Supporting Information for:

H_2 evolution from H_2O via $O\!-\!H$ oxidative addition across a 9,10-diboraanthracene

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General considerations. Unless otherwise noted, all manipulations were carried out using standard Schlenk or glovebox techniques under a N₂ atmosphere. Hexanes, benzene, toluene, and acetonitrile were dried and deoxygenated by argon sparge followed by passage through activated alumina in a solvent purification system from JC Meyer Solvent Systems followed by storage over 4 Å molecular sieves. THF and Et_2O were distilled from sodium-benzophenone ketyl under N_2 followed by storage over 4Å molecular sieves for at least 24 hours prior to use. Non-halogenated and non-nitrile containing solvents were tested with a standard purple solution of sodium benzophenone ketyl in THF to confirm effective oxygen and moisture removal prior to use. All reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. 9,10-bis(2-(diisopropylphosphino)phenyl)-9,10-dihydroboranthrene (B_2P_2), $[Au(B_2P_2)]Cl$, and $[Au(B_2P_2)][K(18-c-6)]$ were synthesized according to literature procedures.¹ Distilled H_2O used for the synthesis of **2**, **2-H₂O**, **4** and **5** was degassed by sparging with argon 15 minutes prior to use. Triethylamine (NEt₃) was distilled from CaH₂ and stored over 3 Å sieves for 24 hours in the dark prior to use. Elemental analyses were performed by Midwest Microlab, LLC, Indianapolis, IN. Deuterated solvents were purchased from Cambridge Isotope Laboratories Inc., degassed, and dried over activated 3Å molecular sieves for at least 24 h prior to use. NMR spectra were recorded on Varian Inova 500 MHz, Bruker Avance 600 MHz, and Bruker NEO 400 MHz spectrometers. Variable Temperature NMR spectra were collected on a Bruker Avance 600 MHz spectrometer that had been pre-referenced with an internal thermometer for accurate temperature readings. ¹H and ¹³C chemical shifts are reported in ppm relative to tetramethylsilane using residual solvent as an internal standard.^{2 11}B chemical shifts are reported in ppm relative to BF₃•Et₂O. Original ¹¹B NMR spectra were processed using MestReNova 10.0.2 with a backwardslinear prediction applied to eliminate background signal from the borosilicate NMR tube. For ¹¹B NMR spectra with peaks overlapping the borosilicate signal, a manual baseline correction was applied.³ IR spectra were recorded using a Bruker Alpha FT-IR with a universal sampling module collecting at 4 cm⁻¹ resolution with 32 scans. Variable temperature dynamic exchange constants were simulated using Spinworks (V4.2.0, Copyright © 2015, Kirk Marat, University of Manitoba) with the DNMR3 simulation module.⁴

X-Ray Crystallography. Single crystals were coated with paratone oil and mounted on cryo-loop glass fibers. X-ray intensity data were collected at 100(2) K on a Bruker APEX2⁵ platform-CCD X-ray diffractometer system using fine-focus Mo K_α radiation ($\lambda = 0.71073$ Å, 50kV/30mA power). The CCD detector was placed at 5.0600 cm from the crystal. Frames were integrated using the Bruker SAINT software package⁶ and using a narrow-frame integration algorithm. Absorption corrections were applied to the raw intensity data using the SADABS program.⁷ The Bruker SHELXTL software package⁸ was used for phase determination and structure refinement. Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms were refined by means of a full matrix least-squares procedure on F^2 . The H-atoms were included in the refinement in calculated positions riding on the atoms to which they were attached. Relevant details for individual data collections are reported in Tables S1–S4.

