**Supplementary Materials**

Isocyanide π-hole Interactions Supported by Aurophilic Forces

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| **Table S1.**Crystal data and structure refinement for **1**. | |
| Identification code | **1** |
| Empirical formula | C7H3AuCl2IN |
| Formula weight | 495.87 |
| Temperature/K | 100.0(7) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 9.54600(10) |
| b/Å | 4.04860(10) |
| c/Å | 25.7236(4) |
| α/° | 90 |
| β/° | 91.8880(10) |
| γ/° | 90 |
| Volume/Å3 | 993.62(3) |
| Z | 4 |
| ρcalcg/cm3 | 3.315 |
| μ/mm–1 | 56.715 |
| F(000) | 872.0 |
| Crystal size/mm3 | 0.08 × 0.05 × 0.02 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 6.876 to 134.958 |
| Index ranges | –11 ≤ h ≤ 8, –4 ≤ k ≤ 4, –30 ≤ l ≤ 30 |
| Reflections collected | 7902 |
| Independent reflections | 1788 [*R*int = 0.0453, *R*sigma = 0.0355] |
| Data/restraints/parameters | 1788/0/109 |
| Goodness-of-fit on *F*2 | 1.058 |
| Final R indexes [I>=2σ(I)] | *R*1 = 0.0271, w*R*2 = 0.0681 |
| Final R indexes [all data] | *R*1 = 0.0280, w*R*2 = 0.0692 |
| Largest diff. peak/hole / e Å-3 | 1.49/–1.61 |