Supporting information

Luminescence responsive intracluster rearrangements of gold(I)-silver(I) clusters triggered by acetonitrile

Xiao-Yun Liu,[a] Yang Yang,[a] Zhen Lei,[a] Zong-Jie Guan[a] and Quan-Ming Wang*[a,b]

[a]Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, P. R. China;

[b]Department of Chemistry, Tsinghua University, Beijing, 100084, P. R. China

E-mail:qmwang@xmu.edu.cn

Contents

I. Experimental detail

II. X-ray Crystallography

III. PXRD measurements

IV. Theoretical calculations

V. Synthesis

VI. Supporting Figures

Figure S1. ^{1}H NMR spectrum of **2-bromo-4-(dimethoxymethyl)pyridine** in $CDCl_3$

Figure S2. ^{1}H NMR spectrum of $\mathbf{L^1}$ in $CDCl_3$

Figure S3. ^{31}P NMR spectrum of $\mathbf{L^1}$ in $CDCl_3$

Figure S4. FT-ICR MS spectrum of $\mathbf{L^1}$ in MeCN solution

Figure S5. ^{1}H NMR spectrum of $\mathbf{[O(AuL^1)_3Ag_1]BF_4}$ in CD_2Cl_2

Figure S6. ^{31}P NMR spectrum of $\mathbf{[O(AuL^1)_3Ag_1]BF_4}$ in CD_2Cl_2

Figure S7. ESI-MS spectrum of $\mathbf{[O(AuL^1)_3Ag_1]BF_4}$ in CH_2Cl_2/MeOH solution

Figure S8. ^{1}H NMR spectrum of $\mathbf{[(C)Au_6Ag_2(L^1)_6](BF_4)_4}$ in CD_2Cl_2

Figure S9. ^{31}P NMR spectrum of $\mathbf{[(C)Au_6Ag_2(L^1)_6](BF_4)_4}$ in CD_2Cl_2

Figure S10. ESI-MS spectrum of $\mathbf{[(C)Au_6Ag_2(L^1)_6](BF_4)_4}$ in CH_2Cl_2/MeOH solution

Figure S11. ^{1}H NMR spectrum of **1** in CD_3CN

Figure S12. ^{31}P NMR spectrum of **1** in CD_3CN

Figure S13. ESI-MS spectrum of **1** in MeCN solution

Figure S14. UV-Vis spectra of **2a** in MeOH and **2b** in MeOH

Figure S15. ESI-MS spectrum of **2a** in MeOH solution

Figure S16. Measured (black trace) and simulated (red trace) isotopic pattems of **2a**

Figure S17. ^{1}H NMR spectrum of **2a** in CD_3OD

Figure S18. ^{1}H NMR spectrum of **2b** in CD_3OD

Figure S19. ^{31}P NMR spectrum of **2a** in CD_3OD

Figure S20. ^{31}P NMR spectrum of **2b** in CD_3OD

Figure S21. ^{1}H NMR spectrum of **2a** in CD_3OD at different concentration

Figure S22. Diffuse reflectance spectra of solid **2a** and **2b**

Figure S23. IR spectra of **2a** and **2b**

Figure S24. Excitation and emission spectra of **2a** in the solid state at room temperature

Figure S25. Excitation and emission spectra of **2b** in the solid state at room temperature

Figure S26. Excitation and emission spectra of **2a** in the solid state at 77K

Figure S27. Excitation and emission spectra of **2b** in the solid state at 77K

Figure S28. Emission spectra of **2a** and **2b** solution (V_{MeOH}:V_{EtOH}=9:1, glass phase) at 77K (420 nm excitation)

Figure S29. Emission spectra in MeOH (2.0×10^{-3} M) at different temperature (excited by 420 nm).

Figure S30. The radio of two isomers in MeOH solution (2.0×10^{-3} M) at different temperature

Figure S31. Luminescence decay profiles of **2a** in solid state at room temperature

Figure S32. Luminescence decay profiles of **2b** in solid state at room temperature

Figure S33. Luminescence decay profiles of **2a** in MeOH at room temperature

Figure S34. Luminescence decay profiles of **2b** in MeOH at room temperature

Figure S35. Molecular structure of **2b** and solvent moleculars

Figure S36. HOMOs and LUMOs of **2a** and **2b**

Table S1. Luminescence data of two isomers at different temperature

Table S2. Coordinate file of **2a**

Table S3. Coordinate file of **2b**

Table S4. Coordinate file of **2a** with MeOH

Table S5. Coordinate file of **2b** with MeOH

Table S6. Coordinate file of **2a** with MeCN

Table S7. Coordinate file of **2b** with MeCN

I. Experimental detail

The C, H, N microanalyses were carried out with a CE instruments EA 1110 elemental analyzer. Luminescence was measured on a Hitachi F-7000 spectrometer. Lifetime and quantum yield were measured on an Edinburgh Analytical Instrument F980. The FT-IR spectra were recorded from KBr pellets in the range 4000-400 cm^{-1} with a Nicolet AVATAR FT-IR360 spectrometer. UV-Vis spectra were recorded on a UV2550 UV-VIS-NIR Spectrophotometer. NMR data were recorded on a Bruker Avance II spectrometer (400 MHz) and Avance III spectrometer (500MHz). Chemical shifts, δ, are reported relative to the external standard 85% H_3PO_4 for ^{31}P NMR. Mass spectrum was recorded on an ESI-TOF-MS spectrometer.

II . X-ray Crystallography

Intensity diffraction data of **2a** were collected on an Agilent SuperNova X-Ray diffractometer using X-ray sources (Mo Kα, λ = 0.71073 Å) at 100K. Intensity diffraction data of **2b** were collected on an Agilent SuperNova X-Ray diffractometer using X-ray sources (Cu Kα, λ = 1.54184 Å) at 100K. Absorption corrections were applied by using the program CrysAlis (multi-scan). A face absorption correction has been performed with **2a** using CrysAlispro 171.37.34. The structures were solved by direct methods. Non-hydrogen atoms except solvent molecules, counteranions and the central carbon atoms of **2a, 2b** were refined anisotropically by least-squares on F_2 using the SHELXTL program. The hydrogen atoms of organic ligands were generated geometrically, while no attempt was made to locate hydrogen atoms of solvent molecules. The counter-anions were not resolved because of the weak data and high symmetry of **2b**. The correct chemical formula reported in CIF includes counter-ions for charge balance. This resulted in two false B level alerts in checkCIF warning that the calculated and reported molecular weights have large difference. The crystals have large solvent accessible voids since a large number of disordered solvent molecules and counter-anions were not resolved.

III. PXRD measurements

Powder X-ray diffraction diagrams (PXRD) were recorded on a Rigaku Ultima IV X-ray diffractometer (35 KV, 15 mA) with CuKα radiation (λ = 0.154056 nm). The calculated diagram obtained from the single crystal data was generated with Mercury software. The raw data of diffraction patterns was treated with the Jade software. Freshly prepared **2a** and **2b** were gently grinded before measurement. After **2a** was soaked with MeCN, the measurement was carried out when the excess MeCN was removed.

Ⅳ. Theoretical calculations

The theoretical calculations were performed with DMol[3] program. The Perdew, Burke and Ernzerh functionals in combination with the generalized gradient approximation (GGA-PBE)[1] was considered in density functional calculations. And the effective core potentials double numerical basis set plus polarization functions (DNP) were used for C, H, O, P, Ag, Au.[2,3]

The structure optimizations have been performed. The two isomers do not represent the only minima.

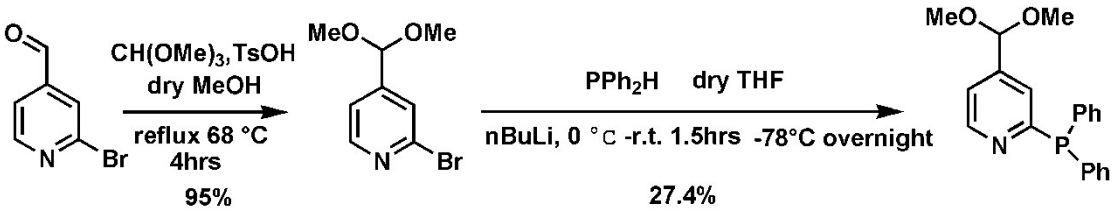
Reference

1 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, 77, 3865-3868.

2 B. Delley, *J. Chem. Phys.*, 1990, 92, 508-517.

3 B. Delley, *Int. J. Quantum Chem.*, 1998, 69, 423-433.

V. Synthesis



Scheme *S 1* Synthesis of L^1

Synthesis of L^1: 4-(dimethoxymethyl)-6-(diphenylphosphino)pyridine

This compound was prepared in a synthetic procedure similar to that of 2-(diphenylphosphino)-5-(dimethoxymethyl)pyridine.

$[C(AuL^1)_6Ag_2](BF_4)_4$ and $[C(AuL^2)_6Ag_2](BF_4)_4$ (**1**) were prepared according to literature methods.

(a) 2-bromo-4-(dimethoxymethyl)pyridine

To a flask 2-Bromo-4-pyridinecarboxaldehyde (10 g, 54.2 mmol), p-toluenesulphonic acid (204 mg, cat.) and trimethylorthoformate (25 mL) were added and sparged with nitrogen. 100 ml dry methanol was injected. The mixture was refluxed at 68°C for 4 hours. After cooling down, 80 ml dichloromethane was added, and then washed with sat.Na_2CO_3 and water. The aqueous layer was extracted with dichloromethane. The combined organic solution was washed with brine, dried with $MgSO_4$ and evaporated to yield a yellow oil (11.9 g, 95%).

^{1}H NMR (400.1 MHz; $CDCl_3$; ppm): δ8.27 (d, J = 5.2 Hz, H = 1, 6-Py), 7.50 (s, H = 1, 3-Py), 7.25 (d, J = 5.2 Hz, H = 1, 5-Py), 5.28 (s, H = 1, C*H*$(OMe)_2$), 3.26 (s, H = 6, -OMe). ^{13}C NMR (100.6 MHz, $CDCl_3$, ppm): δ150.13, 149.76, 142.43, 126.19, 120.86, 100.24, 52.65.