Synthetic Procedures

Au(B₂P₂)OH (2). [Au(B₂P₂)]Cl (1) (0.028 g, 0.035 mmol) was suspended in toluene (4 mL) before adding H₂O (1.9 μ L, 0.11 mmol) followed by NEt₃ (17 μ L, 0.12 mmol) which resulted in the precipitation of a colorless solid over 30 minutes. The reaction was filtered through celite, concentrated *in vacuo* (ca. 1 mL) and added hexanes (3 mL) to precipitate the product. The product was rinsed with hexanes (2 x 1 mL) and dried *in vacuo*. Yield: 0.024 g, 89%. X-ray quality

crystals were grown by layering a concentrated toluene solution with hexanes. ¹H NMR (500 MHz, C_6D_6) δ 8.71 (d, J = 5.7 Hz, 2H), 7.80 (t, J = 6.9 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.30 (m, 2H), 7.08 (m, 4H), 6.88 (m, 4H), 2.05 (m, 4H), 0.82 (d, J = 7.2 Hz, 6H), 0.79 (d, J = 7.2 Hz, 6H), 0.64 (d, J = 7.9 Hz, 6H), 0.61 (d, J = 8.0 Hz, 6H). ³¹P{¹H} NMR (242 MHz, C_6D_6 , 25 °C) δ 48.52 (s). ³¹P NMR (243 MHz, toluene- d_8 , -45 °C) δ 47.47 (d, J = 242.3 Hz), 50.32 (d, J = 241.7 Hz).

¹¹B{¹H} NMR (193 MHz, toluene- d_8 , -45 °C) δ 36.4, -5.6. ¹³C{¹H} NMR (126 MHz, C₆D₆) δ 168.0, 156.9, 135.3, 134.0, 133.4, 131.2, 129.9, 126.7, 124.8, 27.3 (t, *J* = 12.9 Hz), 21.4, 19.3. FT-IR: v_{max} cm⁻¹3662 (OH). MALDI MS Found: m/z 774.2784; Calcd. 774.2797.

Au(B₂P₂)(OH)(H₂O) (2-H₂O). A solution of **2** (0.020 g, 0.026 mmol) in benzene (0.6 mL) was added H₂O (14 µl, 0.39 mmol). The mixture was sonicated and let stand 2 days during which time colorless solid precipitated. The solid was rinsed with n-pentane (1 mL) and briefly dried via N₂ stream for 3 minutes before dissolving the solid in CD₃CN and collected NMR spectra. X-Ray quality crystals of **2-H₂O** were grown by letting a saturated solution as prepared above stand for 3 days. ¹H NMR (400 MHz, CD₃CN) δ 8.13 (d, *J* = 6.3 Hz, 2H), 7.70 – 7.58 (m, 4H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.08 (s, 8H), 2.57 – 2.43 (m, 4H), 2.22 (s, 3H), 0.94 (q, *J* = 7.9 Hz,, 12H), 0.76 (q, *J* = 7.9 Hz, 12H). ³¹P NMR (162 MHz, CD₃CN) δ 48.03 (s). ¹¹B{¹H} NMR (128 MHz, CD₃CN) δ 6.57. Due to the sensitivity of this compound to vacuum, elemental analysis was not obtained.

Reversibility of water binding to 2. A sample of $2-H_2O$ was prepared as described above. Volatiles were then removed from the sample *in vacuo* for 15 minutes (10^{-2} mbar), and the residue was dissolved in C₆D₆ (0.6 mL). The resulting spectrum showed pure **2**. Crystals grown from this material were examined by XRD and confirmed to be **2**.

[Au(B₂P₂)(OH)₂][K(18-c-6)] (4). [Au(B₂P₂)][K(18-c-6)] (**3**) (0.020 g, 0.019 mmol) was dissolved in toluene (4 mL) before adding H₂O (0.72 μL, 0.040 mmol). The reaction was stirred 30 minutes where it became colorless. Volatiles were removed *in vacuo* to yield the product as a colorless solid. Yield: 0.19 g, 92%. X-ray quality crystals and samples suitable for elemental analysis were obtained by layering a concentrated benzene solution with hexanes. ¹H NMR (400 MHz, C₆D₆) δ 9.22 (dd, *J* = 7.6, 1.7 Hz, 2H), 7.84 (t, *J* = 7.7 Hz, 2H), 7.54 (dt, *J* = 8.5, 4.3 Hz, 2H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.25 (dd, *J* = 5.3, 3.4 Hz, 4H), 7.07 (dd, *J* = 5.3, 3.3 Hz, 4H), 3.19 (s, 24H), 2.49 – 2.29 (m, 4H), 1.06 (d, *J* = 7.0 Hz, 6H), 1.02 (d, *J* = 7.0 Hz, 6H), 0.89 (d, *J* = 7.4 Hz, 6H), 0.85 (d, *J* = 7.2 Hz, 6H). ³¹P{¹H</sup> NMR (202 MHz, C₆D₆) δ 45.46 (s).¹¹B{¹H} NMR (128 MHz, C₆D₆) δ -1.10 (s). ¹³C NMR (151 MHz, C₆D₆) δ 174.00, 160.75, 136.32, 135.12, 134.96, 132.63, 131.03, 124.63, 123.72, 69.99, 26.76 (t, *J* = 12.8 Hz), 22.58, 19.00. FT-IR: *v*_{max} cm⁻¹ 3943 (O-H). Anal. Calcd for C₄₈H₇₀AuB₂KO₈P₂: C, 52.66 H, 6.45. Found: C, 53.15 H, 6.25.

