) | 8.2(2) | 1.0000 |
| C(17) | 0.2701(9) | 0.7327(5) | 0.2953(7) | 9.9(3) | 1.0000 |
| C(18) | -0.0989(6) | 0.5322(4) | 0.2719(4) | 7.1(1) | 1.0000 |
| C(19) | 0.3552(9) | 0.6245(5) | 0.4601(5) | 9.3(2) | 1.0000 |
| C(20) | 0.2604(8) | 0.3926(6) | -0.0043(4) | 7.7(2) | 1.0000 |
| C(21) | 0.3578(9) | 0.7232(4) | 0.3740(6) | 10.1(2) | 1.0000 |
| C(22) | -0.2719(7) | 0.5289(5) | 0.2626(5) | 10.3(2) | 1.0000 |
| C(23) | 0.221(1) | 0.6527(6) | 0.1614(8) | 12.4(4) | 1.0000 |
| C(24) | 0.2527(9) | 0.5786(7) | 0.0720(6) | 10.7(3) | 1.0000 |
| C(25) | 0.0922(5) | 0.8687(3) | 0.6952(3) | 3.65(9) | 1.0000 |
| H(1) | 0.1854 | 0.3928 | 0.1830 | 6.7 | 1.0000 |
| H(2) | 0.2002 | 0.5115 | 0.2168 | 6.7 | 1.0000 |
| H(3) | 0.2002 | 0.4594 | 0.2830 | 6.7 | 1.0000 |
| H(4) | 0.1243 | 0.1692 | 0.0708 | 7.2 | 1.0000 |
| H(5) | 0.2874 | 0.1413 | 0.0320 | 7.2 | 1.0000 |
| H(6) | 0.4374 | 0.2200 | 0.1741 | 6.9 | 1.0000 |
| H(7) | 0.3151 | 0.1290 | 0.1666 | 6.9 | 1.0000 |
| H(8) | 0.2412 | 0.2407 | -0.0517 | 7.8 | 1.0000 |
| H(9) | 0.0838 | 0.2860 | -0.0144 | 7.8 | 1.0000 |
| H(10) | 0.2730 | 0.2025 | 0.3230 | 7.5 | 1.0000 |
| H(11) | 0.4242 | 0.2777 | 0.3312 | 7.5 | 1.0000 |
| H(12) | 0.2592 | 0.3458 | 0.4436 | 8.7 | 1.0000 |
| H(13) | 0.1194 | 0.3461 | 0.3717 | 8.7 | 1.0000 |
| H(14) | 0.1542 | 0.5344 | 0.4598 | 8.9 | 1.0000 |
| H(15) | 0.3097 | 0.5268 | 0.5198 | 8.9 | 1.0000 |
| H(16) | 0.3185 | 0.7965 | 0.2988 | 9.0 | 1.0000 |
| H(17) | 0.1583 | 0.7415 | 0.3088 | 9.0 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.4691 | 0.6174 | 0.4631 | 9.1 | 1.0000 |
| H(19) | 0.3378 | 0.6821 | 0.5133 | 9.1 | 1.0000 |
| H(20) | 0.2249 | 0.3980 | -0.0585 | 9.1 | 1.0000 |
| H(21) | 0.3802 | 0.4039 | 0.0078 | 9.1 | 1.0000 |
| H(22) | 0.3542 | 0.7840 | 0.4276 | 9.7 | 1.0000 |
| H(23) | 0.4713 | 0.7156 | 0.3682 | 9.7 | 1.0000 |
| H(24) | 0.0927 | 0.6467 | 0.1485 | 11.2 | 1.0000 |
| H(25) | 0.2407 | 0.7214 | 0.1520 | 11.2 | 1.0000 |
| H(26) | 0.3732 | 0.5818 | 0.0709 | 10.9 | 1.0000 |
| H(27) | 0.2040 | 0.5846 | 0.0183 | 10.9 | 1.0000 |
| H(28) | -0.0748 | 0.3131 | 0.1141 | 5.7 | 1.0000 |
| H(29) | -0.3660 | 0.3115 | 0.0954 | 6.1 | 1.0000 |
| H(30) | -0.4901 | 0.4449 | 0.1900 | 8.3 | 1.0000 |
| H(31) | -0.0280 | 0.5902 | 0.3190 | 8.2 | 1.0000 |
| H(32) | -0.3252 | 0.5877 | 0.3005 | 10.2 | 1.0000 |

($x$ = 0.048)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni0.952 Au0.048 |
| $M_r$ [g mol$^{-1}$] | 816.50 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.142(2) |
| $b$ [Å] | 14.216(5) |
| $c$ [Å] | 16.654(5) |
| $\alpha$ [º] | 112.85(2) |
| $\beta$ [º] | 97.03(2) |
| $\gamma$ [º] | 92.57(2) |
| $D_{calc}$ [g cm$^{-3}$] | 1.546 |
| $V$ [Å$^3$] | 1754(2) |
| Z | 2 |
| $\mu$(Mo$_{K\alpha}$) [cm$^{-1}$] | 48.41 |
| $T$ [K] | 300 |
| no. rflns (measd) | 24119 |
| no. rflns (unique) | 7847 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.089 |