(b) L^1: 2-(diphenylphosphino)-4-(dimethoxymethyl)pyridine

A solution of diphenylphosphine (12.0 mL, 69.2 mmol) in dry THF (80 mL) was cooled to 0 °C in ice water bath. n-BuLi (43.2ml 1.6 M in hexanes, 69.2 mmol) was

injected dropwise over 15 min. The resulted solution was stirred in the bath for 90 min without additional ice to yield a dark red solution. To another flask sparged with nitrogen 2-bromo-4-(dimethoxymethyl)pyridine (8.0 g, 34.5 mmol) and THF (40 ml) were added. Both flasks were cooled to -78 °C. The solution of 2-bromo-4-(dimethoxymethyl)pyridine was slowly injected into the PPh_2Li solution. The reaction mixture was further stirred overnight and allowed to warm up to room temperature. All the next workup was operated with deoxygenated solvents under nitrogen atmosphere. The reaction was stopped by adding water and ester. The aqueous layer was separated and extracted with diethyl ether. The combined organic solution was washed with brine and dried with Na_2SO_4. The final solution was concentrated under reduced pressure to give the crude product, which was purified by flash column chromatography on silica gel (ethyl acetate : hexane = 15 : 85) to afford a pale yellow oil (8.20 g, 71%).

^{1}H NMR (400.1 MHz, $CDCl_3$, ppm): δ8.72 (d, J = 4.8 Hz, H = 1, 6-Py), δ7.30-7.43 (m, H = 10, Ph), 7.27 (d, J = 4.8 Hz, H = 1, 5-Py), 7.20 (s, H = 1, 3-Py), 5.26 (s, H = 1, C*H*$(OMe)_2$), 3.25 (s, H = 6, -OMe). ^{13}C NMR (100.6 MHz, $CDCl_3$, ppm): δ164.16 (d, J_{C-P} = 2.7 Hz), 150.53 (d, J_{C-P} = 11.9 Hz), 146.24 (d, J_{C-P} = 3.0 Hz), 136.20 (d, J_{C-P} = 10.4 Hz), 134.18 (d, J_{C-P} = 19.6 Hz), 129.10, 128.61 (d, J_{C-P} = 7.2 Hz), 125.98 (d, J_{C-P} = 18.6 Hz), 120.29, 101.31, 52.71. ^{31}P NMR (162 MHz, $CDCl_3$, ppm): δ-1.46 (s).

FT-ICR-MS-ESI (MeCN) calculated for $C_{20}H_{21}NO_2P$ $[MH]^+$ m/z: 338.1304; found m/z: 338.1316.

(c) Synthesis of $[O(Au\ L^1)_3Ag]BF_4$

To a solution of L^1 (400 mg, 1.19 mmol) in CH_2Cl_2, $Au(Me_2S)Cl$ (350 mg, 1.19 mmol) was added. After stirring for 20 minutes, the solution was evaporated to dryness to afford a white solid. The white solid was then dissolved with 30 ml acetone. Freshly prepared Ag_2O (605 mg, 2.61 mmol) was added into the above solution, followed by $NaBF_4$ (746 mg 6.78 mmol) and $AgBF_4$ (232 mg, 1.19 mmol). The mixture was stirred for 3 h in the dark before acetone was removed. The solid residue was extracted with CH_2Cl_2 (3×20 ml). The combined solution was concentrated to a

dark brown oil under reduced pressure, which was triturated with ether to afford dark brown solid (407 mg, 54%).

^{1}H NMR (500.2 MHz; CD_2Cl_2; ppm): δ7.83 (broad, H = 3, 6-Py), 7.41-7.57 (m, H = 30, Ph), 7.21 (broad, H = 3, 6-Py), 7.14 (broad, H = 3, 5-Py), 5.28 (s, H = 3, C*H*$(OMe)_2$), 3.33 (s, H = 18, -OMe). ^{13}C NMR (125.8 MHz, CD_2Cl_2, ppm): δ154.14, 153.64, 152.80, 150.90, 133.99, 133.62, 130.19, 128.50, 125.93, 100.74, 53.88. ^{31}P NMR (202.5MHz, CD_2Cl_2, ppm): δ29.50 (s).

ESI-MS (CH_2Cl_2/MeOH=1:4(V:V)): $[AuL]^+$, m/z(%)=534.1 (100%); $[AuL_2]^+$, m/z(%)=871.1 (55.9%).

Anal. Calcd. for $C_{60}H_{60}B_2N_3F_8P_3AgAu_3O_7 \cdot CH_2Cl_2$ (%): C36.90; H 3.15; N 2.12. Found: C 36.93; H 3.57; N 2.01.

(d) Synthesis of $[(C)Au_6Ag_2(L^1)_6](BF_4)_4$

Redistilled Et_3N (25 μl, 0.2 mmol) was added to a solution of $[O(AuL)_3Ag]BF_4$ (340 mg, 0.2 mmol) in dry dichloromethane (6 ml), followed by Me_3SiCHN_2 (100 μl, 2M hexane solution, 0.2 mmol) . After stirring in dark for 3 h, excess $AgBF_4$ (39 mg, in 0.5 ml MeOH, 0.2 mmol) was added. The resulting solution was further stirred for 1 h before filtration. The filtrate was transferred to a tube, and ether was layered on it. After two weeks, yellow-green block crystals (147 mg, 39%) deposited on the glass wall.

^{1}H NMR (400.1 MHz; CD_2Cl_2; ppm): δ7.89 (d, J = 5.2 Hz, H = 6, 6-Py), 7.51 (t, J_{H-H} = 6.0 Hz, H = 12, *p*-Ph), 7.40 (t, J_{H-H} = 8.8 Hz, H = 24, *o*-Ph), 7.28 (t, J_{H-H} = 5.2 Hz, H = 24, *m*-Ph), 7.24 (s, H = 6, *3*-py), 7.14(d, J_{H-H} = 5.2 Hz, H = 6, 5-py), 5.26 (s, H = 3, C*H*$(OMe)_2$), 3.33 (s, H = 18, -OMe). ^{13}C NMR (100.6 MHz, CD_2Cl_2, ppm): δ154.14, 153.64, 152.80, 150.90, 133.99, 133.62, 130.19, 128.50, 125.93, 100.74, 53.88. ^{31}P NMR (162MHz, CD_2Cl_2, ppm): δ32.99 (s).

ESI-MS (CH_2Cl_2/MeOH=1:4(V:V)): $[AuL_2]^+$, m/z(%) = 871.3(100); $[AuL]^+$, m/z(%) = 534.2(14.2%); $[CAu_6Ag_2\ L_6]^{4+}$, m/z(%) = 858.6(15.6%); $[CAu_6Ag\ L_6]^{3+}$, m/z(%) = 1108.4(40.1%).

Anal. Calcd. for $C_{121}H_{120}B_4N_6F_{16}P_6Ag_2Au_6O_{12} \cdot 2CH_2Cl_2$ (%): C37.39; H 3.16; N 2.13.

Found: C 37.37; H 3.72; N 2.36.

(e) Synthesis of $[(C)Au_6Ag_2(L^2)_6](BF_4)_4$ (1)

To a flask containing $[(C)Au_6Ag_2(L^1)_6](BF_4)_4$ (300 mg, 79.5 mmol) was added 1.5 mL of trifluoracetic acid. The solution was strired at room temperature for 24 h, then diluted with 1 mL of dichloromethane and filtered. The filtrate was added into a thin tube, and diethyl ether was layered on it. Green-yellow crystals (213 mg) were obtained in 1 week. Yield: 76%.

^{1}H NMR(500.2 MHz, CD_3CN, ppm): δ9.90 (s, H=6, -CHO), δ7.96 (broad, H = 6, 6-Py), δ7.59 (s, H = 6, 3-py), δ7.49 (t, H = 24, *o*-Ph), δ7.41 (t, H = 12, *p*-Ph), δ7.35(d, H = 6, 5-py), δ7.19(t, H=24, *m*-Ph)

^{13}C NMR(125.8 MHz, CD_3CN, ppm): δ191.85, 156.95, 156.29, 155.59, 143.65, 135.71, 134.30, 131.04, 129.30, 126.48.

^{31}P NMR(162 MHz, CD_3CN, ppm): δ33.28 (s).

ESI-MS (MeCN):[$CAu_6Ag_2(L^2)_6]^{4+}$, *m/z* =789.52; $[CAu_6Ag_1(L^2)_6]^{3+}$, *m/z* =1416.39; $[CAu_6(L^2)_6]^{2+}$, *m/z* =1470.15; $[CAu_6(L^2)_6AgBF_4]^{2+}$, *m/z* =1568.09.

Anal. Calcd. for $C_{109}H_{84}B_4N_6F_{16}P_6Ag_2Au_6O_6$ $10H_2O$（%）: C, 35.53; H, 2.844; N: 2.280. Found: C, 35.47; H, 2.635; N, 2.488;

(f) Synthesis of $[(C)Au_6Ag_2(L^3)_6](BF_4)_4$ (2a)

1 (35 mg, 10 mmol) was added 2 mL of acetone and 60 μL30% H_2O_2 was injected, The mixture was stirred at room temperature for 48 h before the solvent was removed. The solid residue was extracted with 2 mL MeOH, and the solution was filtered. The filtrate was added into a thin tube, and diethyl ether was layered on it. Yellow block crystal(27 mg) were obtained after about 2 weeks. Yield: 76%.

IR(KBr):ν =1727 cm^{-1} (C=O). Lifetime: τ_1 = 1.09±0.06 μs (24.93%), τ_2 = 3.75±0.03 μs (75.07%) in the solid state. Quantum yield (solid state): 36%.

^{1}H NMR(500.2 MHz, CD_3OD, ppm): δ7.87 (d, H=6, 6-Py), δ7.74 (s, H = 6, 3-Py), δ7.49-7.43, (broad, H = 42, *o*-Ph+ *p*-Ph+5-Py), δ7.30 (broad, H=24, *m*-Ph).

