

## Supporting information for the dissertation

### Theophylline-derived N-heterocyclic carbenes and their metal complexes

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Tables of Crystal data and structure refinement obtained in this project

#### Content

|  |             |
|--|-------------|
| <b>X-Ray data of compound (5a)</b> .....   | <b>(1)</b>  |
| <b>X-Ray data of compound (7a)</b> .....   | <b>(2)</b>  |
| <b>X-Ray data of compound (7b)</b> .....   | <b>(3)</b>  |
| <b>X-Ray data of compound (Ag1)</b> .....  | <b>(4)</b>  |
| <b>X-Ray data of compound (Ag2)</b> .....  | <b>(5)</b>  |
| <b>X-Ray data of compound (Ag4)</b> .....  | <b>(6)</b>  |
| <b>X-Ray data of compound (Ag5)</b> .....  | <b>(7)</b>  |
| <b>X-Ray data of compound (Ag6)</b> .....  | <b>(8)</b>  |
| <b>X-Ray data of compound (Au2)</b> .....  | <b>(9)</b>  |
| <b>X-Ray data of compound (Au4)</b> .....  | <b>(10)</b> |
| <b>X-Ray data of compound (Au5)</b> .....  | <b>(11)</b> |
| <b>X-Ray data of compound (Pd1)</b> .....  | <b>(12)</b> |
| <b>X-Ray data of compound (Pd2)</b> .....  | <b>(13)</b> |
| <b>X-Ray data of compound (Ag8)</b> .....  | <b>(14)</b> |
| <b>X-Ray data of compound (Ag9)</b> .....  | <b>(15)</b> |
| <b>X-Ray data of compound (Ag10)</b> ..... | <b>(16)</b> |

## Compound 5a

|  |  |
|--|--|
| Identification code                            | acsan209_auto  |
| Empirical formula                              | BrONCHPF   |
| Formula weight                                 | N/A  |
| Temperature/K                                  | N/A  |
| Crystal system                                 | monoclinic   |
| Space group                                    | P2 <sub>1</sub> /c   |
| a/Å  | 10.4281(3)   |
| b/Å  | 8.3009(2)  |
| c/Å  | 19.3075(6)   |
| $\alpha/^\circ$                                | 90   |
| $\beta/^\circ$                                 | 91.498(3)  |
| $\gamma/^\circ$                                | 90   |
| Volume/Å <sup>3</sup>                          | 1670.74  |
| Z  | 1  |
| $\rho_{\text{calc}}/\text{cm}^3$               | N/A  |
| $\mu/\text{mm}^{-1}$                           | N/A  |
| F(000)   | N/A  |
| Crystal size/mm <sup>3</sup>                   | N/A × N/A × N/A  |
| Radiation                                      | N/A ( $\lambda$ = N/A)   |
| 2 $\Theta$ range for data collection/ $^\circ$ | N/A to N/A   |
| Index ranges                                   | $100 \leq h \leq -100, 100 \leq k \leq -100, 100 \leq l \leq -100$ |
| Reflections collected                          | N/A  |
| Independent reflections                        | N/A [ $R_{\text{int}}$ = N/A, $R_{\text{sigma}}$ = N/A]            |
| Data/restraints/parameters                     | N/A/N/A/N/A  |
| Goodness-of-fit on $F^2$                       | N/A  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = N/A, $wR_2$ = N/A  |
| Final R indexes [all data]                     | $R_1$ = N/A, $wR_2$ = N/A  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | N/A/N/A  |