| $wR2$ (all data) | 0.153 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | 1.11006(7) | 0.09514(6) | 0.95331(4) | 4.40(2) | 0.385(1) |
| S(1) | 1.1147(2) | -0.0059(1) | 0.8173(1) | 4.57(4) | 1.0000 |
| S(2) | 0.9324(2) | 0.1870(1) | 0.9184(1) | 4.67(4) | 1.0000 |
| S(3) | 0.7814(2) | 0.1767(2) | 0.7387(1) | 5.37(5) | 1.0000 |
| S(4) | 0.9501(2) | 0.0017(1) | 0.6475(1) | 4.86(4) | 1.0000 |
| S(5) | 1.2767(2) | -0.0004(1) | 0.9883(1) | 4.76(4) | 1.0000 |
| S(6) | 1.1202(2) | 0.2005(2) | 1.0891(1) | 4.89(4) | 1.0000 |
| S(7) | 1.2967(2) | 0.1957(2) | 1.2587(1) | 5.71(5) | 1.0000 |
| S(8) | 1.4393(2) | 0.0100(2) | 1.1656(1) | 4.96(5) | 1.0000 |
| S(9) | 0.7299(3) | 0.0882(2) | 0.5428(1) | 6.69(6) | 1.0000 |
| S(10) | 1.5181(2) | 0.1071(2) | 1.3608(1) | 7.23(6) | 1.0000 |
| O(1) | 0.7354(5) | 0.7092(4) | 1.4213(3) | 5.7(1) | 1.0000 |
| O(2) | 0.7574(5) | 0.7354(4) | 1.2666(3) | 5.7(1) | 1.0000 |
| O(4) | 0.7123(7) | 0.3523(5) | 1.2776(5) | 7.8(2) | 1.0000 |
| O(5) | 0.7999(6) | 0.5272(5) | 1.4371(4) | 7.1(2) | 1.0000 |
| O(6) | 0.7167(6) | 0.3637(4) | 1.1145(4) | 7.0(2) | 1.0000 |
| O(7) | 0.6864(6) | 0.5547(5) | 1.1072(3) | 7.0(2) | 1.0000 |
| N(2) | 0.8468(5) | 0.5460(4) | 1.2745(3) | 4.2(1) | 1.0000 |
| C(2) | 1.2445(6) | 0.1444(5) | 1.1438(4) | 4.2(2) | 1.0000 |
| C(3) | 1.0299(6) | 0.5480(5) | 1.2821(4) | 4.1(2) | 1.0000 |
| C(4) | 0.9856(6) | 0.0483(5) | 0.7619(4) | 3.8(1) | 1.0000 |
| C(5) | 1.1267(7) | 0.6287(5) | 1.3472(4) | 4.8(2) | 1.0000 |
| C(6) | 1.3130(6) | 0.0577(5) | 1.1013(4) | 3.7(1) | 1.0000 |
| C(7) | 0.8169(7) | 0.0889(5) | 0.6380(4) | 4.8(2) | 1.0000 |
| C(8) | 1.4227(7) | 0.1034(6) | 1.2666(4) | 5.2(2) | 1.0000 |
| C(9) | 1.2969(7) | 0.6306(6) | 1.3569(5) | 5.5(2) | 1.0000 |
| C(10) | 0.7987(10) | 0.7063(9) | 1.5032(5) | 7.9(3) | 1.0000 |
| C(11) | 0.7584(9) | 0.8076(7) | 1.4208(5) | 6.4(2) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(12) | 0.6795(8) | 0.8044(6) | 1.3350(6) | 6.4(2) | 1.0000 |
| C(13) | 0.6932(9) | 0.7334(7) | 1.1819(6) | 6.9(3) | 1.0000 |
| C(14) | 1.3673(8) | 0.5515(7) | 1.3017(6) | 7.7(2) | 1.0000 |
| C(15) | 0.728(1) | 0.2645(8) | 1.200(1) | 10.0(4) | 1.0000 |
| C(16) | 1.1001(8) | 0.4680(6) | 1.2279(6) | 7.9(2) | 1.0000 |
| C(17) | 0.7610(10) | 0.6498(9) | 1.1135(6) | 7.6(3) | 1.0000 |
| C(18) | 0.727(1) | 0.4678(10) | 1.0373(6) | 8.6(3) | 1.0000 |
| C(19) | 0.639(1) | 0.2788(8) | 1.1229(9) | 10.3(4) | 1.0000 |
| C(20) | 0.7372(10) | 0.6076(9) | 1.5045(5) | 7.6(3) | 1.0000 |
| C(21) | 0.796(1) | 0.347(1) | 1.354(1) | 11.1(5) | 1.0000 |
| C(22) | 0.646(1) | 0.3759(9) | 1.0386(7) | 9.5(3) | 1.0000 |
| C(23) | 1.2721(8) | 0.4716(7) | 1.2368(7) | 10.5(3) | 1.0000 |
| C(24) | 0.743(1) | 0.427(1) | 1.4322(8) | 10.1(4) | 1.0000 |
| C(25) | 0.9055(6) | 0.1305(5) | 0.8049(4) | 3.8(1) | 1.0000 |
| H(1) | 0.9157 | 0.7140 | 1.5134 | 8.2 | 1.0000 |
| H(2) | 0.7596 | 0.7612 | 1.5512 | 8.2 | 1.0000 |