^{13}C NMR(125.8 MHz, CD_3CN, ppm): δ167.21, 155.83, 155.29, 146.29, 135.53, 134.88 131.53, 131.18, 128.08, 127.04.

^{31}P NMR(162 MHz, CD_3OD, ppm): δ33.55 (s).

ESI-MS (MeOH):[$CAu_6(L^3)_6Ag_1]^{3+}$, *m/z*=1048.39; $[CAu_6(L^3)_5Ag_1(L^3\text{-}H)_1]^{2+}$, *m/z*=1572.08; $[CAu_6(L^3)_4Ag_1(L^3\text{-}H)_2Na]^{2+}$, *m/z*=1583.07; $[CAu_6(L^3)_3Ag_1(L^3\text{-}H)_3Na_2]^{2+}$, *m/z*=1594.06; $[CAu_6(L^3)_4Ag_2(L^3\text{-}H)_2]^{2+}$, *m/z*=1625.02.

Anal. Calcd. for $C_{109}H_{84}B_4N_6O_{12}F_{16}P_6Ag_2Au_6$ $4H_2O$ (%): C, 35.64; H, 2.524; N , 2.288. Found : C, 35.66; H, 2.794; N, 2.488.

(g) Synthesis of $[(C)Au_6Ag_2(L^3)_6](BF_4)_4$ (2b)

Compound **2a** (40.0 mg, 11.4 mmol) was dissolved in 2 mL of MeOH in a thin tube, and MeCN was layered on it. Red crystals (10.5mg) were obtained after about 1 week. Yield: 26%.

IR(KBr):ν =1727 cm^{-1} (C=O). Lifetime: τ_1 = 1.34±0.02 μs (62.81%), τ_2 = 3.23±0.04 μs (37.19%) in the solid state. Quantum yield (solid state): 42%.

^{1}H NMR(500.2 MHz, CD_3OD, ppm): δ7.87 (d, H=6, 6-Py), δ7.74 (s, H = 6, 3-Py), δ7.49-7.43, (broad, H = 42, *o*-Ph+ *p*-Ph+5-Py), δ7.30 (broad, H=24, *m*-Ph).

^{31}P NMR(162 MHz, CD_3OD, ppm): δ33.56 (s)

Anal. Calcd. for $C_{109}H_{84}B_4N_6O_{12}F_{16}P_6Ag_2Au_6$ MeCN (%): C, 36.53; H, 2.463; N: 2.688. Found: C, 37.42; H, 2.728; N, 2.554.

VI. Supporting Figures

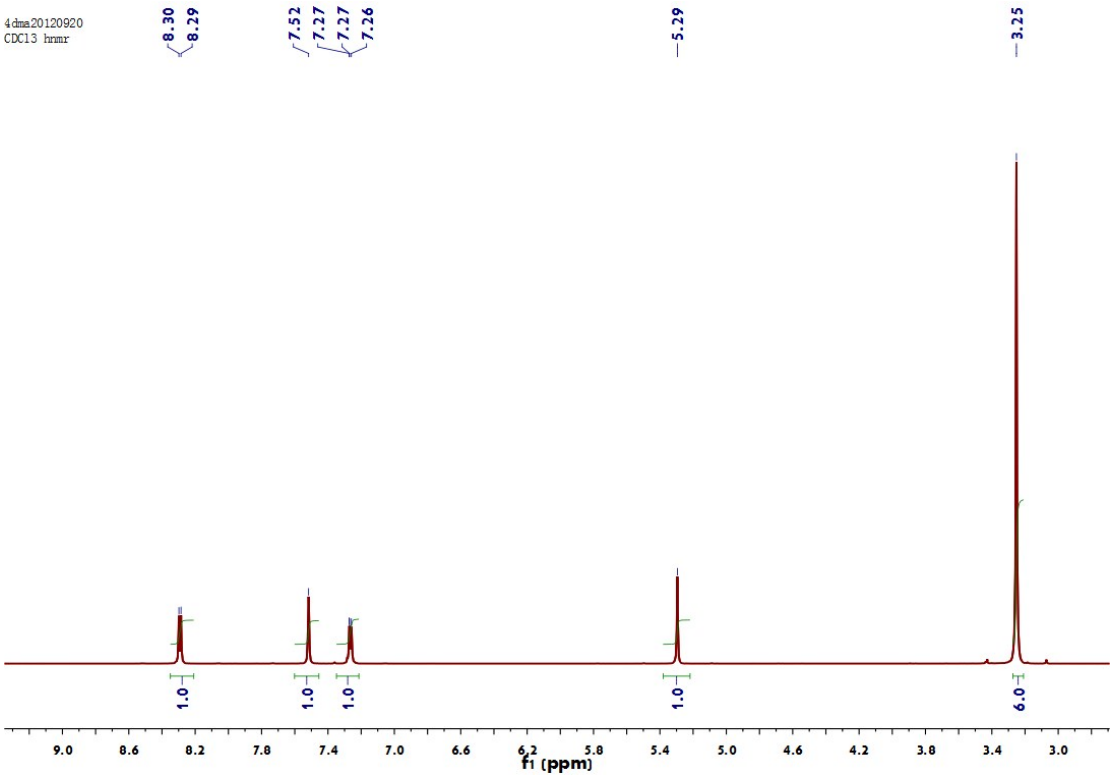


Figure S1. ^{1}H NMR spectrum of **2-bromo-4-(dimethoxymethyl)pyridine** in $CDCl_3$

