Gold(III) complexation in the presence of the macropolyhedral hydridoborate cluster $[B_{20}H_{18}]^{2-}$

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SUPPORTING INFORMATION

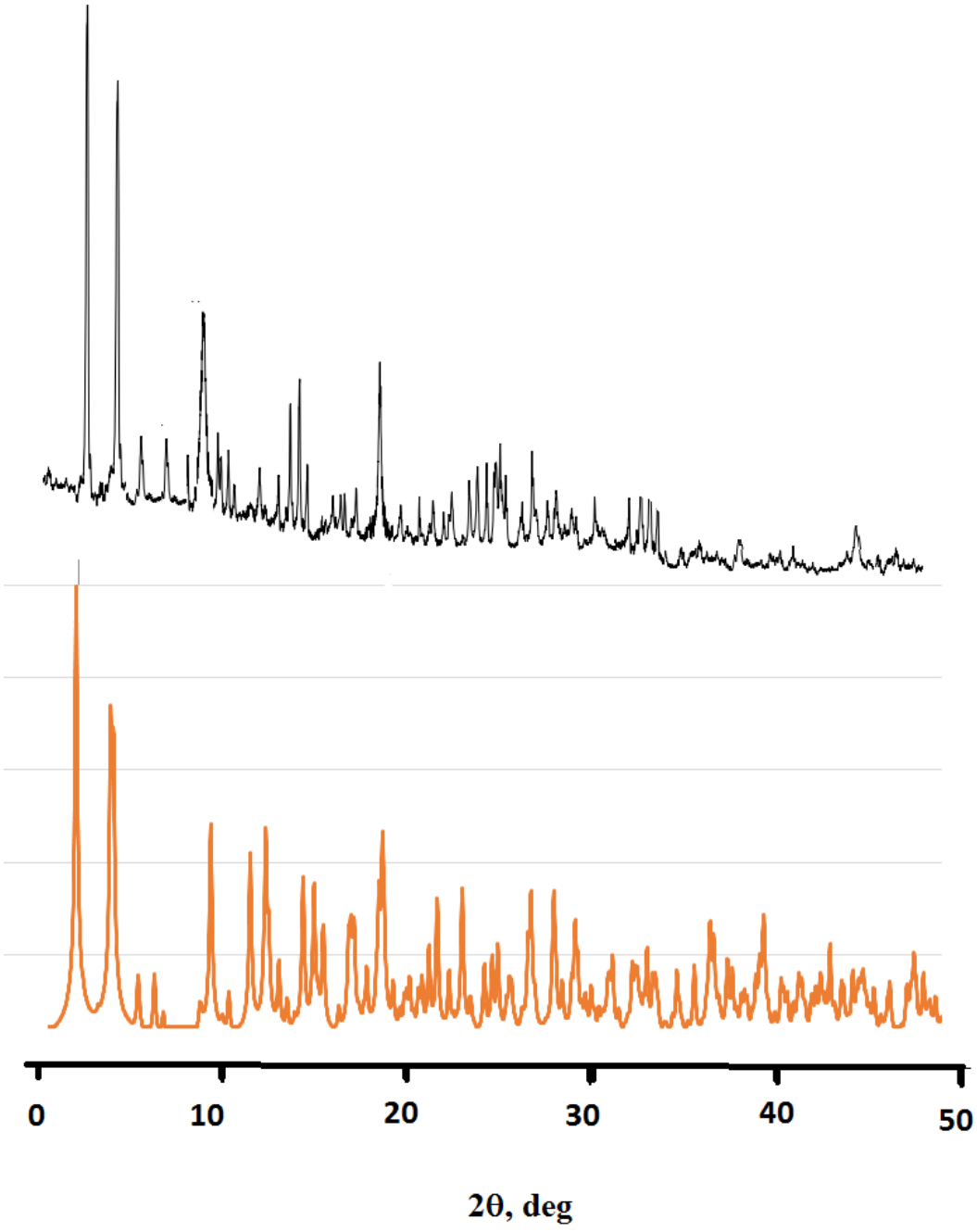

Figure S1. Calculated (orange) and experimental (black) X-ray powder diffraction patterns of complex **1**·2CH_3CN.