| H(3) | 0.7130 | 0.8585 | 1.4682 | 7.3 | 1.0000 |
| H(4) | 0.8759 | 0.8302 | 1.4289 | 7.3 | 1.0000 |
| H(5) | 0.6827 | 0.8705 | 1.3326 | 7.6 | 1.0000 |
| H(6) | 0.5618 | 0.7790 | 1.3251 | 7.6 | 1.0000 |
| H(7) | 0.5735 | 0.7242 | 1.1677 | 8.0 | 1.0000 |
| H(8) | 0.7270 | 0.7969 | 1.1741 | 8.0 | 1.0000 |
| H(9) | 0.8425 | 0.2563 | 1.1925 | 9.7 | 1.0000 |
| H(10) | 0.6816 | 0.2020 | 1.2028 | 9.7 | 1.0000 |
| H(11) | 0.8770 | 0.6517 | 1.1287 | 9.0 | 1.0000 |
| H(12) | 0.7380 | 0.6505 | 1.0556 | 9.0 | 1.0000 |
| H(13) | 0.6879 | 0.4721 | 0.9804 | 9.7 | 1.0000 |
| H(14) | 0.8439 | 0.4641 | 1.0402 | 9.7 | 1.0000 |
| H(15) | 0.5283 | 0.2862 | 1.1338 | 10.2 | 1.0000 |
| H(16) | 0.6421 | 0.2160 | 1.0729 | 10.2 | 1.0000 |
| H(17) | 0.6198 | 0.5998 | 1.4957 | 9.0 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.7768 | 0.6066 | 1.5615 | 9.0 | 1.0000 |
| H(19) | 0.7652 | 0.2791 | 1.3525 | 11.0 | 1.0000 |
| H(20) | 0.9117 | 0.3537 | 1.3540 | 11.0 | 1.0000 |
| H(21) | 0.6616 | 0.3178 | 0.9866 | 9.6 | 1.0000 |
| H(22) | 0.5305 | 0.3824 | 1.0375 | 9.6 | 1.0000 |
| H(23) | 0.7995 | 0.4196 | 1.4854 | 11.2 | 1.0000 |
| H(24) | 0.6299 | 0.4202 | 1.4320 | 11.2 | 1.0000 |
| H(25) | 0.8106 | 0.5468 | 1.3271 | 6.9 | 1.0000 |
| H(26) | 0.8110 | 0.6044 | 1.2648 | 6.9 | 1.0000 |
| H(27) | 0.7968 | 0.4855 | 1.2262 | 6.9 | 1.0000 |
| H(28) | 1.0731 | 0.6864 | 1.3871 | 6.0 | 1.0000 |
| H(29) | 1.3655 | 0.6901 | 1.4042 | 6.9 | 1.0000 |
| H(30) | 1.4887 | 0.5546 | 1.3112 | 8.6 | 1.0000 |
| H(31) | 1.0293 | 0.4093 | 1.1807 | 8.5 | 1.0000 |
| H(32) | 1.3275 | 0.4146 | 1.1989 | 10.2 | 1.0000 |

($x$ = 0.065)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni0.935 Au0.065 |
| $M_r$ [g mol$^{-1}$] | 818.86 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.1357(8) |
| $b$ [Å] | 14.223(1) |
| $c$ [Å] | 16.675(2) |
| $\alpha$ [º] | 112.818(5) |
| $\beta$ [º] | 97.046(5) |
| $\gamma$ [º] | 92.651(5) |
| $D_{calc}$ [g cm$^{-3}$] | 1.549 |
| $V$ [Å$^3$] | 1755.8(9) |
| Z | 2 |
| $\mu$(Mo$_{K\alpha}$) [cm$^{-1}$] | 48.36 |
| $T$ [K] | 300 |
| no. rflns (measd) | 17020 |
| no. rflns (unique) | 7775 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.064 |
| $wR2$ (all data) | 0.108 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | 1.11011(5) | -0.40478(3) | -1.04676(3) | 3.719(10) | 0.3957(8) |
| S(1) | 1.1147(1) | -0.50581(8) | -1.18283(6) | 4.02(2) | 1.0000 |
| S(2) | 0.9311(1) | -0.31305(8) | -1.08223(6) | 4.02(2) | 1.0000 |
| S(3) | 1.2968(1) | -0.30408(10) | -0.74147(7) | 5.07(3) | 1.0000 |
| S(4) | 1.1201(1) | -0.29933(8) | -0.91091(6) | 4.29(2) | 1.0000 |
| S(5) | 1.4399(1) | -0.48935(9) | -0.83413(7) | 4.42(3) | 1.0000 |
| S(6) | 0.7813(1) | -0.32350(9) | -1.26133(7) | 4.80(3) | 1.0000 |
| S(7) | 0.9498(1) | -0.49832(8) | -1.35268(7) | 4.26(2) | 1.0000 |
| S(8) | 1.2780(1) | -0.50005(8) | -1.01133(6) | 4.23(2) | 1.0000 |