## Compound 7a

|  |   |
|--|---|
| Identification code                            | ACSANA101_auto  |
| Empirical formula                              | C <sub>11</sub> I <sub>3</sub> N <sub>4</sub> O <sub>2</sub>  |
| Formula weight                                 | 615.97  |
| Temperature/K                                  | 150   |
| Crystal system                                 | orthorhombic  |
| Space group                                    | Pbca  |
| a/Å  | 16.4024(7)  |
| b/Å  | 12.7108(5)  |
| c/Å  | 16.5807(7)  |
| $\alpha/^\circ$                                | 90  |
| $\beta/^\circ$                                 | 90  |
| $\gamma/^\circ$                                | 90  |
| Volume/Å <sup>3</sup>                          | 3456.9(2)   |
| Z  | 8   |
| $\rho_{\text{calc}}/\text{g}/\text{cm}^3$      | 2.367   |
| $\mu/\text{mm}^{-1}$                           | 5.431   |
| F(000)   | 2272.0  |
| Crystal size/mm <sup>3</sup>                   | 0.15 × 0.1 × 0.08   |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)                          |
| 2 $\Theta$ range for data collection/ $^\circ$ | 4.74 to 59.028  |
| Index ranges                                   | -21 ≤ h ≤ 10, -16 ≤ k ≤ 16, -21 ≤ l ≤ 22                      |
| Reflections collected                          | 11284   |
| Independent reflections                        | 4149 [R <sub>int</sub> = 0.0309, R <sub>sigma</sub> = 0.0334] |
| Data/restraints/parameters                     | 4149/0/184  |
| Goodness-of-fit on F <sup>2</sup>              | 1.092   |
| Final R indexes [I ≥ 2 $\sigma$ (I)]           | R <sub>1</sub> = 0.0320, wR <sub>2</sub> = 0.0679             |
| Final R indexes [all data]                     | R <sub>1</sub> = 0.0453, wR <sub>2</sub> = 0.0745             |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.72/-1.37  |

## Compound 7b

|  |  |
|--|--|
| Identification code                            | ACSANBi08_auto   |
| Empirical formula                              | C <sub>10</sub> H <sub>14</sub> I <sub>2</sub> N <sub>4</sub> O <sub>2</sub> |
| Formula weight                                 | 476.05   |
| Temperature/K                                  | 150  |
| Crystal system                                 | monoclinic   |
| Space group                                    | P2 <sub>1</sub>  |
| a/Å  | 8.6935(4)  |
| b/Å  | 7.6364(3)  |
| c/Å  | 11.0967(5)   |
| $\alpha/^\circ$                                | 90   |
| $\beta/^\circ$                                 | 99.790(4)  |
| $\gamma/^\circ$                                | 90   |
| Volume/Å <sup>3</sup>                          | 725.96(6)  |
| Z  | 2  |
| $\rho_{\text{calc}}/\text{g}/\text{cm}^3$      | 2.178  |
| $\mu/\text{mm}^{-1}$                           | 4.333  |
| F(000)   | 448.0  |
| Crystal size/mm <sup>3</sup>                   | 0.09 × 0.06 × 0.04   |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)   |
| 2 $\Theta$ range for data collection/ $^\circ$ | 4.754 to 58.636  |
| Index ranges                                   | -11 ≤ h ≤ 7, -10 ≤ k ≤ 6, -14 ≤ l ≤ 14                                       |
| Reflections collected                          | 3461   |
| Independent reflections                        | 2365 [ $R_{\text{int}}$ = 0.0275, $R_{\text{sigma}}$ = 0.0472]               |
| Data/restraints/parameters                     | 2365/1/166   |
| Goodness-of-fit on F <sup>2</sup>              | 1.072  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0331, $wR_2$ = 0.0741  |
| Final R indexes [all data]                     | $R_1$ = 0.0367, $wR_2$ = 0.0764  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.81/-0.79   |
| Flack parameter                                | -0.06(5)   |