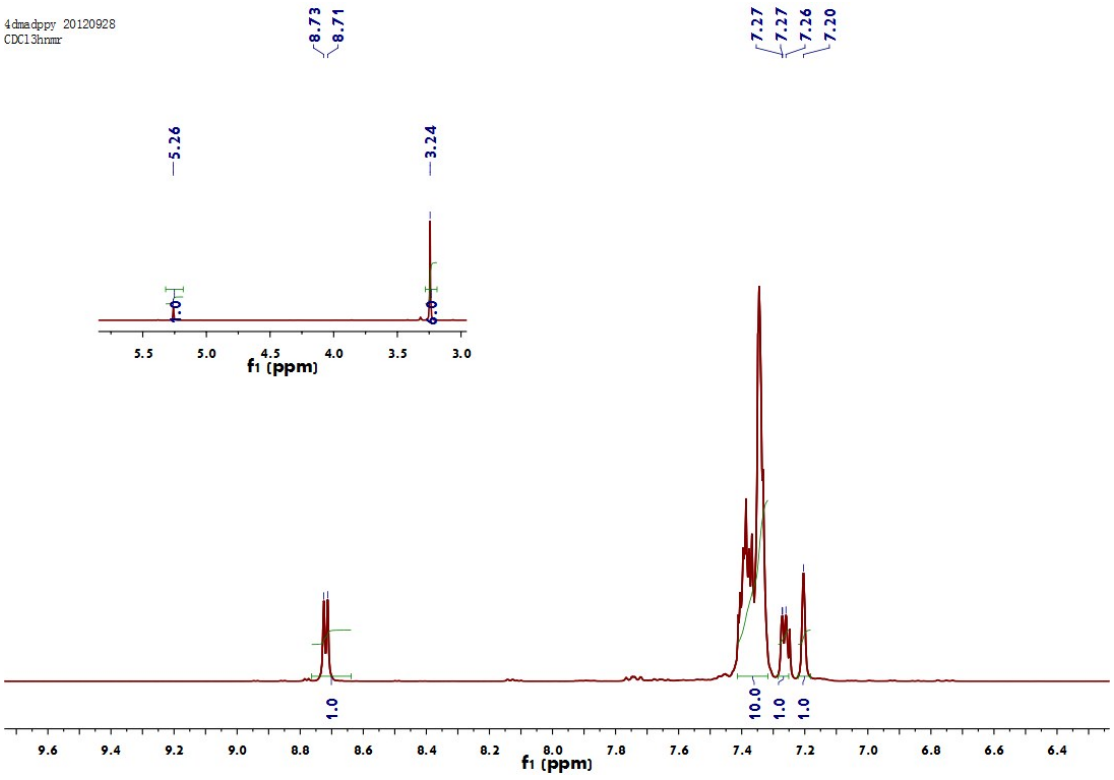


Figure S2. ^{1}H NMR spectrum of $\mathbf{L^1}$ in $CDCl_3$

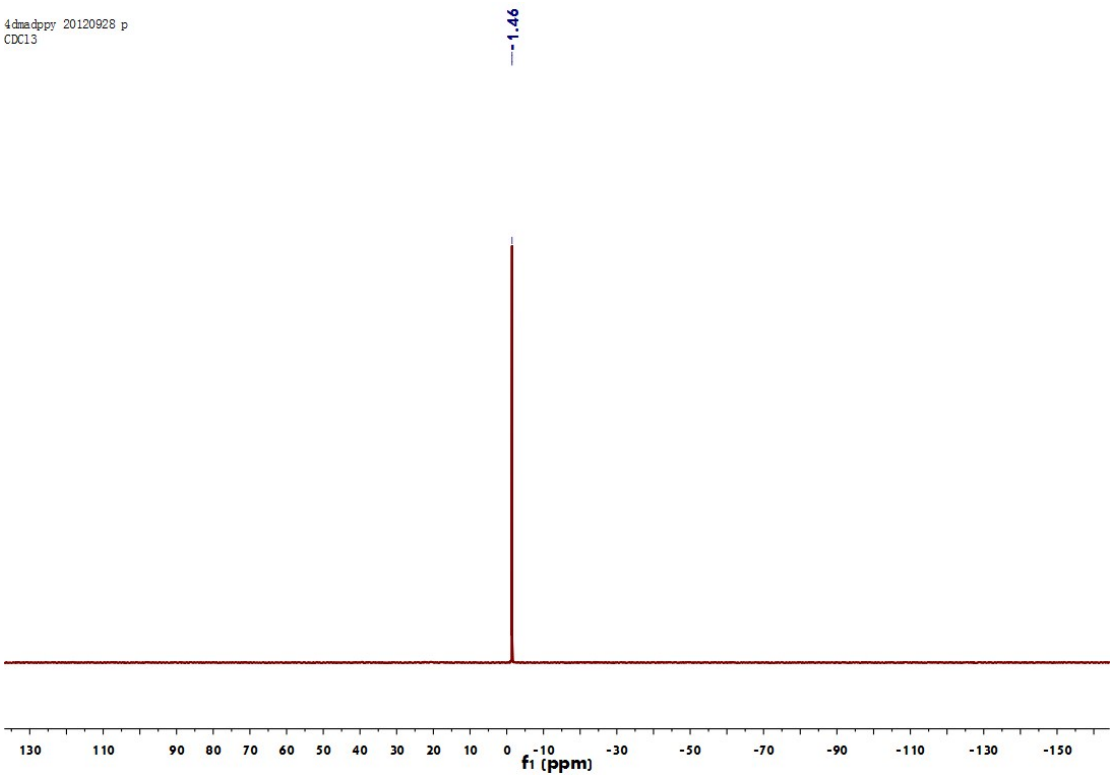


Figure S3. ^{31}P NMR spectrum of $\mathbf{L^1}$ in $CDCl_3$

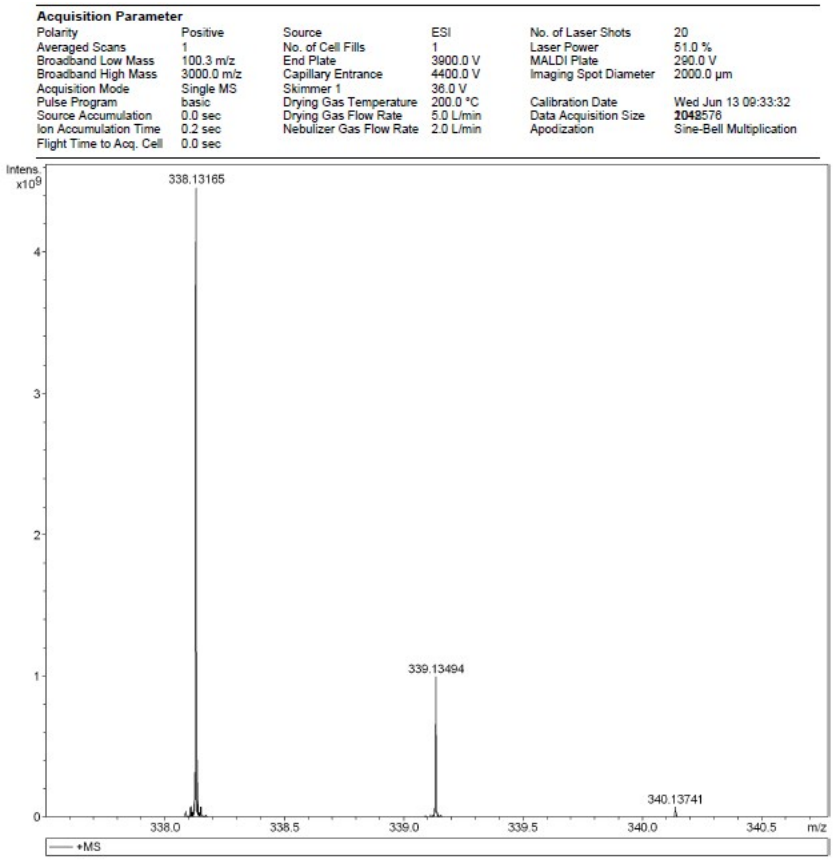


Figure S4. FT-ICR MS spectrum of $\mathbf{L^1}$ in MeCN solution

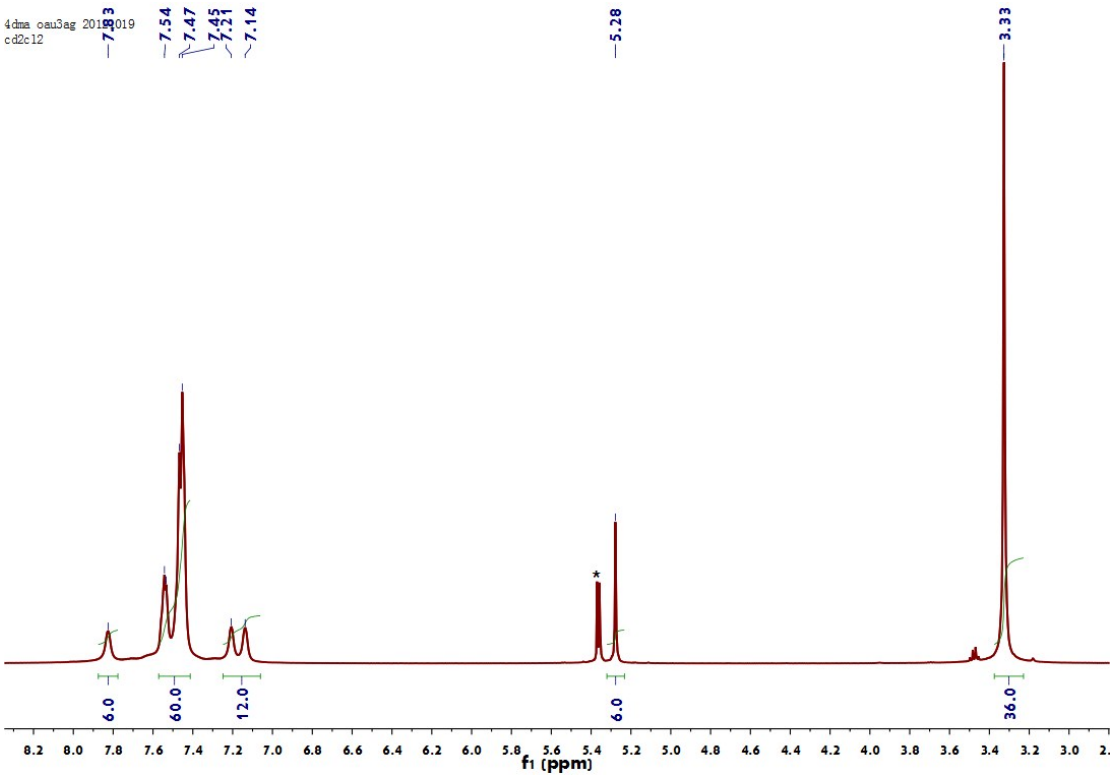