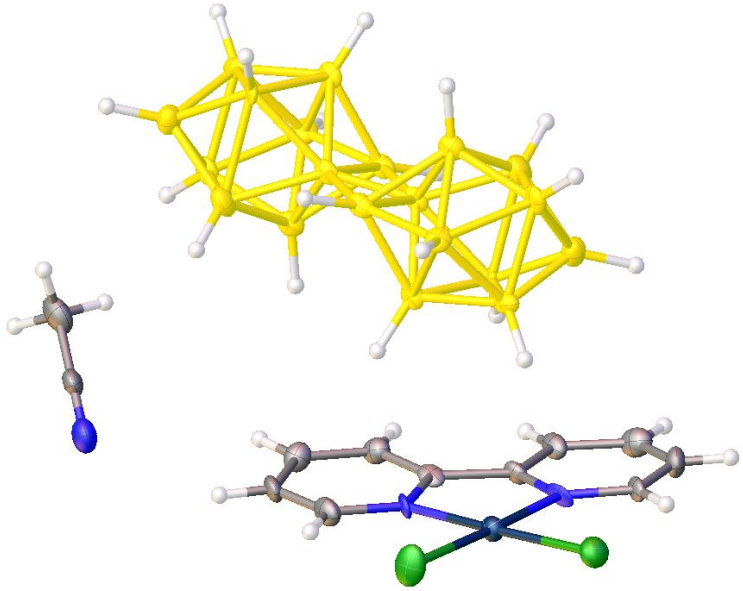

Figure S2. Molecular view of **1**·2CH_3CN in representation of atoms with thermal ellipsoids (p = 50%).

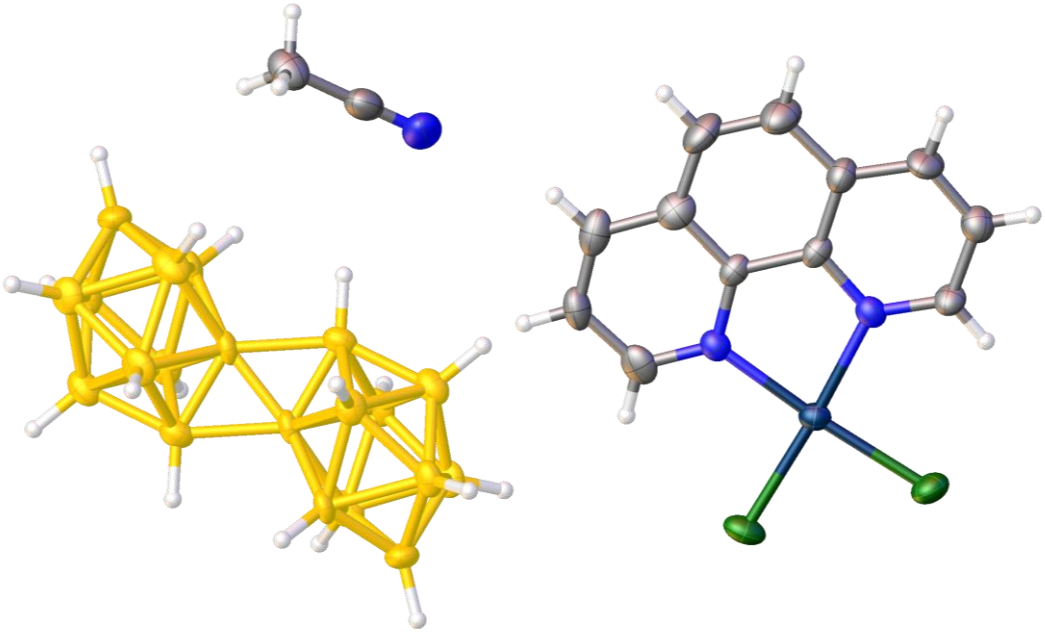

Figure S3. Molecular view of **2**·2CH_3CN in representation of atoms with thermal ellipsoids (*p* = 50%).