## Compound Ag1

|  |  |
|--|--|
| Identification code                            | wit_ACSANAg3_auto  |
| Empirical formula                              | C <sub>22</sub> H <sub>28</sub> AgF <sub>6</sub> N <sub>8</sub> O <sub>4</sub> P |
| Formula weight                                 | 721.36   |
| Temperature/K                                  | 293(2)   |
| Crystal system                                 | monoclinic   |
| Space group                                    | P2 <sub>1</sub> /n   |
| a/Å  | 10.1738(13)  |
| b/Å  | 12.350(3)  |
| c/Å  | 22.750(3)  |
| $\alpha/^\circ$                                | 90   |
| $\beta/^\circ$                                 | 91.518(14)   |
| $\gamma/^\circ$                                | 90   |
| Volume/Å <sup>3</sup>                          | 2857.6(8)  |
| Z  | 4  |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.677  |
| $\mu/\text{mm}^{-1}$                           | 0.845  |
| F(000)   | 1456.0   |
| Crystal size/mm <sup>3</sup>                   | ? × ? × ?  |
| Radiation                                      | MoK $\alpha$ ( $\lambda$ = 0.71073)  |
| 2 $\Theta$ range for data collection/ $^\circ$ | 5.188 to 66.686  |
| Index ranges                                   | -13 ≤ h ≤ 13, -13 ≤ k ≤ 18, -33 ≤ l ≤ 18   |
| Reflections collected                          | 17571  |
| Independent reflections                        | 9757 [ $R_{\text{int}}$ = 0.1198, $R_{\text{sigma}}$ = 0.2696]                   |
| Data/restraints/parameters                     | 9757/0/385   |
| Goodness-of-fit on F <sup>2</sup>              | 0.872  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.1007, $wR_2$ = 0.2236  |
| Final R indexes [all data]                     | $R_1$ = 0.3140, $wR_2$ = 0.3293  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.79/-1.20   |

## Compound Ag2

|   |  |
|---|--|
| Identification code                         | SANco1_Ag1_auto  |
| Empirical formula                           | C <sub>12</sub> H <sub>19</sub> AgF <sub>6</sub> N <sub>5</sub> O <sub>2</sub> P |
| Formula weight                              | 518.16   |
| Temperature/K                               | 150.0(3)   |
| Crystal system                              | monoclinic   |
| Space group                                 | P2 <sub>1</sub> /n   |
| a/Å   | 20.5351(7)   |
| b/Å   | 9.2214(2)  |
| c/Å   | 21.0163(7)   |
| α/°   | 90   |
| β/°   | 112.420(4)   |
| γ/°   | 90   |
| Volume/Å <sup>3</sup>                       | 3678.9(2)  |
| Z   | 8  |
| ρ <sub>calc</sub> /cm <sup>3</sup>          | 1.871  |
| μ/mm <sup>-1</sup>                          | 1.259  |
| F(000)                                      | 2064.0   |
| Crystal size/mm <sup>3</sup>                | 0.155 × 0.124 × 0.121  |
| Radiation                                   | Mo Kα (λ = 0.71073)  |
| 2Θ range for data collection/°              | 4.72 to 52.742   |
| Index ranges                                | -25 ≤ h ≤ 25, -10 ≤ k ≤ 11, -24 ≤ l ≤ 26   |
| Reflections collected                       | 24839  |
| Independent reflections                     | 7513 [R <sub>int</sub> = 0.0369, R <sub>sigma</sub> = 0.0364]                    |
| Data/restraints/parameters                  | 7513/73/524  |
| Goodness-of-fit on F <sup>2</sup>           | 1.039  |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0368, wR <sub>2</sub> = 0.0841                                |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0490, wR <sub>2</sub> = 0.0884                                |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.94/-1.18   |

## Compound Ag4

|   |  |
|---|--|
| Identification code                         | ACSAN200_auto  |
| Empirical formula                           | C <sub>11</sub> H <sub>18</sub> AgBrF <sub>6</sub> N <sub>5</sub> O <sub>2</sub> P |
| Formula weight                              | 585.05   |
| Temperature/K                               | 150  |
| Crystal system                              | monoclinic   |
| Space group                                 | P2 <sub>1</sub> /c   |
| a/Å   | 8.6351(3)  |
| b/Å   | 23.3138(8)   |
| c/Å   | 9.3991(3)  |
| α/°   | 90   |
| β/°   | 94.554(3)  |
| γ/°   | 90   |
| Volume/Å <sup>3</sup>                       | 1886.22(11)  |
| Z   | 4  |
| ρ <sub>calc</sub> /cm <sup>3</sup>          | 2.060  |
| μ/mm <sup>-1</sup>                          | 3.346  |
| F(000)                                      | 1144.0   |
| Crystal size/mm <sup>3</sup>                | 0.07 × 0.05 × 0.03   |
| Radiation                                   | Mo Kα (λ = 0.71073)  |
| 2θ range for data collection/°              | 4.686 to 58.66   |
| Index ranges                                | -11 ≤ h ≤ 10, -30 ≤ k ≤ 31, -12 ≤ l ≤ 12   |
| Reflections collected                       | 10551  |
| Independent reflections                     | 4373 [R <sub>int</sub> = 0.0258, R <sub>sigma</sub> = 0.0386]                      |
| Data/restraints/parameters                  | 4373/0/248   |
| Goodness-of-fit on F <sup>2</sup>           | 1.039  |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0333, wR <sub>2</sub> = 0.0669                                  |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0461, wR <sub>2</sub> = 0.0722                                  |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.84/-0.69   |