Figure S5. ^{1}H NMR spectrum of **[O(AuL^{1})$_3$Ag$_1$]BF$_4$** in CD_2Cl_2

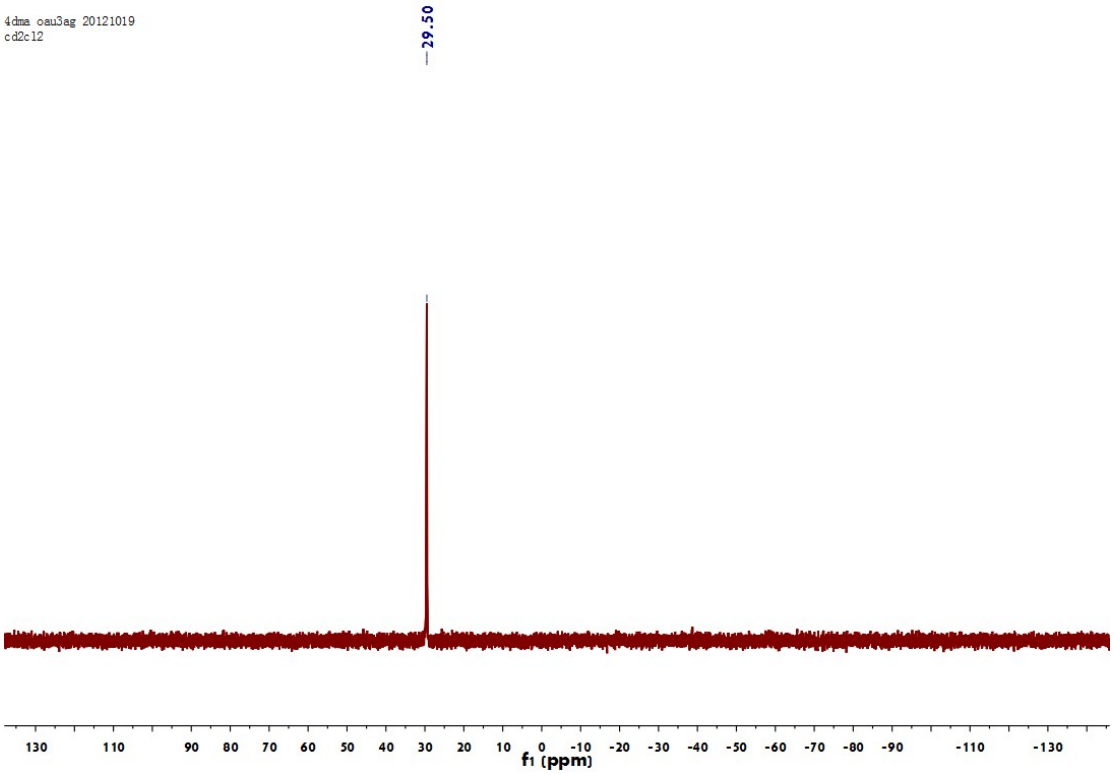


Figure S6. ^{31}P NMR spectrum of **[O(AuL^{1})$_3$Ag$_1$]BF$_4$** in CD_2Cl_2

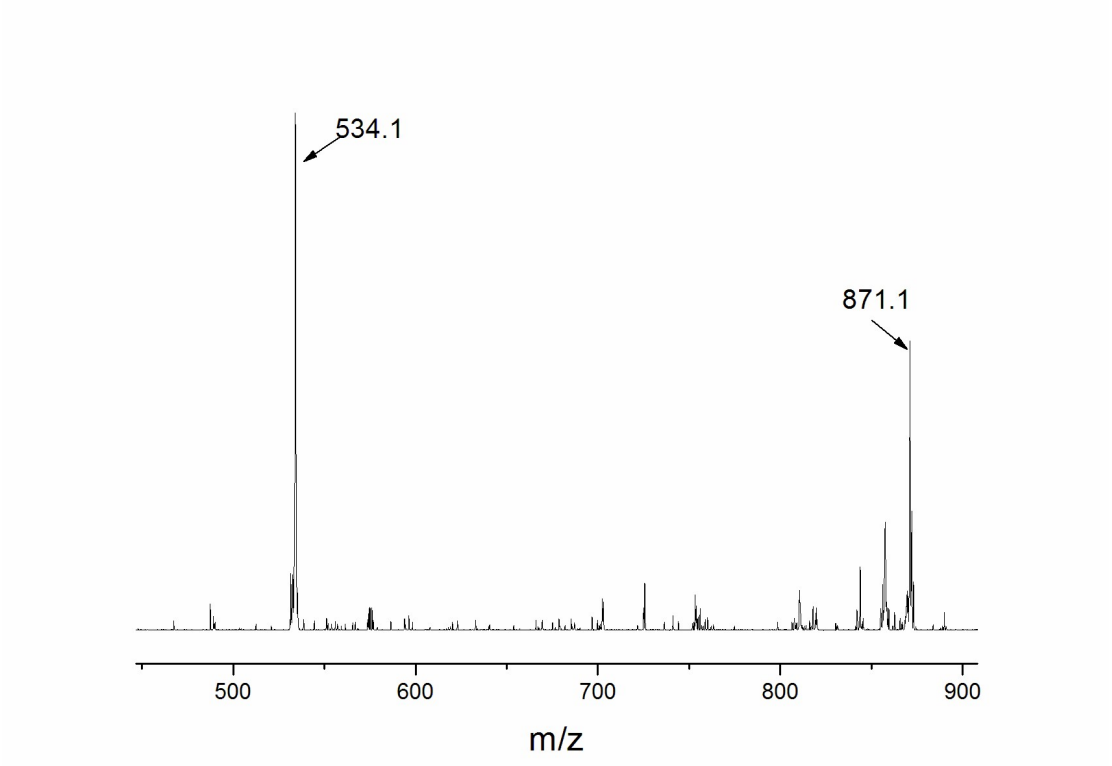


Figure S7. ESI-MS spectrum of **$[O(AuL^1)_3Ag_1]BF_4$** in CH_2Cl_2/MeOH solution

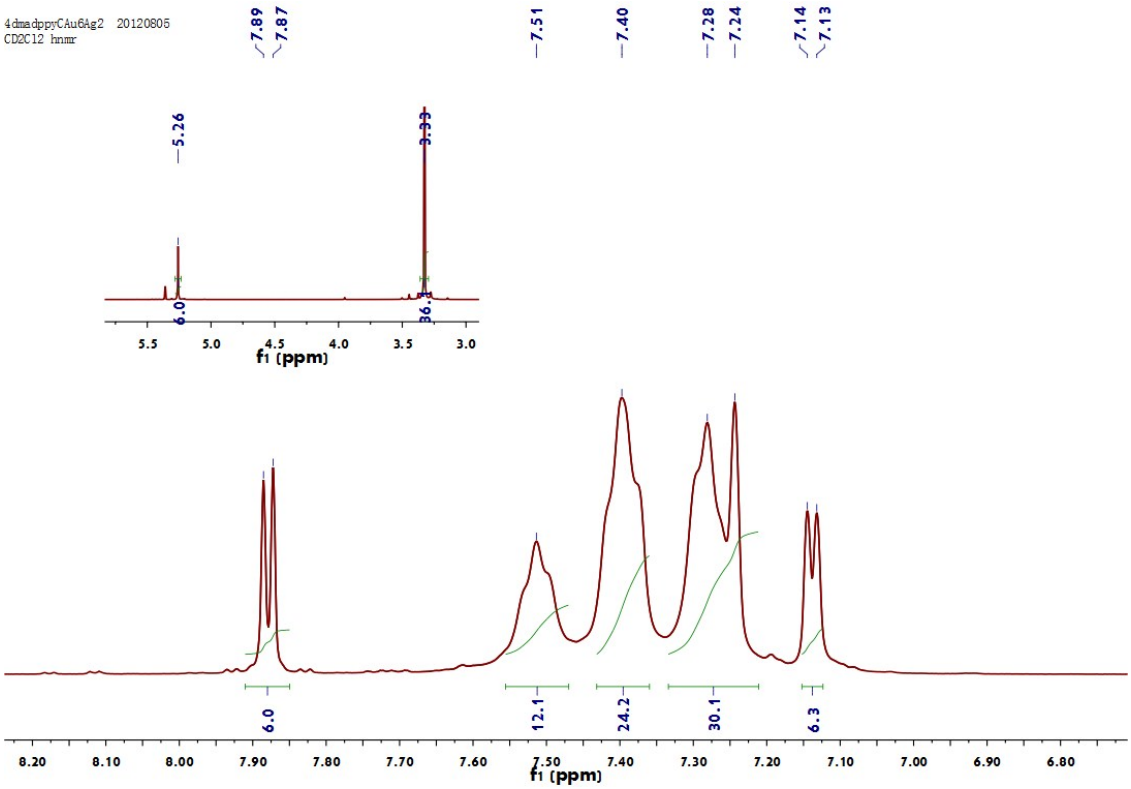