| S(9) | 0.7304(2) | -0.41190(10) | -1.45717(8) | 6.10(3) | 1.0000 |
| S(10) | 1.5180(2) | -0.3931(1) | -0.63944(8) | 6.69(4) | 1.0000 |
| O(2) | 0.7564(3) | 0.2358(2) | -0.7332(2) | 4.91(7) | 1.0000 |
| O(3) | 0.7346(3) | 0.2094(2) | -0.5783(2) | 4.98(7) | 1.0000 |
| O(5) | 0.7177(4) | -0.1358(2) | -0.8848(3) | 6.31(9) | 1.0000 |
| O(6) | 0.7999(4) | 0.0271(3) | -0.5632(2) | 6.30(10) | 1.0000 |
| O(7) | 0.7125(4) | -0.1475(3) | -0.7225(3) | 7.1(1) | 1.0000 |
| O(8) | 0.6859(4) | 0.0542(3) | -0.8925(2) | 6.18(9) | 1.0000 |
| N(1) | 0.8476(3) | 0.0466(2) | -0.7253(2) | 3.63(7) | 1.0000 |
| C(2) | 1.3140(4) | -0.4415(3) | -0.8985(2) | 3.26(8) | 1.0000 |
| C(4) | 1.0306(4) | 0.0483(3) | -0.7173(3) | 3.51(8) | 1.0000 |
| C(5) | 1.4224(5) | -0.3958(3) | -0.7328(3) | 4.32(10) | 1.0000 |
| C(6) | 1.1284(5) | 0.1300(3) | -0.6522(3) | 4.24(9) | 1.0000 |
| C(7) | 0.9838(4) | -0.4518(3) | -1.2385(2) | 3.29(8) | 1.0000 |
| C(8) | 1.2979(5) | 0.1305(3) | -0.6430(3) | 5.2(1) | 1.0000 |
| C(9) | 0.8144(5) | -0.4120(3) | -1.3629(3) | 4.06(9) | 1.0000 |
| C(10) | 0.7596(6) | 0.3083(3) | -0.5792(3) | 5.7(1) | 1.0000 |
| C(11) | 0.7996(6) | 0.2082(5) | -0.4961(3) | 6.7(1) | 1.0000 |
| C(12) | 0.7602(7) | 0.1496(5) | -0.8863(4) | 7.1(2) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(13) | 0.6791(5) | 0.3048(3) | -0.6647(4) | 5.5(1) | 1.0000 |
| C(14) | 1.3681(5) | 0.0519(4) | -0.6978(4) | 7.0(1) | 1.0000 |
| C(15) | 0.7391(7) | 0.1062(6) | -0.4967(4) | 7.6(2) | 1.0000 |
| C(16) | 0.6438(7) | -0.1246(5) | -0.9611(5) | 8.9(2) | 1.0000 |
| C(17) | 0.6933(6) | 0.2340(4) | -0.8165(4) | 6.3(1) | 1.0000 |
| C(18) | 1.0994(5) | -0.0309(4) | -0.7725(4) | 6.9(1) | 1.0000 |
| C(19) | 0.7307(8) | -0.2342(4) | -0.7995(6) | 9.1(2) | 1.0000 |
| C(20) | 0.7940(9) | -0.1530(6) | -0.6464(7) | 10.0(3) | 1.0000 |
| C(21) | 0.6402(7) | -0.2227(4) | -0.8760(6) | 9.5(2) | 1.0000 |
| C(22) | 0.7265(7) | -0.0320(6) | -0.9634(3) | 7.8(2) | 1.0000 |
| C(23) | 0.7450(9) | -0.0715(7) | -0.5671(6) | 9.8(3) | 1.0000 |
| C(24) | 1.2718(6) | -0.0286(4) | -0.7632(5) | 9.6(2) | 1.0000 |
| C(25) | 1.2461(4) | -0.3554(3) | -0.8556(2) | 3.56(8) | 1.0000 |
| C(26) | 0.9067(4) | -0.3690(3) | -1.1954(2) | 3.31(8) | 1.0000 |
| H(1) | 0.7109 | 0.3578 | -0.5307 | 5.3 | 1.0000 |
| H(2) | 0.8760 | 0.3318 | -0.5683 | 5.3 | 1.0000 |
| H(3) | 0.9135 | 0.2170 | -0.4840 | 6.0 | 1.0000 |
| H(4) | 0.7534 | 0.2612 | -0.4492 | 6.0 | 1.0000 |
| H(5) | 0.8754 | 0.1494 | -0.8725 | 6.1 | 1.0000 |
| H(6) | 0.7326 | 0.1510 | -0.9425 | 6.1 | 1.0000 |
| H(7) | 0.6837 | 0.3693 | -0.6676 | 5.6 | 1.0000 |
| H(8) | 0.5625 | 0.2779 | -0.6749 | 5.6 | 1.0000 |
| H(9) | 0.6219 | 0.1039 | -0.5036 | 7.2 | 1.0000 |
| H(10) | 0.7803 | 0.1111 | -0.4385 | 7.2 | 1.0000 |
| H(11) | 0.6694 | -0.1845 | -1.0103 | 7.7 | 1.0000 |
| H(12) | 0.5323 | -0.1236 | -0.9622 | 7.7 | 1.0000 |
| H(13) | 0.5795 | 0.2240 | -0.8308 | 6.0 | 1.0000 |