## Compound Ag5

|  |   |
|--|---|
| Identification code                            | ACSAN108Ag_auto   |
| Empirical formula                              | C <sub>12</sub> H <sub>16</sub> AgClN <sub>4</sub> O <sub>2</sub> |
| Formula weight                                 | 391.61  |
| Temperature/K                                  | 150   |
| Crystal system                                 | triclinic   |
| Space group                                    | P-1   |
| a/Å  | 7.9251(6)   |
| b/Å  | 8.2653(5)   |
| c/Å  | 12.3614(9)  |
| $\alpha/^\circ$                                | 96.196(6)   |
| $\beta/^\circ$                                 | 100.134(6)  |
| $\gamma/^\circ$                                | 116.471(7)  |
| Volume/Å <sup>3</sup>                          | 697.38(9)   |
| Z  | 2   |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.865   |
| $\mu/\text{mm}^{-1}$                           | 1.643   |
| F(000)   | 392.0   |
| Crystal size/mm <sup>3</sup>                   | 0.07 × 0.05 × 0.03  |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)                              |
| 2 $\Theta$ range for data collection/ $^\circ$ | 5.634 to 58.15  |
| Index ranges                                   | -10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -16 ≤ l ≤ 16                          |
| Reflections collected                          | 5975  |
| Independent reflections                        | 3183 [ $R_{\text{int}}$ = 0.0279, $R_{\text{sigma}}$ = 0.0470]    |
| Data/restraints/parameters                     | 3183/0/184  |
| Goodness-of-fit on F <sup>2</sup>              | 1.080   |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0327, $wR_2$ = 0.0721                                   |
| Final R indexes [all data]                     | $R_1$ = 0.0400, $wR_2$ = 0.0758                                   |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.62/-0.44  |



## Compound Ag6

|  |  |
|--|--|
| Identification code                            | ACSANai03Ac_auto   |
| Empirical formula                              | C <sub>26</sub> H <sub>42</sub> Ag <sub>2</sub> N <sub>8</sub> O <sub>12</sub> |
| Formula weight                                 | 874.41   |
| Temperature/K                                  | 150  |
| Crystal system                                 | triclinic  |
| Space group                                    | P-1  |
| a/Å  | 9.4848(5)  |
| b/Å  | 13.3279(10)  |
| c/Å  | 14.4146(7)   |
| $\alpha/^\circ$                                | 79.084(5)  |
| $\beta/^\circ$                                 | 71.287(5)  |
| $\gamma/^\circ$                                | 75.994(6)  |
| Volume/Å <sup>3</sup>                          | 1662.13(19)  |
| Z  | 2  |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.747  |
| $\mu/\text{mm}^{-1}$                           | 1.250  |
| F(000)   | 888.0  |
| Crystal size/mm <sup>3</sup>                   | 0.09 × 0.06 × 0.03   |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)   |
| 2 $\Theta$ range for data collection/ $^\circ$ | 4.622 to 58.718  |
| Index ranges                                   | -11 ≤ h ≤ 12, -17 ≤ k ≤ 15, -19 ≤ l ≤ 17                                       |
| Reflections collected                          | 14982  |
| Independent reflections                        | 7565 [ $R_{\text{int}}$ = 0.0281, $R_{\text{sigma}}$ = 0.0424]                 |
| Data/restraints/parameters                     | 7565/24/471  |
| Goodness-of-fit on F <sup>2</sup>              | 1.082  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0386, $wR_2$ = 0.0870  |
| Final R indexes [all data]                     | $R_1$ = 0.0489, $wR_2$ = 0.0921  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 1.43/-1.16   |