Figure S8. ^{1}H NMR spectrum of **$[(C)Au_6Ag_2(L^1)_6](BF_4)_4$** in CD_2Cl_2

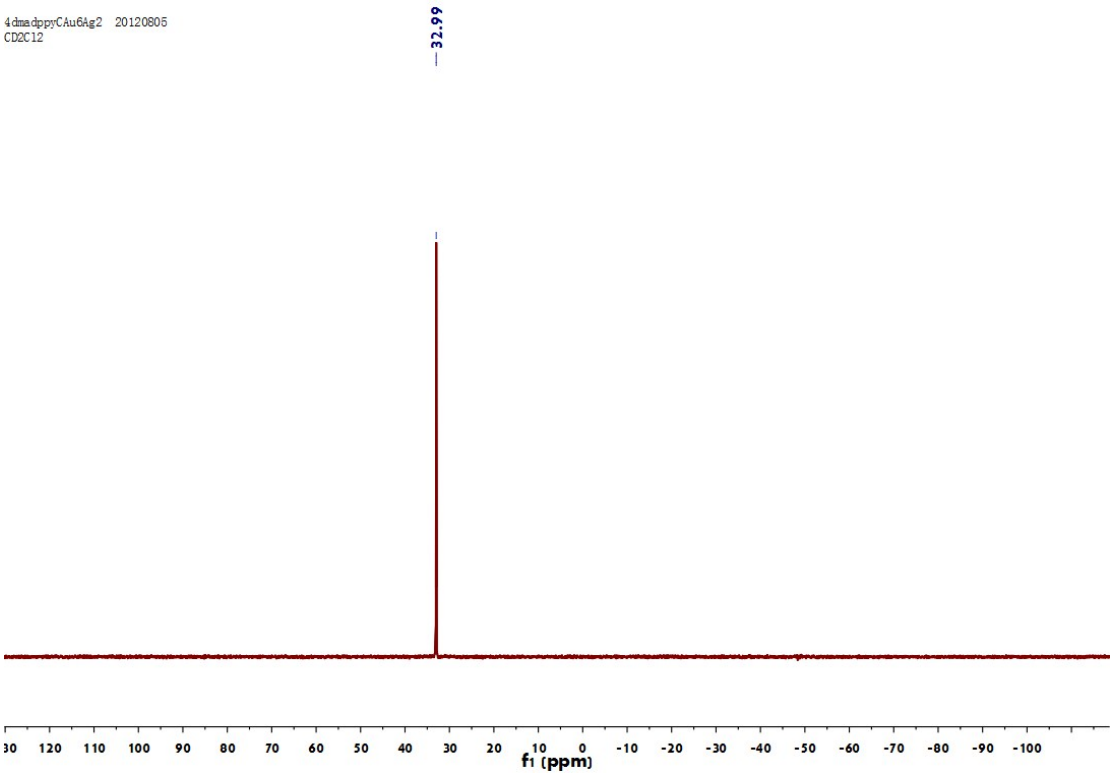


Figure S9. ^{31}P NMR spectrum of **[(C)Au$_6$Ag$_2$(L^1)$_6$](BF$_4$)$_4$** in CD_2Cl_2

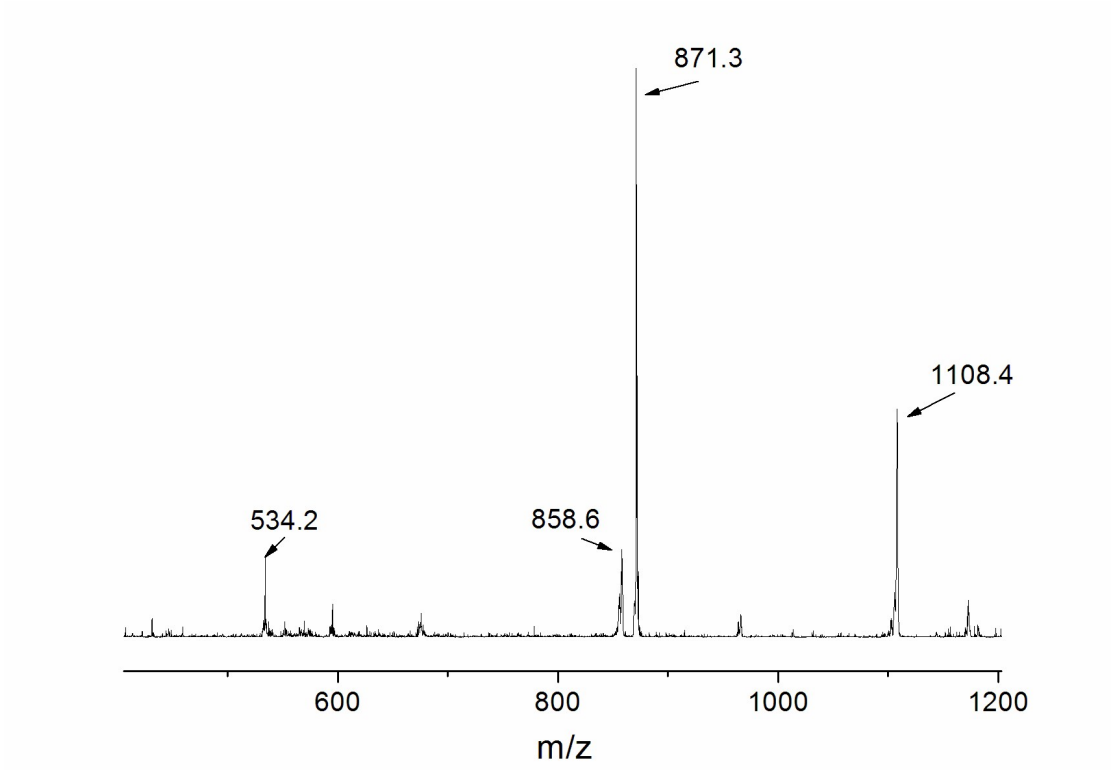


Figure S10. ESI-MS spectrum of **[(C)Au$_6$Ag$_2$(L^1)$_6$](BF$_4$)$_4$** in CH_2Cl_2/MeOH solution