| H(14) | 0.7373 | 0.2938 | -0.8242 | 6.0 | 1.0000 |
| H(15) | 0.8435 | -0.2388 | -0.8024 | 7.5 | 1.0000 |
| H(16) | 0.6789 | -0.2927 | -0.7954 | 7.5 | 1.0000 |
| H(17) | 0.7633 | -0.2191 | -0.6519 | 9.1 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.9068 | -0.1423 | -0.6503 | 9.1 | 1.0000 |
| H(19) | 0.5370 | -0.2151 | -0.8664 | 8.5 | 1.0000 |
| H(20) | 0.6614 | -0.2815 | -0.9217 | 8.5 | 1.0000 |
| H(21) | 0.6872 | -0.0274 | -1.0176 | 8.1 | 1.0000 |
| H(22) | 0.8449 | -0.0325 | -0.9574 | 8.1 | 1.0000 |
| H(23) | 0.8019 | -0.0839 | -0.5181 | 8.8 | 1.0000 |
| H(24) | 0.6295 | -0.0812 | -0.5681 | 8.8 | 1.0000 |
| H(25) | 0.8158 | 0.1076 | -0.6826 | 4.8 | 1.0000 |
| H(26) | 0.8023 | 0.0428 | -0.7829 | 4.8 | 1.0000 |
| H(27) | 0.7992 | -0.0112 | -0.7180 | 4.8 | 1.0000 |
| H(28) | 1.0754 | 0.1878 | -0.6162 | 4.0 | 1.0000 |
| H(29) | 1.3657 | 0.1860 | -0.5947 | 5.2 | 1.0000 |
| H(30) | 1.4869 | 0.0562 | -0.6891 | 6.4 | 1.0000 |
| H(31) | 1.0316 | -0.0868 | -0.8183 | 6.5 | 1.0000 |
| H(32) | 1.3267 | -0.0863 | -0.7978 | 8.5 | 1.0000 |

($x = 0.091$)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Ni0.909 Au0.091 |
| $M_r$ [g mol$^{-1}$] | 822.45 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.14(2) |
| $b$ [Å] | 14.19(5) |
| $c$ [Å] | 16.66(5) |
| $\alpha$ [º] | 112.81(10) |
| $\beta$ [º] | 96.91(10) |
| $\gamma$ [º] | 92.8(1) |
| $D_{calc}$ [g cm$^{-3}$] | 1.559 |
| $V$ [Å$^3$] | 1752(30) |
| Z | 2 |
| $\mu(Mo_{K\alpha})$ [cm$^{-1}$] | 48.45 |
| $T$ [K] | 300 |
| no. rflns (measd) | 24966 |
| no. rflns (unique) | 7847 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.097 |
| $wR2$ (all data) | 0.175 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | -0.1098(1) | 0.40470(8) | 1.04660(6) | 4.42(3) | 0.419(2) |
| S(1) | 0.0689(3) | 0.3134(2) | 1.0824(2) | 4.78(7) | 1.0000 |
| S(2) | -0.1146(3) | 0.5060(2) | 1.1832(2) | 4.75(7) | 1.0000 |
| S(3) | -0.2963(4) | 0.3041(3) | 0.7411(2) | 5.86(8) | 1.0000 |
| S(4) | -0.4393(3) | 0.4889(2) | 0.8337(2) | 5.24(8) | 1.0000 |
| S(5) | -0.1192(3) | 0.2992(2) | 0.9103(2) | 4.99(7) | 1.0000 |
| S(6) | 0.0502(4) | 0.4982(2) | 1.3526(2) | 5.09(7) | 1.0000 |
| S(7) | -0.2775(3) | 0.4998(2) | 1.0112(2) | 4.97(7) | 1.0000 |
| S(8) | 0.2185(3) | 0.3238(2) | 1.2615(2) | 5.45(8) | 1.0000 |
| S(9) | 0.2688(4) | 0.4121(3) | 1.4575(2) | 6.82(9) | 1.0000 |
| S(10) | -0.5175(4) | 0.3924(3) | 0.6393(2) | 7.4(1) | 1.0000 |
| O(2) | 0.2455(8) | -0.2361(6) | 0.7322(5) | 5.5(2) | 1.0000 |
| O(3) | 0.2819(9) | 0.1375(7) | 0.8838(6) | 6.9(2) | 1.0000 |
| O(5) | 0.2645(9) | -0.2096(6) | 0.5781(5) | 5.5(2) | 1.0000 |
| O(6) | 0.287(1) | 0.1474(7) | 0.7228(9) | 8.2(3) | 1.0000 |
| O(7) | 0.3166(9) | -0.0562(7) | 0.8908(5) | 6.6(2) | 1.0000 |
| O(8) | 0.1999(9) | -0.0283(7) | 0.5624(6) | 7.0(3) | 1.0000 |
| N(2) | 0.1538(9) | -0.0471(6) | 0.7252(5) | 4.6(2) | 1.0000 |
| C(2) | -0.312(1) | 0.4410(8) | 0.8996(7) | 4.2(3) | 1.0000 |