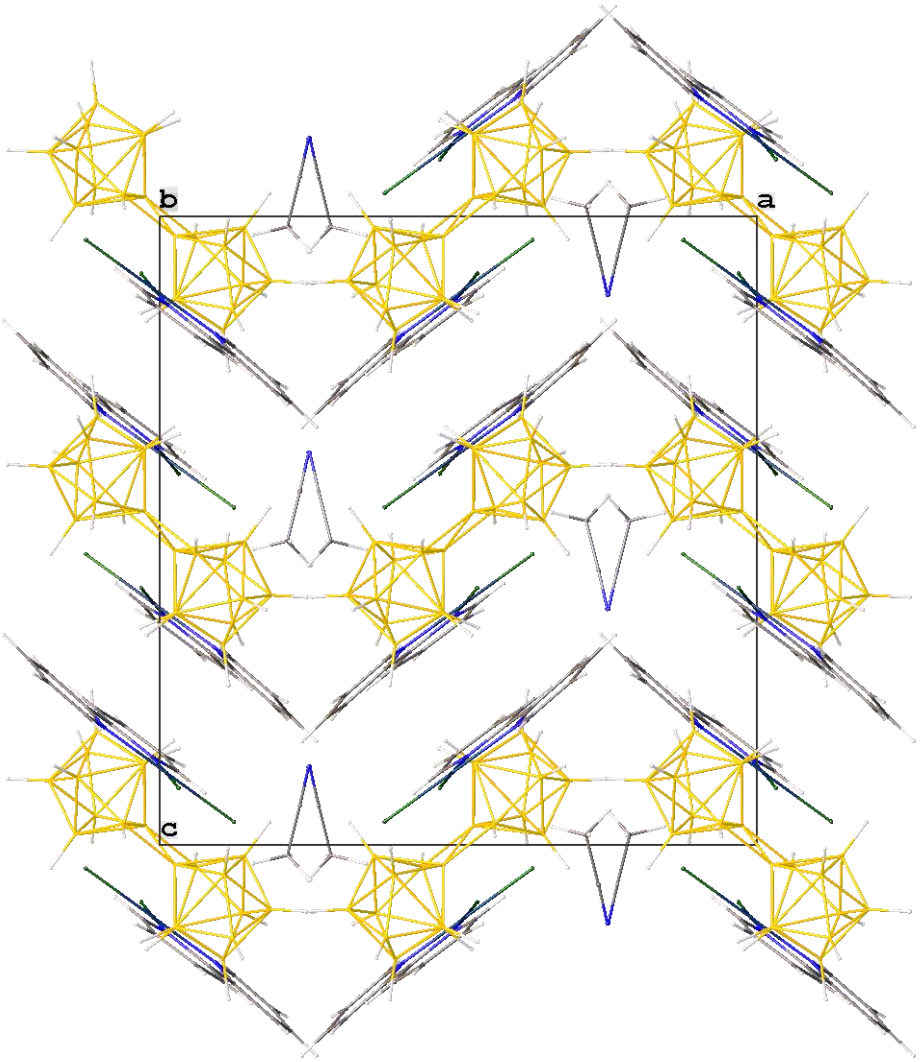

Figure S4. Crystal packing of **1**·2CH_3CN.