## Compound Au2

|  |  |
|--|--|
| Identification code                            | ACSANA30AgAu   |
| Empirical formula                              | C <sub>24</sub> H <sub>32</sub> AuF <sub>6</sub> N <sub>8</sub> O <sub>4</sub> P |
| Formula weight                                 | 838.51   |
| Temperature/K                                  | 150  |
| Crystal system                                 | monoclinic   |
| Space group                                    | C2/c   |
| a/Å  | 12.7118(5)   |
| b/Å  | 15.8181(6)   |
| c/Å  | 15.2061(9)   |
| $\alpha/^\circ$                                | 90   |
| $\beta/^\circ$                                 | 108.841(6)   |
| $\gamma/^\circ$                                | 90   |
| Volume/Å <sup>3</sup>                          | 2893.8(3)  |
| Z  | 4  |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.925  |
| $\mu/\text{mm}^{-1}$                           | 5.225  |
| F(000)   | 1648.0   |
| Crystal size/mm <sup>3</sup>                   | 0.2 × 0.07 × 0.03  |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)   |
| 2 $\Theta$ range for data collection/ $^\circ$ | 4.462 to 58.878  |
| Index ranges                                   | -16 ≤ h ≤ 17, -19 ≤ k ≤ 21, -20 ≤ l ≤ 20   |
| Reflections collected                          | 6895   |
| Independent reflections                        | 3400 [ $R_{\text{int}}$ = 0.0283, $R_{\text{sigma}}$ = 0.0515]                   |
| Data/restraints/parameters                     | 3400/0/204   |
| Goodness-of-fit on F <sup>2</sup>              | 1.055  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0520, $wR_2$ = 0.1141  |
| Final R indexes [all data]                     | $R_1$ = 0.0744, $wR_2$ = 0.1343  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 1.82/-2.75   |

## Compound Au4

|                                   |  |                          |
|-----------------------------------|--|--------------------------|
| Identification code               | 16120  |                          |
| Empirical formula                 | C <sub>11</sub> H <sub>14</sub> Au I N <sub>4</sub> O <sub>2</sub> |                          |
| Color                             | yellow   |                          |
| Formula weight                    | 558.13 g · mol <sup>-1</sup>                                       |                          |
| Temperature                       | 100(2) K   |                          |
| Wavelength                        | 0.71073 Å  |                          |
| Crystal system                    | MONOCLINIC   |                          |
| Space group                       | <b>P2<sub>1</sub>/c, (no. 14)</b>                                  |                          |
| Unit cell dimensions              | a = 10.4598(2) Å   | α = 90°.                 |
|                                   | b = 15.8718(3) Å   | β = 93.7910(10)°.        |
|                                   | c = 8.50610(10) Å  | γ = 90°.                 |
| Volume                            | 1409.06(4) Å <sup>3</sup>  |                          |
| Z                                 | 4  |                          |
| Density (calculated)              | 2.631 Mg · m <sup>-3</sup>   |                          |
| Absorption coefficient            | 12.635 mm <sup>-1</sup>  |                          |
| F(000)                            | 1024 e   |                          |
| Crystal size                      | 0.084 x 0.051 x 0.041 mm <sup>3</sup>                              |                          |
| θ range for data collection       | 2.335 to 39.490°.  |                          |
| Index ranges                      | -18 ≤ h ≤ 18, -28 ≤ k ≤ 28, -15 ≤ l ≤ 15                           |                          |
| Reflections collected             | 322802   |                          |
| Independent reflections           | 8445 [R <sub>int</sub> = 0.0634]                                   |                          |
| Reflections with I > 2σ(I)        | 7690   |                          |
| Completeness to θ = 25.242°       | 100.0 %  |                          |
| Absorption correction             | Gaussian   |                          |
| Max. and min. transmission        | 0.75 and 0.54  |                          |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                        |                          |
| Data / restraints / parameters    | 8445 / 0 / 175   |                          |
| Goodness-of-fit on F <sup>2</sup> | 1.039  |                          |
| Final R indices [I > 2σ(I)]       | R <sub>1</sub> = 0.0165  | wR <sup>2</sup> = 0.0372 |
| R indices (all data)              | R <sub>1</sub> = 0.0200  | wR <sup>2</sup> = 0.0382 |
| Largest diff. peak and hole       | 1.8 and -0.8 e · Å <sup>-3</sup>                                   |                          |