| C(3) | 0.093(1) | 0.3696(8) | 1.1951(6) | 3.8(2) | 1.0000 |
| C(4) | -0.028(1) | -0.0484(8) | 0.7173(7) | 4.1(3) | 1.0000 |
| C(5) | -0.129(1) | -0.1293(8) | 0.6542(7) | 4.8(3) | 1.0000 |
| C(6) | 0.015(1) | 0.4512(8) | 1.2379(6) | 3.9(2) | 1.0000 |
| C(7) | -0.428(1) | 0.3963(9) | 0.7348(7) | 5.2(3) | 1.0000 |
| C(8) | 0.186(1) | 0.4115(8) | 1.3615(6) | 4.7(3) | 1.0000 |
| C(9) | -0.297(1) | -0.1317(9) | 0.6434(7) | 5.6(3) | 1.0000 |
| C(10) | 0.242(1) | -0.3084(10) | 0.5789(8) | 6.7(4) | 1.0000 |
| C(11) | 0.243(2) | -0.151(1) | 0.884(1) | 9.1(5) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(12) | 0.319(1) | -0.3044(9) | 0.666(1) | 7.3(4) | 1.0000 |
| C(13) | 0.203(2) | -0.207(1) | 0.4964(8) | 7.8(4) | 1.0000 |
| C(14) | 0.261(2) | -0.107(1) | 0.4961(9) | 8.4(5) | 1.0000 |
| C(15) | 0.303(2) | -0.235(1) | 0.820(1) | 7.3(4) | 1.0000 |
| C(16) | 0.360(2) | 0.223(1) | 0.877(1) | 10.7(6) | 1.0000 |
| C(17) | -0.095(1) | 0.0297(9) | 0.7705(9) | 8.1(4) | 1.0000 |
| C(18) | 0.349(2) | 0.123(1) | 0.959(1) | 10.7(5) | 1.0000 |
| C(19) | 0.268(2) | 0.234(1) | 0.797(2) | 10.2(6) | 1.0000 |
| C(20) | 0.272(2) | 0.031(1) | 0.9651(8) | 8.5(4) | 1.0000 |
| C(21) | 0.206(2) | 0.151(1) | 0.646(2) | 10.4(7) | 1.0000 |
| C(22) | -0.367(1) | -0.0526(10) | 0.697(1) | 7.9(4) | 1.0000 |
| C(23) | 0.258(2) | 0.072(2) | 0.566(1) | 10.7(7) | 1.0000 |
| C(24) | -0.270(2) | 0.030(1) | 0.7658(10) | 9.8(4) | 1.0000 |
| C(25) | -0.243(1) | 0.3535(8) | 0.8541(6) | 3.9(2) | 1.0000 |
| H(1) | 0.1243 | -0.3339 | 0.5673 | 6.2 | 1.0000 |
| H(2) | 0.2904 | -0.3591 | 0.5306 | 6.2 | 1.0000 |
| H(3) | 0.2598 | -0.1544 | 0.9399 | 7.0 | 1.0000 |
| H(4) | 0.1229 | -0.1525 | 0.8674 | 7.0 | 1.0000 |
| H(5) | 0.4365 | -0.2782 | 0.6750 | 6.6 | 1.0000 |
| H(6) | 0.3148 | -0.3692 | 0.6685 | 6.6 | 1.0000 |
| H(7) | 0.2450 | -0.2595 | 0.4470 | 7.0 | 1.0000 |
| H(8) | 0.0839 | -0.2180 | 0.4823 | 7.0 | 1.0000 |
| H(9) | 0.2195 | -0.1040 | 0.4424 | 7.9 | 1.0000 |
| H(10) | 0.3758 | -0.0988 | 0.5078 | 7.9 | 1.0000 |
| H(11) | 0.2655 | -0.2964 | 0.8229 | 6.7 | 1.0000 |
| H(12) | 0.4217 | -0.2247 | 0.8305 | 6.7 | 1.0000 |
| H(13) | 0.3422 | 0.2812 | 0.9257 | 9.8 | 1.0000 |
| H(14) | 0.4672 | 0.2157 | 0.8702 | 9.8 | 1.0000 |
| H(15) | 0.4652 | 0.1217 | 0.9675 | 9.5 | 1.0000 |
| H(16) | 0.3251 | 0.1817 | 1.0132 | 9.5 | 1.0000 |
| H(17) | 0.3180 | 0.2932 | 0.7937 | 8.4 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.1547 | 0.2385 | 0.8014 | 8.4 | 1.0000 |
| H(19) | 0.1540 | 0.0317 | 0.9599 | 8.6 | 1.0000 |
| H(20) | 0.3114 | 0.0255 | 1.0194 | 8.6 | 1.0000 |
| H(21) | 0.0869 | 0.1429 | 0.6447 | 9.3 | 1.0000 |
| H(22) | 0.2309 | 0.2193 | 0.6460 | 9.3 | 1.0000 |
| H(23) | 0.3682 | 0.0859 | 0.5752 | 10.8 | 1.0000 |
| H(24) | 0.2001 | 0.0855 | 0.5203 | 10.8 | 1.0000 |
| H(25) | 0.1866 | -0.1081 | 0.6842 | 5.6 | 1.0000 |
| H(26) | 0.2007 | 0.0106 | 0.7161 | 5.6 | 1.0000 |