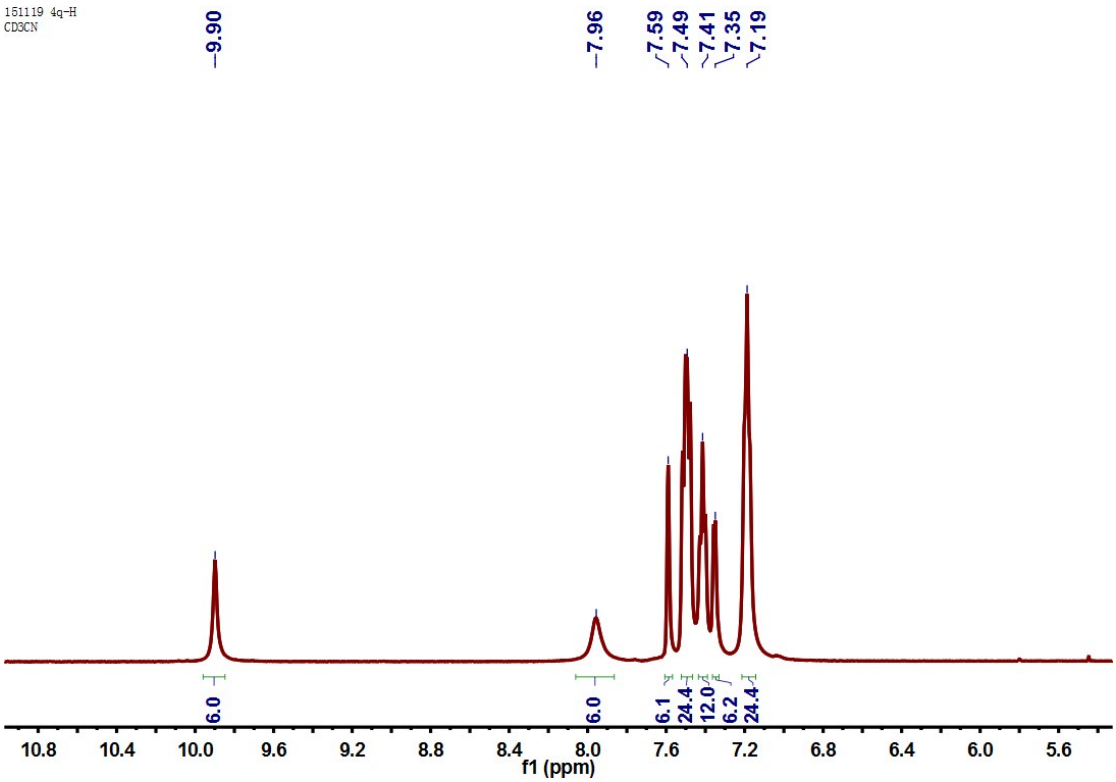


Figure S11. ^{1}H NMR spectrum of **1** in CD_3CN

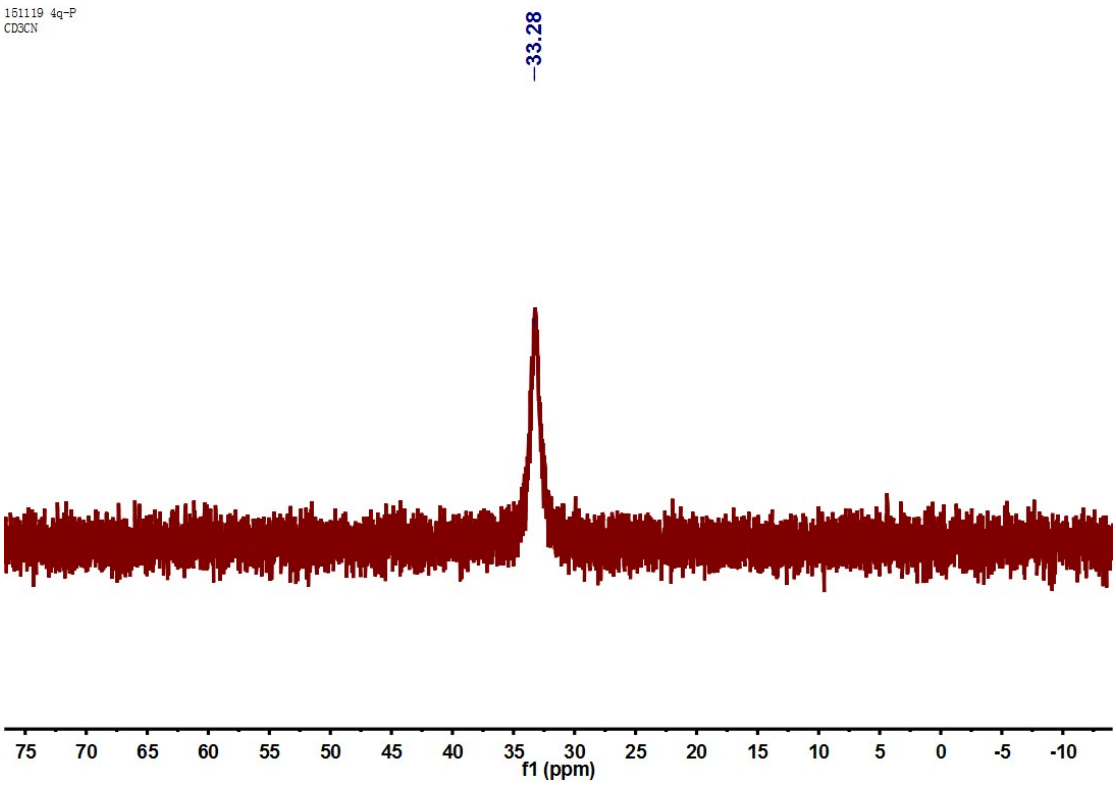


Figure S12. ^{31}P NMR spectrum of **1** in CD_3CN

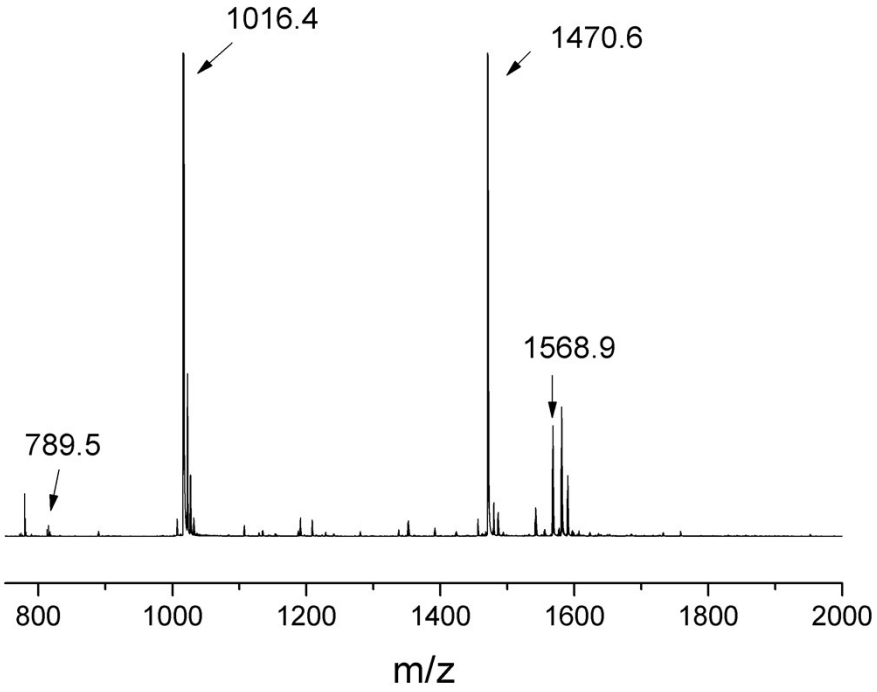


Figure S13. ESI-MS spectrum of **1** in MeCN solution

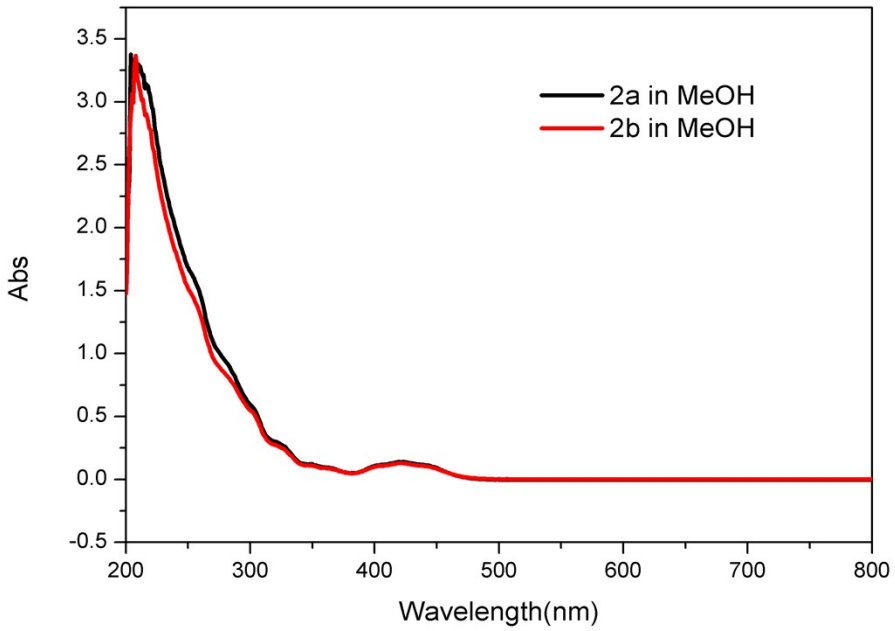


Figure S14. UV-Vis spectra of **2a** in MeOH and **2b** in MeOH

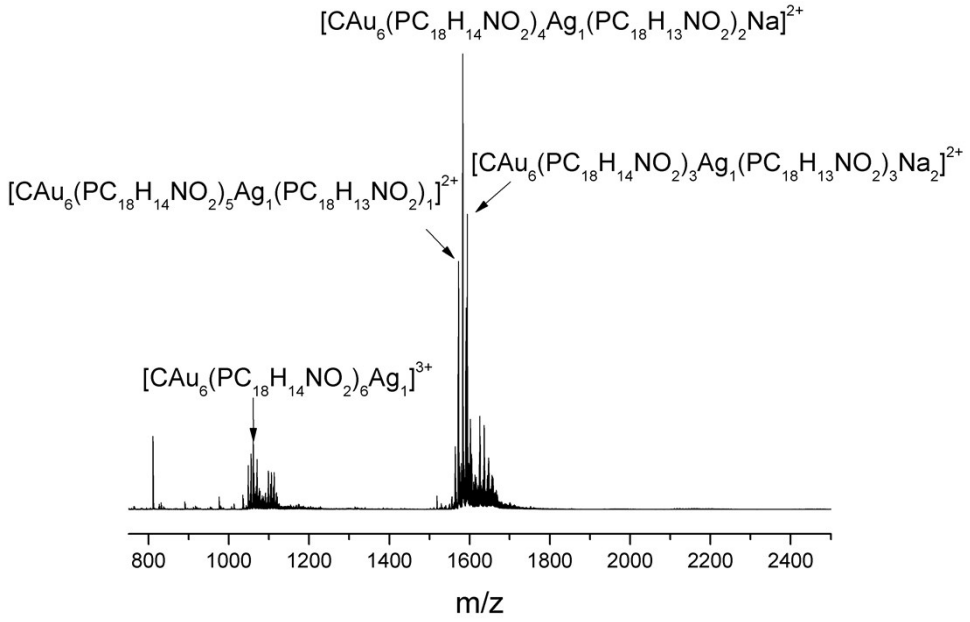


Figure S15. ESI-MS spectrum of **2a** in MeOH solution

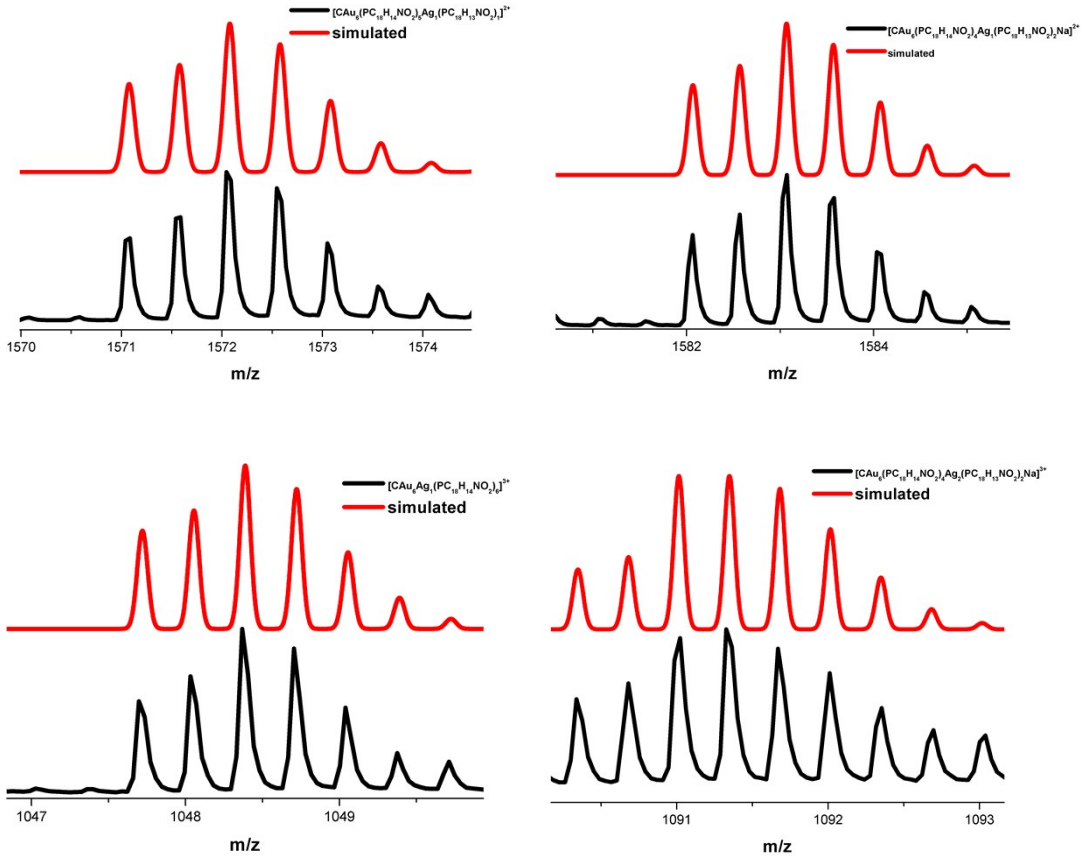


Figure S16. Measured (black trace) and simulated (red trace) isotopic pattems of **2a**