## Compound Au5

|   |  |
|---|--|
| Identification code                         | ACsanAiAu05_auto   |
| Empirical formula                           | C <sub>12</sub> H <sub>16</sub> AuIN <sub>4</sub> O <sub>2</sub> |
| Formula weight                              | 572.15   |
| Temperature/K                               | 150  |
| Crystal system                              | monoclinic   |
| Space group                                 | P2 <sub>1</sub> /n   |
| a/Å   | 9.9991(5)  |
| b/Å   | 13.1781(7)   |
| c/Å   | 12.0503(7)   |
| α/°   | 90   |
| β/°   | 98.646(5)  |
| γ/°   | 90   |
| Volume/Å <sup>3</sup>                       | 1569.81(15)  |
| Z   | 4  |
| ρ <sub>calc</sub> /cm <sup>3</sup>          | 2.421  |
| μ/mm <sup>-1</sup>                          | 11.344   |
| F(000)                                      | 1056.0   |
| Crystal size/mm <sup>3</sup>                | 0.11 × 0.08 × 0.06   |
| Radiation                                   | Mo Kα (λ = 0.71073)  |
| 2θ range for data collection/°              | 4.944 to 58.466  |
| Index ranges                                | -13 ≤ h ≤ 12, -10 ≤ k ≤ 17, -16 ≤ l ≤ 16                         |
| Reflections collected                       | 7952   |
| Independent reflections                     | 3660 [R <sub>int</sub> = 0.0285, R <sub>sigma</sub> = 0.0407]    |
| Data/restraints/parameters                  | 3660/66/313  |
| Goodness-of-fit on F <sup>2</sup>           | 1.062  |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0281, wR <sub>2</sub> = 0.0576                |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0362, wR <sub>2</sub> = 0.0625                |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 2.09/-1.12   |

## Compound Pd1

|  |   |
|--|---|
| Identification code                            | ACSANaPd1_full_auto   |
| Empirical formula                              | C <sub>16</sub> H <sub>19</sub> I <sub>2</sub> N <sub>5</sub> O <sub>2</sub> Pd |
| Formula weight                                 | 673.56  |
| Temperature/K                                  | 150   |
| Crystal system                                 | orthorhombic  |
| Space group                                    | P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>                                   |
| a/Å  | 9.1010(3)   |
| b/Å  | 10.3910(4)  |
| c/Å  | 21.9112(6)  |
| $\alpha/^\circ$                                | 90  |
| $\beta/^\circ$                                 | 90  |
| $\gamma/^\circ$                                | 90  |
| Volume/Å <sup>3</sup>                          | 2072.13(12)   |
| Z  | 4   |
| $\rho_{\text{calc}}/\text{g}/\text{cm}^3$      | 2.159   |
| $\mu/\text{mm}^{-1}$                           | 3.895   |
| F(000)   | 1272.0  |
| Crystal size/mm <sup>3</sup>                   | 0.08 × 0.05 × 0.03  |
| Radiation                                      | Mo K $\alpha$ ( $\lambda$ = 0.71073)  |
| 2 $\Theta$ range for data collection/ $^\circ$ | 4.846 to 58.752   |
| Index ranges                                   | -10 ≤ h ≤ 12, -14 ≤ k ≤ 11, -30 ≤ l ≤ 25  |
| Reflections collected                          | 7737  |
| Independent reflections                        | 4443 [ $R_{\text{int}}$ = 0.0220, $R_{\text{sigma}}$ = 0.0384]                  |
| Data/restraints/parameters                     | 4443/0/238  |
| Goodness-of-fit on F <sup>2</sup>              | 1.029   |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0260, $wR_2$ = 0.0489   |
| Final R indexes [all data]                     | $R_1$ = 0.0301, $wR_2$ = 0.0504   |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.61/-0.67  |
| Flack parameter                                | -0.021(18)  |