| H(27) | 0.2007 | -0.0397 | 0.7839 | 5.6 | 1.0000 |
| H(28) | -0.0752 | -0.1882 | 0.6174 | 4.6 | 1.0000 |
| H(29) | -0.3663 | -0.1861 | 0.5958 | 5.9 | 1.0000 |
| H(30) | -0.0264 | 0.0893 | 0.8151 | 7.8 | 1.0000 |
| H(31) | -0.4849 | -0.0568 | 0.6865 | 7.9 | 1.0000 |
| H(32) | -0.3277 | 0.0857 | 0.8030 | 9.9 | 1.0000 |

($x$ = 1)

| | |
|---|---|
| Formula | C24 H32 NO6 S10 Au |
| $M_r$ [g mol$^{-1}$] | 948.14 |
| crystal system | triclinic |
| space group | $P\bar{1}$ |
| $a$ [Å] | 8.293(4) |
| $b$ [Å] | 14.425(10) |
| $c$ [Å] | 16.95(1) |
| $\alpha$ [º] | 111.68(3) |
| $\beta$ [º] | 96.11(3) |
| $\gamma$ [º] | 94.69(3) |
| $D_{calc}$ [g cm$^{-3}$] | 1.697 |
| $V$ [Å$^3$] | 1856(2) |
| Z | 2 |
| $\mu$(Mo$_{K\alpha}$) [cm$^{-1}$] | 45.73 |
| $T$ [K] | 300 |
| no. rflns (measd) | 22240 |
| no. rflns (unique) | 7768 |
| no. params | 380 |
| $R1$ (I>2σ(I)) | 0.086 |
| $wR2$ (all data) | 0.182 |

| Atom | x | y | z | $B_{eq}$ | occ |
|---|---|---|---|---|---|
| Au(1) | 0.10696(7) | 0.09689(5) | 0.95265(4) | 3.61(1) | 1.004(5) |
| S(1) | 0.1194(5) | 0.2065(4) | 1.0972(3) | 5.0(1) | 1.0000 |
| S(2) | 0.1096(5) | -0.0094(3) | 0.8080(3) | 4.57(9) | 1.0000 |
| S(3) | 0.4477(5) | 0.0165(4) | 1.1671(3) | 5.0(1) | 1.0000 |
| S(4) | -0.0559(5) | 0.0036(3) | 0.6449(3) | 4.79(10) | 1.0000 |
| S(5) | 0.2958(5) | 0.0025(3) | 0.9905(2) | 4.63(10) | 1.0000 |
| S(6) | -0.2257(5) | 0.1760(4) | 0.7357(3) | 5.4(1) | 1.0000 |
| S(7) | -0.0871(5) | 0.1891(3) | 0.9135(3) | 4.67(10) | 1.0000 |
| S(8) | -0.2730(7) | 0.0891(4) | 0.5411(3) | 6.7(1) | 1.0000 |
| S(9) | 0.2964(6) | 0.1952(4) | 1.2598(3) | 5.7(1) | 1.0000 |
| S(10) | 0.5201(7) | 0.1072(5) | 1.3599(3) | 7.1(1) | 1.0000 |
| O(1) | 0.279(2) | 0.647(1) | 0.716(1) | 8.5(5) | 1.0000 |
| O(2) | 0.249(1) | 0.2633(10) | 0.7337(8) | 6.0(3) | 1.0000 |
| O(5) | 0.266(1) | 0.2895(10) | 0.5785(8) | 5.9(3) | 1.0000 |
| O(6) | 0.316(2) | 0.442(1) | 0.8887(8) | 7.7(4) | 1.0000 |
| O(7) | 0.282(2) | 0.634(1) | 0.883(1) | 8.4(4) | 1.0000 |
| O(8) | 0.194(2) | 0.470(1) | 0.563(1) | 8.0(5) | 1.0000 |
| N(1) | 0.151(1) | 0.453(1) | 0.7240(9) | 5.0(3) | 1.0000 |
| C(1) | -0.026(2) | 0.051(1) | 0.7592(9) | 3.9(3) | 1.0000 |
| C(2) | -0.030(2) | 0.447(1) | 0.716(1) | 4.8(4) | 1.0000 |
| C(3) | 0.424(2) | 0.110(1) | 1.268(1) | 5.2(4) | 1.0000 |
| C(5) | -0.100(2) | 0.129(1) | 0.7995(9) | 4.2(4) | 1.0000 |
| C(6) | 0.253(3) | 0.566(3) | 0.565(3) | 12(1) | 1.0000 |
| C(7) | 0.251(2) | 0.145(1) | 1.1448(9) | 4.0(3) | 1.0000 |
| C(9) | -0.191(2) | 0.090(1) | 0.633(1) | 5.4(4) | 1.0000 |
| C(11) | 0.319(2) | 0.193(2) | 0.662(2) | 6.8(6) | 1.0000 |
| C(12) | -0.125(2) | 0.372(1) | 0.650(1) | 5.4(4) | 1.0000 |
| C(13) | -0.272(3) | 0.519(2) | 0.767(2) | 12.2(8) | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C(14) | 0.244(3) | 0.338(3) | 0.879(2) | 9.4(8) | 1.0000 |
| C(15) | -0.296(2) | 0.363(1) | 0.638(1) | 6.4(5) | 1.0000 |