[Au(B₂P₂)(H)(OH)][K(18-c-6)] (5). [Au(B₂P₂)][K(18-c-6)] (**3**) (0.020 g, 0.019 mmol) was dissolved in THF (1 mL) before adding a solution of water (0.34 μL, 0.019 mmol) in THF (2 mL) dropwise over 5 minutes at 0 °C. The reaction was stirred 30 minutes where it became colorless. The reaction was concentrated *in vacuo* (ca. 0.3 mL) and added pentane (2 mL) before being placed at -35 °C overnight. The next day, colorless crystals had formed that were decanted from the mother liquor, rinsed with hexanes (ca. 1 mL) and dried *in vacuo* to yield **4** in ~80 % purity (as judged by ³¹P NMR) with the sole byproduct being **5**. X-ray quality crystals were grown by layering a concentrated benzene solution with hexanes. ¹H NMR (400 MHz, C₆D₆) δ 9.24 (dd, *J* = 7.3, 3.3 Hz, 1H), 8.58 (s, 1H), 7.83 (t, *J* = 7.1 Hz, 1H), 7.70 (t, *J* = 7.2 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.3 Hz, 2H), 7.31 (d, *J* = 6.9 Hz, 2H), 7.23 (d, *J* = 6.7 Hz, 2H), 7.11 (t, *J* = 6.6 Hz, 2H), 7.06 (t, *J* = 6.5 Hz, 2H), 4.57 – 3.81 (4-line signal, *J*_{B-H} = 72.0 Hz, 1H), 3.13 (s, 24H), 2.39 (tq, *J* = 14.2, 7.0

Hz, 4H), 1.05 (dt, J = 13.2, 6.4 Hz, 12H), 0.92 (d, J = 3.4 Hz, 3H), 0.91 (d, J = 3.4 Hz, 3H), 0.88 (d, J = 3.7 Hz, 3H), 0.86 (d, J = 3.7 Hz, 3H). ³¹P NMR (162 MHz, C₆D₆) δ 48.27 (d, J = 276.9 Hz). ¹¹B NMR (128 MHz, C₆D₆) δ -0.85, -9.73 (d, J = 75.7 Hz). ¹³C NMR (151 MHz, C₆D₆) δ 175.5, 161.6, 159.8, 143.3 (d, J = 14.9 Hz), 136.3, 136.2, 135.5, 135.3, 134.1, 133.8, 133.2, 132.6, 132.2, 131.3 (d, J = 29.3 Hz), 124.6, 124.0, 123.5 (d, J = 6.3 Hz), 123.0, 70.0, 27.0 (d, J = 7.3 Hz), 26.8 (d, J = 6.9 Hz), 22.5 (d, J = 7.7 Hz), 22.4 (d, J = 7.7 Hz), 19.2, 19.1. FT-IR: v_{max} cm⁻¹ 3643 (O-H), 2130 (B-H). As this compound could only be generated in ~80% purity as judged by NMR, elemental analysis data would have been misleading and was not collected.



Figure S1. ¹H NMR spectra of 0.2 M Au(B_2P_2)Cl (**1**) in CD₃CN:D₂O solvent mixtures over variable time periods. Spectra 5-1 are of a 0.2 M solution of pure **1** in 5) CD₃CN with no D₂O 4) CD₃CN:D₂O (4:1) after 15 minutes, 3) CD₃CN:D₂O (4:1) after 14 hours 2) CD₃CN:D₂O (4:1) after 34 hours and, 1) CD₃CN:D₂O (2:1) after 72 hours.