## Compound Pd2

|   |   |
|---|---|
| Identification code                         | ACSANBiPd02_auto  |
| Empirical formula                           | C <sub>15</sub> H <sub>18</sub> I <sub>3</sub> N <sub>5</sub> O <sub>2</sub> Pd |
| Formula weight                              | 787.44  |
| Temperature/K                               | 150   |
| Crystal system                              | monoclinic  |
| Space group                                 | P2 <sub>1</sub> /c  |
| a/Å   | 8.1355(2)   |
| b/Å   | 10.9028(3)  |
| c/Å   | 24.7444(6)  |
| α/°   | 90  |
| β/°   | 90.296(2)   |
| γ/°   | 90  |
| Volume/Å <sup>3</sup>                       | 2194.79(10)   |
| Z   | 4   |
| ρ <sub>calc</sub> /g/cm <sup>3</sup>        | 2.383   |
| μ/mm <sup>-1</sup>                          | 5.084   |
| F(000)                                      | 1456.0  |
| Crystal size/mm <sup>3</sup>                | 0.06 × 0.02 × 0.02  |
| Radiation                                   | Mo Kα (λ = 0.71073)   |
| 2θ range for data collection/°              | 4.98 to 58.968  |
| Index ranges                                | -10 ≤ h ≤ 6, -14 ≤ k ≤ 14, -33 ≤ l ≤ 33   |
| Reflections collected                       | 12708   |
| Independent reflections                     | 5222 [R <sub>int</sub> = 0.0340, R <sub>sigma</sub> = 0.0487]                   |
| Data/restraints/parameters                  | 5222/0/238  |
| Goodness-of-fit on F <sup>2</sup>           | 1.055   |
| Final R indexes [I >= 2σ (I)]               | R <sub>1</sub> = 0.0404, wR <sub>2</sub> = 0.0824                               |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0605, wR <sub>2</sub> = 0.0906                               |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.98/-1.91  |

## Compound Ag8

|  |  |
|--|--|
| Identification code                            | ACSANT5Ag_auto   |
| Empirical formula                              | C <sub>34</sub> H <sub>40</sub> AgF <sub>6</sub> N <sub>8</sub> O <sub>4</sub> PS <sub>2</sub> |
| Formula weight                                 | 941.70   |
| Temperature/K                                  | 200  |
| Crystal system                                 | monoclinic   |
| Space group                                    | P2 <sub>1</sub> /c   |
| a/Å  | 9.1542(7)  |
| b/Å  | 14.5513(9)   |
| c/Å  | 14.0959(9)   |
| $\alpha/^\circ$                                | 90   |
| $\beta/^\circ$                                 | 91.123(6)  |
| $\gamma/^\circ$                                | 90   |
| Volume/Å <sup>3</sup>                          | 1877.3(2)  |
| Z  | 2  |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.666  |
| $\mu/\text{mm}^{-1}$                           | 0.772  |
| F(000)   | 960.0  |
| Crystal size/mm <sup>3</sup>                   | 0.123 × 0.031 × 0.016  |
| Radiation                                      | MoK $\alpha$ ( $\lambda$ = 0.71073)  |
| 2 $\Theta$ range for data collection/ $^\circ$ | 5.258 to 66.698  |
| Index ranges                                   | -13 ≤ h ≤ 13, -22 ≤ k ≤ 22, -21 ≤ l ≤ 13   |
| Reflections collected                          | 17008  |
| Independent reflections                        | 6819 [ $R_{\text{int}}$ = 0.0301, $R_{\text{sigma}}$ = 0.0377]                                 |
| Data/restraints/parameters                     | 6819/0/259   |
| Goodness-of-fit on F <sup>2</sup>              | 1.032  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0350, $wR_2$ = 0.0848  |
| Final R indexes [all data]                     | $R_1$ = 0.0551, $wR_2$ = 0.0957  |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 0.59/-0.35   |