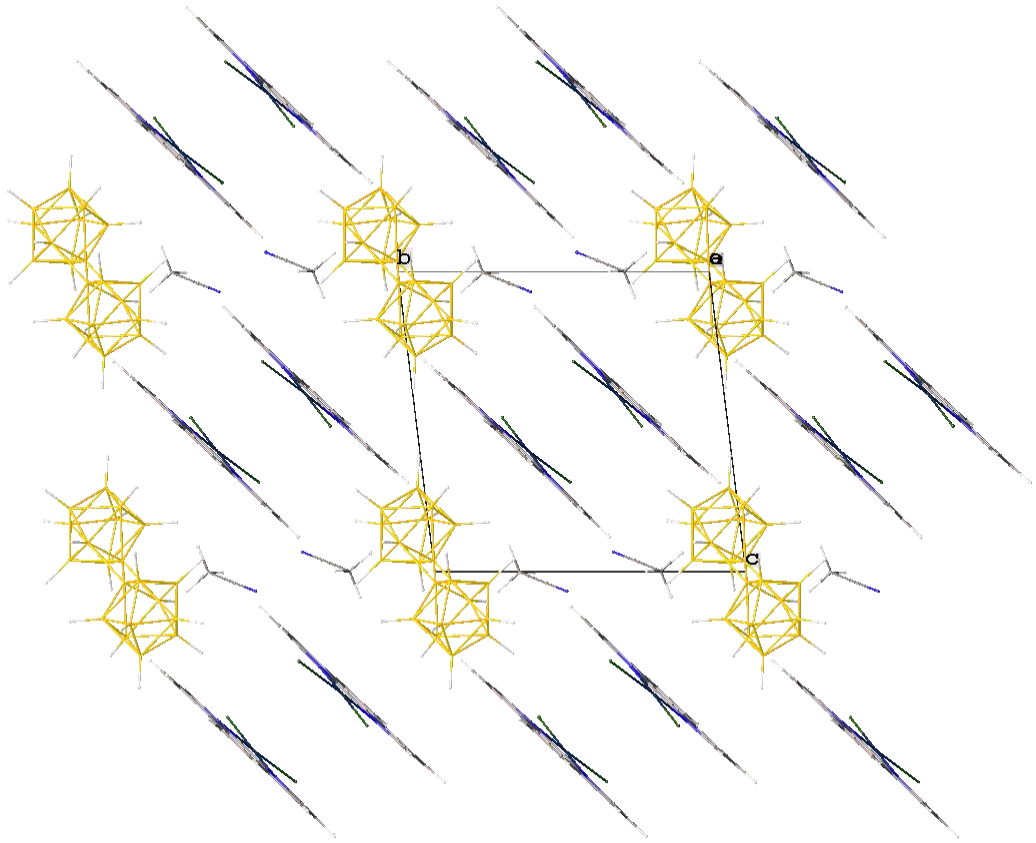

Figure S5. Crystal packing of **2**·2CH_3CN.

Table S1. Crystal structure data and refinement details for **1**·2CH_3CN and **2**·2CH_3CN.

Complex	**1**·2CH_3CN
Composition	$C_{24}H_{40}Au_2B_{20}Cl_4N_6$
F_w	1164.55
Crystal system	orthorhombic
Space group	Pbca
a, Å	15.99(3)
b, Å	15.83(3)
c, Å	16.89(3)
β, °	90
V, Å^3	4276(14)
Z	4
D_{calcd}, g cm^{-3}	1.809
μ(MoK_α), cm^{-1}	7.134
F(000), e	2208
hkl range	$-21 \le h \le 13$
	$-22 \le k \le 20$
	$-24 \le l \le 17$
Refl. measured	17033
Refl. unique	6323
Refl. observed	3519
R_{int}	0.197
Param. refined / constr	254 / 36
$R(F)/wR(F^2)$[a] (I > 2σ(I))	0.060 / 0.134
$R(F)/wR(F^2)$[a] (all refl.)	0.110 / 0.152
GoF (F^2)[b]	0.95
$\Delta\rho_{fin}$ (max/min), e Å^{-3}	5.05/-3.18

[a] R1= ||Fo|–|Fc||/Σ|Fo|, wR2= [Σw(Fo^2–Fc^2)□/Σw(Fo^2)^2]$^{1/2}$, w = [σ^2(Fo^2) +(0.05P)^2]$^{-1}$, where P = (Max(Fo^2, 0) +2Fc^2)/3; [b] GoF = [Σw(Fo^2–Fc^2)^2/(n$_{obs}$ –n$_{param}$)]$^{1/2}$

Contd.

Complex	**2**·2CH_3CN
Composition	$C_{28}H_{40}Au_2B_{20}Cl_4N_6$
F_w	1212.59
Crystal system	triclinic
Space group	P-1
a, Å	10.350(14)
b, Å	10.817(14)
c, Å	11.037(11)
α, °	92.56(5)
β, °	110.69(5)
γ, °	100.88(6)
V, Å^3	1127(2)
Z	1
D_{calcd}, g cm^{-3}	1.787
μ(MoK_α), cm^{-1}	6.772
F(000), e	576.0
hkl range	-12 ≤ h ≤ 12
	-13 ≤ k ≤ 13
	-11 ≤ l ≤ 13
Refl. measured	12068
Refl. unique	4409
Refl. observed	3680
R_{int}	0.0571
Param. refined / constr	254 / 0
$R(F)/wR(F^2)$[a] (I > 2σ(I))	0.0489/ 0.0728
$R(F)/wR(F^2)$[a] (all refl.)	0.0633/ 0.0779
GoF (F^2)[b]	1.135
$\Delta\rho_{fin}$ (max/min), e Å^{-3}	1.73/-2.06

[a] R1= ||Fo|–|Fc||/Σ|Fo|, wR2= [Σw(Fo^2–Fc^2)□/Σw(Fo^2)^2]$^{1/2}$, w = [σ^2(Fo^2) +(0.05P)^2]$^{-1}$, where P = (Max(Fo^2, 0) +2Fc^2)/3; [b] GoF = [Σw(Fo^2–Fc^2)^2/(n$_{obs}$ –n$_{param}$)]$^{1/2}$