Figure S2. ³¹P NMR spectra of 0.2 M Au(B_2P_2)Cl (1) in CD₃CN:D₂O solvent mixtures over variable time periods. Spectra 5-1 are of a 0.2 M solution of pure 1 in 5) CD₃CN with no D₂O 4) CD₃CN:D₂O (4:1) after 15 minutes, 3) CD₃CN:D₂O (4:1) after 14 hours 2) CD₃CN:D₂O (4:1) after 34 hours and, 1) CD₃CN:D₂O (2:1) after 72 hours.



Figure S4. ³¹P NMR spectrum of $Au(B_2P_2)OH$ (2) recorded at 242 MHz in C_6D_6 .



Figure S5. ³¹P VT-NMR spectra of Au(B_2P_2)OH (**2**) recorded at 242 MHz in toluene- d_8 . Spectra 10-1 were collected at 22, 0, -5, -12, -15, -18, -22, -25, -29 and -45 °C, respectively.



Figure S6. 13 C NMR spectrum of Au(B₂P₂)OH (2) recorded at 126 MHz in C₆D₆.



Figure S7. ¹H NMR spectrum of Au(B_2P_2)OH (**2**) recorded at 600 MHz in toluene- d_8 at -45 °C.





Figure S9. ¹¹B NMR spectrum of Au(B_2P_2)OH (2) recorded at 242 MHz in toluene- d_8 at -45° C.



Figure S10. ³¹P NMR spectra used to calculate Guttman-Becket acceptor numbers (ANs) of $Au(B_2P_2)Cl(1)$, $Au(B_2P_2)OH(2)$, $[Au(B_2P_2)][BAr^F_4]$ and pure triethylphosphine oxide listed from 4-1, respectively. All spectra were recorded at 242 MHz in THF- d_8 at 23° C.





Figure S12. ³¹P NMR spectrum of $Au(B_2P_2)(OH)(H_2O)$ (2-H₂O) recorded at 162 MHz in CD₃CN.



Figure S13. ¹¹B NMR spectrum of Au(B₂P₂)(OH)(H₂O) (2-H₂O) recorded at 128 MHz in CD₃CN.



Figure S14. ¹H NMR spectrum of $[Au(B_2P_2)(H)(OH)][K(18-c-6)]$ (5) recorded at 400 MHz in C₆D₆.



Figure S16. ¹¹B NMR spectrum of $[Au(B_2P_2)(H)(OH)][K(18-c-6)]$ (5) recorded at 128 MHz in C₆D₆.



Figure S18. ¹H NMR spectrum of $[Au(B_2P_2)(OH)_2][K(18-c-6)]$ (4) recorded at 400 MHz in C_6D_6 .



Figure S20. ¹¹B NMR spectrum of [Au(B₂P₂)(OH)₂][K(18-c-6)] (4) recorded at 128 MHz in C₆D₆.



Figure S21. ¹³C NMR spectrum of $[Au(B_2P_2)(OH)_2][K(18-c-6)]$ (4) recorded at 151 MHz in C_6D_6





freq. of 0 ppm: 242.835682 MHz processed size: 16384 complex points LB: 3.000 GF: 0.0000 Hz/cm: 90.069 ppm/cm: 0.37089

Figure S22. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at 22 °C and its simulation (top).



Figure S23. VT-³¹P NMR spectrum of Au(B_2P_2)OH (2) recorded at 242 MHz in toluene- d_8 at 0 °C and its simulation (top).

SpinWorks 4: 6-47-AuB2P2OH_VT_-5C_coaexps-31P-dtol-9_25_17



Figure S24. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at -5 °C and its simulation (top).



Figure S25. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at -12 °C and its simulation (top).

SpinWorks 4: 6-47-AuB2P2OH_VT_-15C-31P-dtol-9_25_17



Figure S26. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at -15 °C and its simulation (top).



Figure S27. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at –18 °C and its simulation (top).





Figure S28. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at -22 °C and its simulation (top).



Figure S29. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at –25 °C and its simulation (top).