## Compound Ag9

|                                   |  |                          |
|-----------------------------------|--|--------------------------|
| Identification code               | 16118  |                          |
| Empirical formula                 | C <sub>34</sub> H <sub>40</sub> AgF <sub>6</sub> N <sub>8</sub> O <sub>4</sub> PS <sub>2</sub> |                          |
| Color                             | colourless   |                          |
| Formula weight                    | 941.70   | g · mol <sup>-1</sup>    |
| Temperature                       | 200(2)   | K                        |
| Wavelength                        | 0.71073  | Å                        |
| Crystal system                    | MONOCLINIC   |                          |
| Space group                       | <b>C2/c, (no. 15)</b>  |                          |
| Unit cell dimensions              | a = 11.3414(12) Å  | α = 90°.                 |
|                                   | b = 12.1604(12) Å  | β = 93.703(4)°.          |
|                                   | c = 27.598(3) Å  | γ = 90°.                 |
| Volume                            | 3798.3(7)  | Å <sup>3</sup>           |
| Z                                 | 4  |                          |
| Density (calculated)              | 1.647  | Mg · m <sup>-3</sup>     |
| Absorption coefficient            | 0.763  | mm <sup>-1</sup>         |
| F(000)                            | 1920   | e                        |
| Crystal size                      | 0.081 x 0.062 x 0.014  | mm <sup>3</sup>          |
| θ range for data collection       | 2.458 to 26.507°.  |                          |
| Index ranges                      | -14 ≤ h ≤ 14, -15 ≤ k ≤ 15, -34 ≤ l ≤ 34   |                          |
| Reflections collected             | 81536  |                          |
| Independent reflections           | 3936 [R <sub>int</sub> = 0.1778]   |                          |
| Reflections with I > 2σ(I)        | 2955   |                          |
| Completeness to θ = 25.242°       | 99.9 %   |                          |
| Absorption correction             | Gaussian   |                          |
| Max. and min. transmission        | 1.00 and 0.99  |                          |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>  |                          |
| Data / restraints / parameters    | 3936 / 0 / 267   |                          |
| Goodness-of-fit on F <sup>2</sup> | 1.084  |                          |
| Final R indices [I > 2σ(I)]       | R <sub>1</sub> = 0.0579  | wR <sup>2</sup> = 0.1283 |
| R indices (all data)              | R <sub>1</sub> = 0.0865  | wR <sup>2</sup> = 0.1404 |
| Largest diff. peak and hole       | 0.8 and -0.8   | e · Å <sup>-3</sup>      |



## Compound Ag10

|  |   |
|--|---|
| Identification code                            | 16276final-cpl  |
| Empirical formula                              | C <sub>67.25</sub> H <sub>77</sub> Ag <sub>4</sub> N <sub>10</sub> O <sub>22</sub> S <sub>6</sub> |
| Formula weight                                 | 2001.22   |
| Temperature/K                                  | 100(2)  |
| Crystal system                                 | triclinic   |
| Space group                                    | P-1   |
| a/Å  | 8.1784(3)   |
| b/Å  | 17.3634(7)  |
| c/Å  | 26.8726(10)   |
| $\alpha/^\circ$                                | 99.223(2)   |
| $\beta/^\circ$                                 | 95.638(2)   |
| $\gamma/^\circ$                                | 95.050(2)   |
| Volume/Å <sup>3</sup>                          | 3727.5(2)   |
| Z  | 2   |
| $\rho_{\text{calc}}/\text{cm}^3$               | 1.783   |
| $\mu/\text{mm}^{-1}$                           | 1.286   |
| F(000)   | 2021.0  |
| Crystal size/mm <sup>3</sup>                   | 0.183 × 0.101 × 0.097   |
| Radiation                                      | Mo-K $\alpha$ ( $\lambda$ = 0.71073)  |
| 2 $\Theta$ range for data collection/ $^\circ$ | 2.39 to 66.232  |
| Index ranges                                   | -12 ≤ h ≤ 12, -26 ≤ k ≤ 26, -41 ≤ l ≤ 41  |
| Reflections collected                          | 245098  |
| Independent reflections                        | 28320 [ $R_{\text{int}}$ = 0.0721, $R_{\text{sigma}}$ = 0.0474]                                   |
| Data/restraints/parameters                     | 28320/0/987   |
| Goodness-of-fit on F <sup>2</sup>              | 1.016   |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0391, $wR_2$ = 0.0783   |
| Final R indexes [all data]                     | $R_1$ = 0.0716, $wR_2$ = 0.0884   |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 1.19/-1.78  |