| C(17) | 0.209(3) | 0.290(2) | 0.495(1) | 9.0(7) | 1.0000 |
| C(18) | 0.264(3) | 0.732(2) | 0.796(3) | 12(1) | 1.0000 |
| C(19) | 0.277(3) | 0.527(2) | 0.961(1) | 9.0(7) | 1.0000 |
| C(20) | -0.363(2) | 0.445(2) | 0.698(2) | 7.9(6) | 1.0000 |
| C(21) | 0.361(3) | 0.626(2) | 0.960(2) | 11.3(8) | 1.0000 |
| C(22) | 0.259(3) | 0.392(3) | 0.497(2) | 10.2(10) | 1.0000 |
| C(23) | 0.363(3) | 0.717(2) | 0.873(3) | 13(1) | 1.0000 |
| C(24) | 0.197(4) | 0.646(3) | 0.639(4) | 16(1) | 1.0000 |
| C(25) | 0.240(2) | 0.192(1) | 0.580(1) | 7.5(5) | 1.0000 |
| C(26) | -0.099(2) | 0.525(2) | 0.777(2) | 8.9(6) | 1.0000 |
| C(27) | 0.318(2) | 0.066(1) | 1.104(1) | 4.5(4) | 1.0000 |
| C(28) | 0.318(3) | 0.264(2) | 0.815(2) | 8.0(7) | 1.0000 |
| H(1) | 0.3634 | 0.5855 | 0.5712 | 10.3 | 1.0000 |
| H(2) | 0.1956 | 0.5845 | 0.5206 | 10.3 | 1.0000 |
| H(3) | 0.4328 | 0.2184 | 0.6711 | 8.2 | 1.0000 |
| H(4) | 0.3064 | 0.1298 | 0.6651 | 8.2 | 1.0000 |
| H(5) | 0.2397 | 0.3489 | 0.9441 | 11.1 | 1.0000 |
| H(6) | 0.1185 | 0.3434 | 0.8657 | 11.1 | 1.0000 |
| H(7) | 0.2542 | 0.2416 | 0.4538 | 5.7 | 1.0000 |
| H(8) | 0.0940 | 0.2779 | 0.4866 | 5.7 | 1.0000 |
| H(9) | 0.3129 | 0.7994 | 0.7985 | 10.7 | 1.0000 |
| H(10) | 0.1537 | 0.7410 | 0.8063 | 10.7 | 1.0000 |
| H(11) | 0.1693 | 0.5347 | 0.9691 | 7.5 | 1.0000 |
| H(12) | 0.3359 | 0.5334 | 1.0195 | 7.5 | 1.0000 |
| H(13) | 0.4687 | 0.6225 | 0.9459 | 10.2 | 1.0000 |
| H(14) | 0.3484 | 0.6863 | 1.0001 | 10.2 | 1.0000 |
| H(15) | 0.2284 | 0.3910 | 0.4435 | 6.7 | 1.0000 |
| H(16) | 0.3786 | 0.4032 | 0.5111 | 6.7 | 1.0000 |
| H(17) | 0.3583 | 0.7758 | 0.9289 | 11.3 | 1.0000 |

| | | | | | |
|---|---|---|---|---|---|
| H(18) | 0.4680 | 0.7104 | 0.8679 | 11.3 | 1.0000 |
| H(19) | 0.0904 | 0.6342 | 0.6453 | 12.2 | 1.0000 |
| H(20) | 0.2273 | 0.7130 | 0.6434 | 12.2 | 1.0000 |
| H(21) | 0.1281 | 0.1656 | 0.5677 | 2.9 | 1.0000 |
| H(22) | 0.2924 | 0.1444 | 0.5328 | 2.9 | 1.0000 |
| H(23) | 0.3123 | 0.2253 | 0.8438 | 21.4 | 1.0000 |
| H(24) | 0.4313 | 0.3152 | 0.8459 | 21.4 | 1.0000 |
| H(25) | 0.1853 | 0.3927 | 0.7303 | 7.5 | 1.0000 |
| H(26) | 0.1886 | 0.4594 | 0.6765 | 7.5 | 1.0000 |
| H(27) | 0.2042 | 0.5089 | 0.7758 | 7.5 | 1.0000 |
| H(28) | -0.0724 | 0.3198 | 0.6102 | 5.8 | 1.0000 |
| H(29) | -0.3203 | 0.5702 | 0.8096 | 6.8 | 1.0000 |
| H(30) | -0.3654 | 0.3110 | 0.5933 | 7.2 | 1.0000 |
| H(31) | -0.4811 | 0.4484 | 0.6919 | 7.8 | 1.0000 |
| H(32) | -0.0275 | 0.5781 | 0.8233 | 3.5 | 1.0000 |

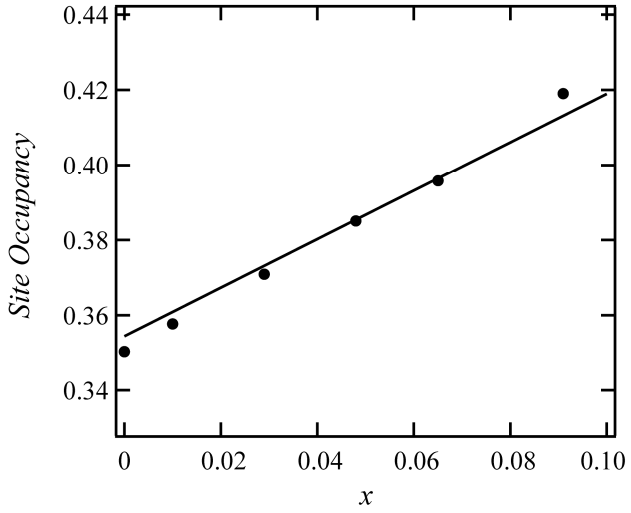


**Figure S2**. The occupancy of M site in $[M(dmit)_2]^-$, in which M site was assigned tentatively to Au, plotted against $x$. The solid line is calculated using the electron number of $Ni^{3+}$ and $Au^{3+}$ ions. (see text)

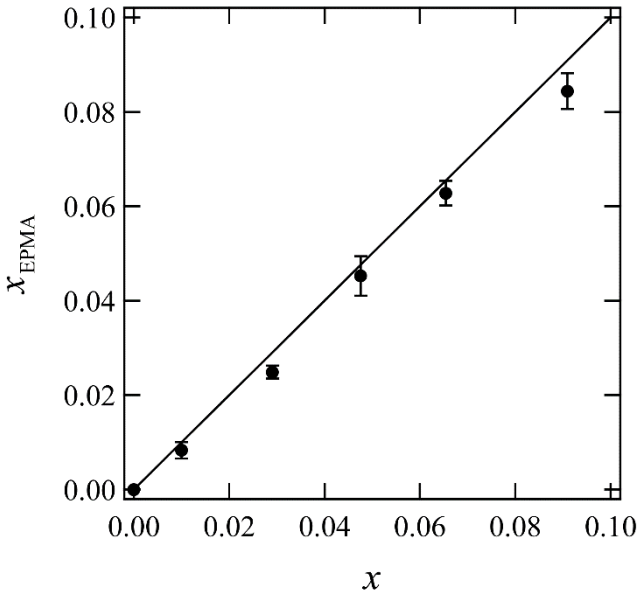


**Figure S3**. Plot of Au concentration (Au / (Au + Ni), $x_{EPMA}$) analyzed by EPMA vs. $x$.