Figure S30. VT-³¹P NMR spectrum of Au(B_2P_2)OH (**2**) (bottom) recorded at 242 MHz in toluene- d_8 at -45 °C and its simulation (top).



Figure S31. Eyring plot constructed from the simulated rates calculated from VT-³¹P NMR measurements of Au(B_2P_2)OH (**2**) in toluene- d_8 . The slope, intercept and R² value are inlayed and were used to extract thermal parameters of activation.



Figure S32. FT-IR spectrum of Au(B₂P₂)OH (2).



Figure S33. FT-IR spectrum of [Au(B₂P₂)(H)(OH)][K(18-c-6)] (5).



Figure S34. FT-IR spectrum of [Au(B₂P₂)(OH)₂][K(18-c-6)] (4).



Figure S35. Labelled thermal ellipsoid plot (50%) for $Au(B_2P_2)OH$ (2).



Figure S36. Labelled thermal ellipsoid plot (50%) for $Au(B_2P_2)(OH)(H_2O)$ (2-H₂O).



Figure S37. Labelled thermal ellipsoid plot (50%) for $[Au(B_2P_2)(H)(OH)][K(18-c-6)]$ (5).



Figure S38. Labelled thermal ellipsoid plot (50%) for $[Au(B_2P_2)(OH)_2][K(18-c-6)]$ (4).

Table S1. Crystal data and structure refinement for $Au(B_2P_2)OH(2)$.

Identification code	hh246JT122r_0m	
Empirical formula	$G_{36}H_{45}AuB_2OP_2$	
Formula weight	774.24 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	<i>a</i> = 19.5549(3) Å	α = 90°.
	<i>b</i> = 17.1275(3) Å	<i>β</i> = 90°.
	<i>c</i> = 19.6848(3) Å	γ = 90°.
Volume	6592.96(18) Å ³	
Z	8	
Density (calculated)	1.560 mg/m ³	
Absorption coefficient	4.588 mm ⁻¹	
F(000)	3104	
Crystal size	0.368 x 0.302 x 0.198 mm ³	
artheta range for data collection	1.889 to 30.506°.	
Index ranges	$-27 \le h \le 27, -24 \le k \le 24, -28 \le l \le 28$	
Reflections collected	236655	
Independent reflections	10069 [<i>R</i> _{int} = 0.0290]	
Completeness to ϑ = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10069 / 0 / 388	
Goodness-of-fit on F ²	1.053	
Final R indices $[l > 2\sigma_l]$	$R_1 = 0.0148, wR_2 = 0.0344$	
R indices (all data)	$R_1 = 0.0203, wR_2 = 0.0369$	
Largest diff. peak and hole	0.733 and –0.305 e/Å ³	

Table S2. Crystal data and structure refinement for $[Au(B_2P_2)](OH)(H_2O)$ (2-H₂O).

Identification code	hh232JT116_0m	
Empirical formula	$C_{45}H_{56}AuB_2O_2P_2$	
Formula weight	909.42 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	<i>a</i> = 11.1923(3) Å	$\alpha = 84.3144(5)^{\circ}.$
	<i>b</i> = 13.0857(4) Å	$\beta = 74.4558(5)^{\circ}.$
	<i>c</i> = 15.6457(5) Å	$\gamma = 68.8762(5)^{\circ}.$
Volume	2059.29(11) Å ³	
Z	2	
Density (calculated)	1.467 mg/m ³	
Absorption coefficient	3.686 mm ⁻¹	
F(000)	922	
Crystal size	0.484 x 0.343 x 0.211 mm ³	
artheta range for data collection	1.668 to 28.282°.	
Index ranges	$-14 \le h \le 14, -17 \le k \le 17, -20 \le l \le 20$	
Reflections collected	42609	
Independent reflections	10216 [<i>R</i> _{int} = 0.0150]	
Completeness to ϑ = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	10216 / 493 / 559	
Goodness-of-fit on F ²	1.058	
Final R indices $[l > 2\sigma_l]$	R1 = 0.0137, wR2 = 0.0345	
R indices (all data)	R1 = 0.0145, wR2 = 0.0347	
Largest diff. peak and hole	1.164 and –0.398 e/Å ³	

Table S3. Crystal data and structure refinement for $[Au(B_2P_2)(H)(OH)][K(18-c-6)]$ (5).

Identification code	hh264JT130	
Empirical formula	C ₄₈ H _{69.47} AuB ₂ KO _{7.53} P ₂	
Formula weight	1086.53 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	<i>a</i> = 11.5721(3) Å	$\alpha = 77.4593(5)^{\circ}.$
	<i>b</i> = 13.3494(4) Å	$\beta = 77.1738(5)^{\circ}.$
	<i>c</i> = 17.4347(5) Å	$\gamma = 68.9764(5)^{\circ}.$
Volume	2423.17(12) Å ³	
Ζ	2	
Density (calculated)	1.489 mg/m ³	
Absorption coefficient	3.237 mm ⁻¹	
F(000)	1111	
Crystal size	0.442 x 0.355 x 0.336 mm ³	
artheta range for data collection	1.653 to 28.282°	
Index ranges	–15 ≤ h ≤ 15, –17 ≤ k ≤ 17, –23 ≤ l ≤ 23	
Reflections collected	84102	
Independent reflections	12016 [<i>R</i> _{int} = 0.0197]	
Completeness to ϑ = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	12016 / 1216 / 923	
Goodness-of-fit on F ²	1.076	
Final R indices $[l > 2\sigma_l]$	$R_1 = 0.0141, wR_2 = 0.0355$	
<i>R</i> indices (all data, 0.75 Å)	$R_1 = 0.0148, wR_2 = 0.0357$	
Largest diff. peak and hole	0.607 and –0.558 e/Å ³	
Final <i>R</i> indices [<i>l</i> > 2σ _i] <i>R</i> indices (all data, 0.75 Å) Largest diff. peak and hole	$R_1 = 0.0141, wR_2 = 0.0355$ $R_1 = 0.0148, wR_2 = 0.0357$ $0.607 \text{ and } -0.558 \text{ e/Å}^3$	

Table S4. Crystal data and structure refinement for $[Au(B_2P_2)(OH)_2][K(18-c-6)]$ (4).

hh207JT102_0m	
$C_{53}H_{81}AuB_2KO_{8.50}P_2$	
1173.80 g/mol	
100(2) K	
0.71073 Å	
Monoclinic	
P 21/n	
<i>a</i> = 12.4601(4) Å	<i>α</i> = 90°.
<i>b</i> = 27.1704(10) Å	$\beta = 94.0898(6)^{\circ}.$
<i>c</i> = 16.4408(6) Å	γ = 90°.
5551.8(3) Å ³	
4	
1.404 mg/m ³	
2.833 mm ⁻¹	
2420	
0.425 x 0.339 x 0.115 mm ³	
1.499 to 29.130°.	
–17 ≤ h ≤ 17, –37 ≤ k ≤ 37, –22 ≤ l ≤ 22	
121598	
14933 [<i>R</i> _{int} = 0.0320]	
100.0 %	
Semi-empirical from equivalents	
Full-matrix least-squares on <i>F</i> ²	
14933 / 472 / 700	
1.055	
$R_1 = 0.0213, wR_2 = 0.0479$	
$R_1 = 0.0264, wR_2 = 0.0498$	
0.815 and –1.115 e/ų	
	hh207JT102_0m $C_{53}H_{81}AuB_2KO_{8.50}P_2$ 1173.80 g/mol 100(2) K 0.71073 Å Monoclinic P 21/n a = 12.4601(4) Å b = 27.1704(10) Å c = 16.4408(6) Å 5551.8(3) Å ³ 4 1.404 mg/m ³ 2.833 mm ⁻¹ 2420 0.425 x 0.339 x 0.115 mm ³ 1.499 to 29.130°. $-17 \le h \le 17, -37 \le k \le 37, -21$ 121598 14933 [$R_{int} = 0.0320$] 100.0 % Semi-empirical from equival Full-matrix least-squares on 14933 / 472 / 700 1.055 $R_1 = 0.0213, wR_2 = 0.0479$ $R_1 = 0.0264, wR_2 = 0.0498$ 0.815 and $-1.115 e/Å^3$

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