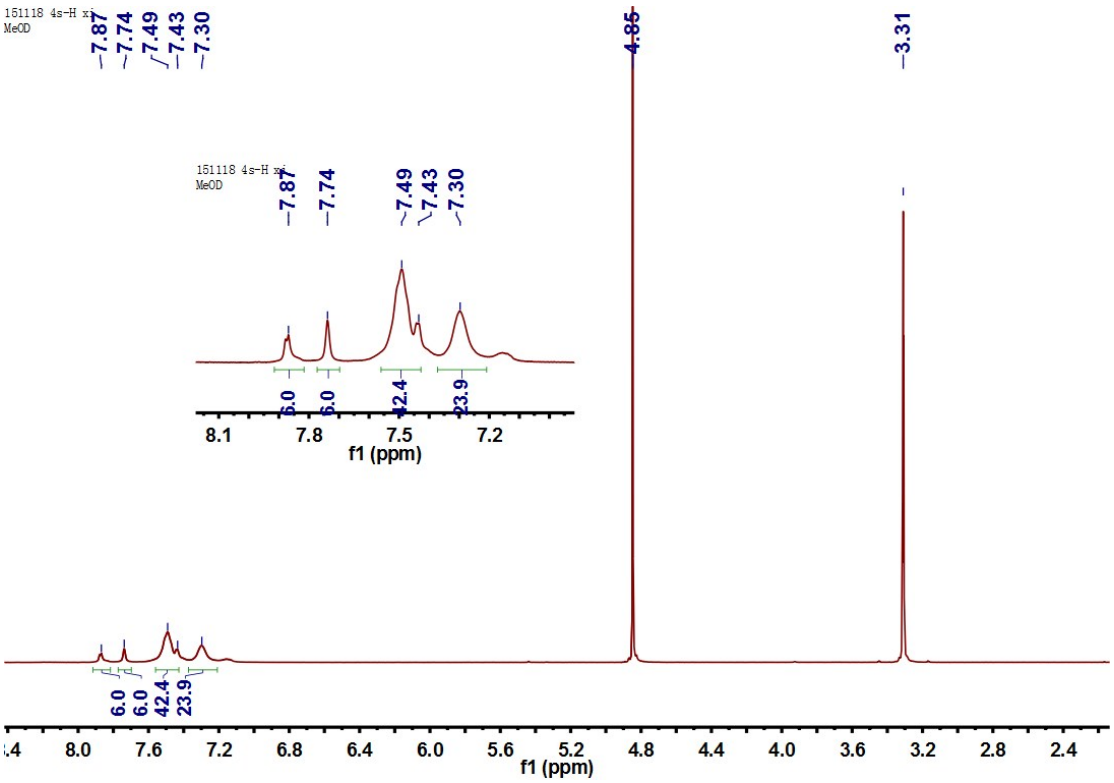


Figure S17. ^{1}H NMR spectrum of **2a** in CD_3OD

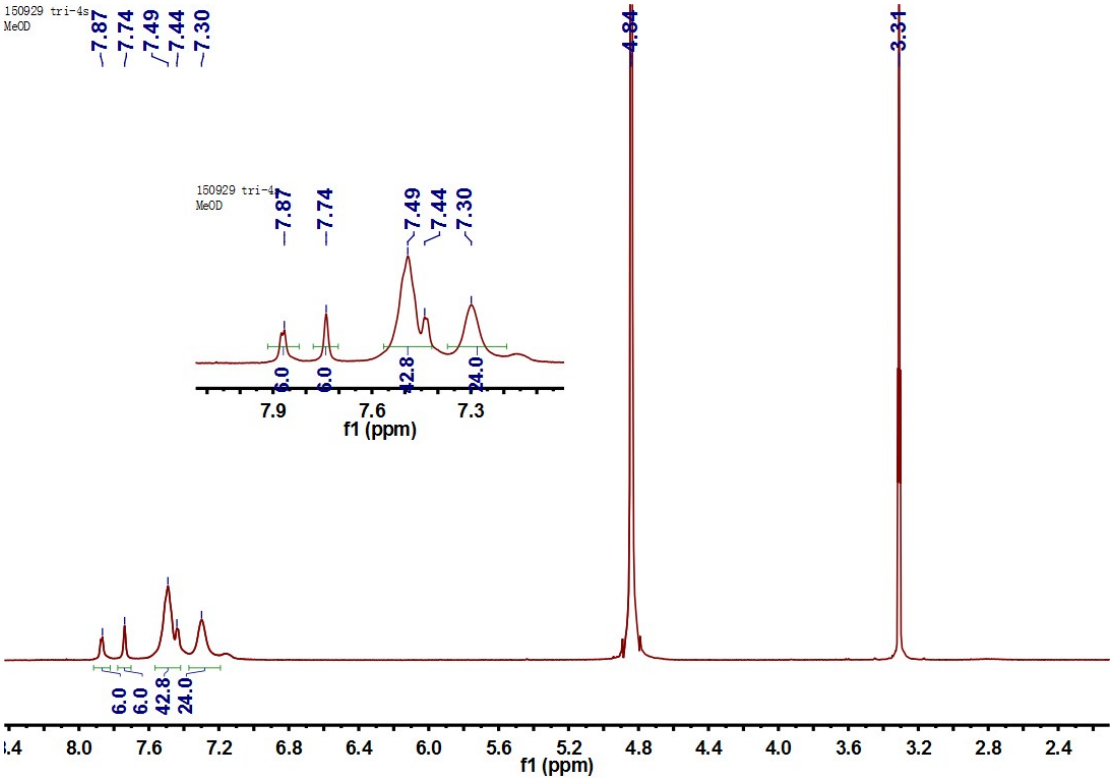


Figure S18. ^{1}H NMR spectrum of **2b** in CD_3OD

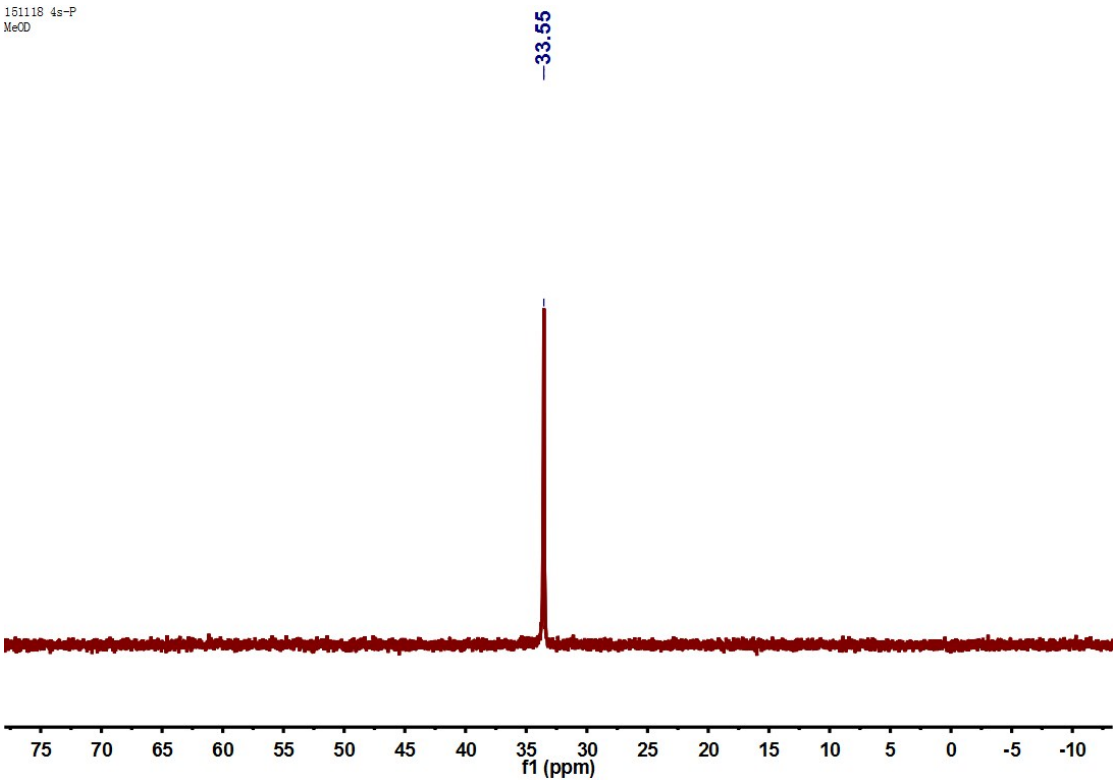


Figure S19. ^{31}P NMR spectrum of **2a** in CD_3OD

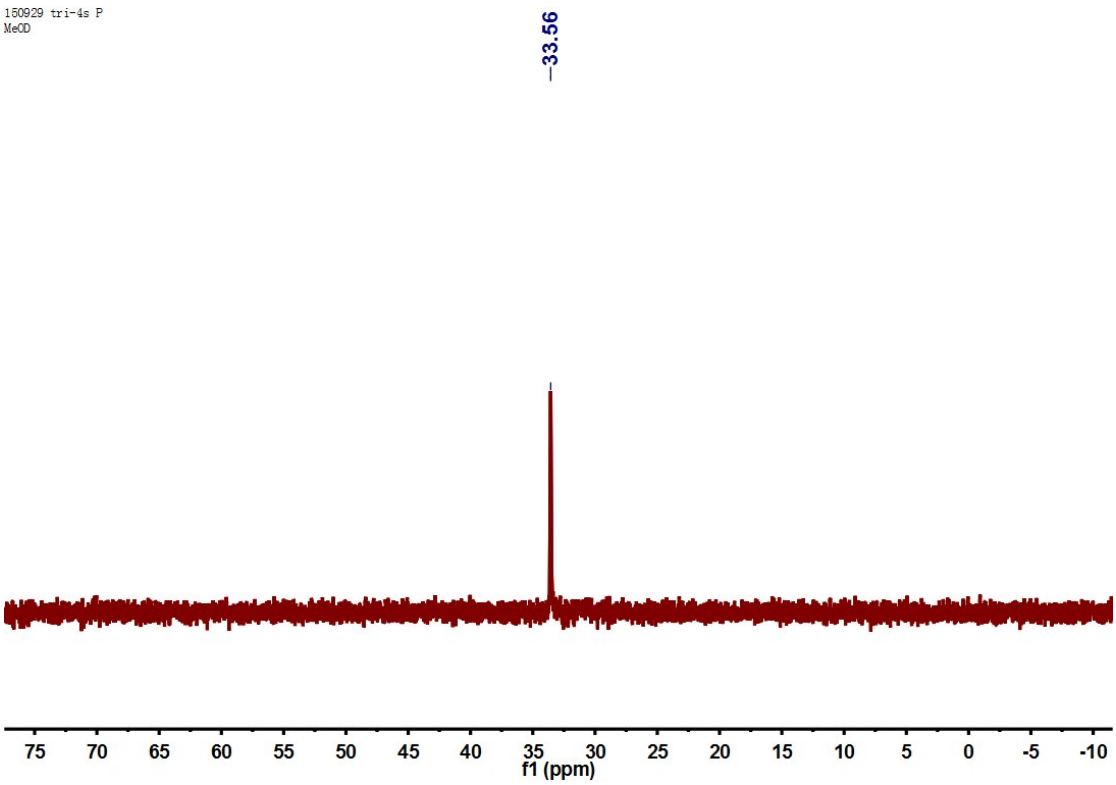


Figure S20. ^{31}P NMR spectrum of **2b** in CD_3OD

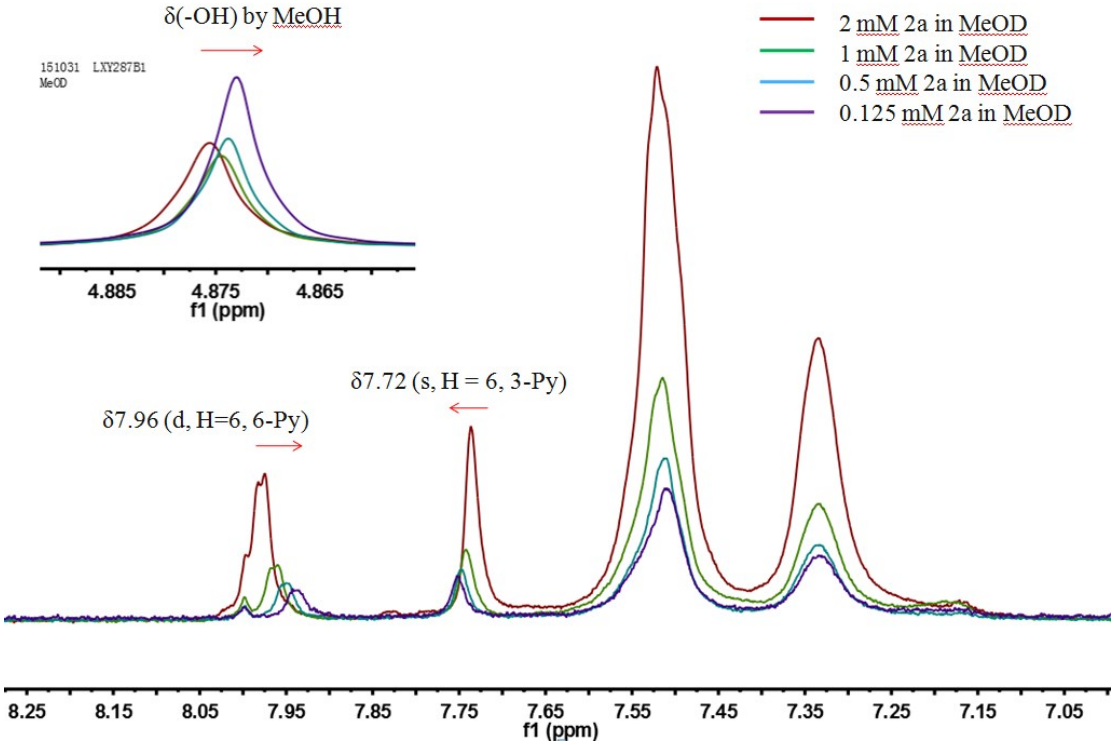


Figure S21. ^{1}H NMR spectrum of **2a** in CD_3OD at different concentration

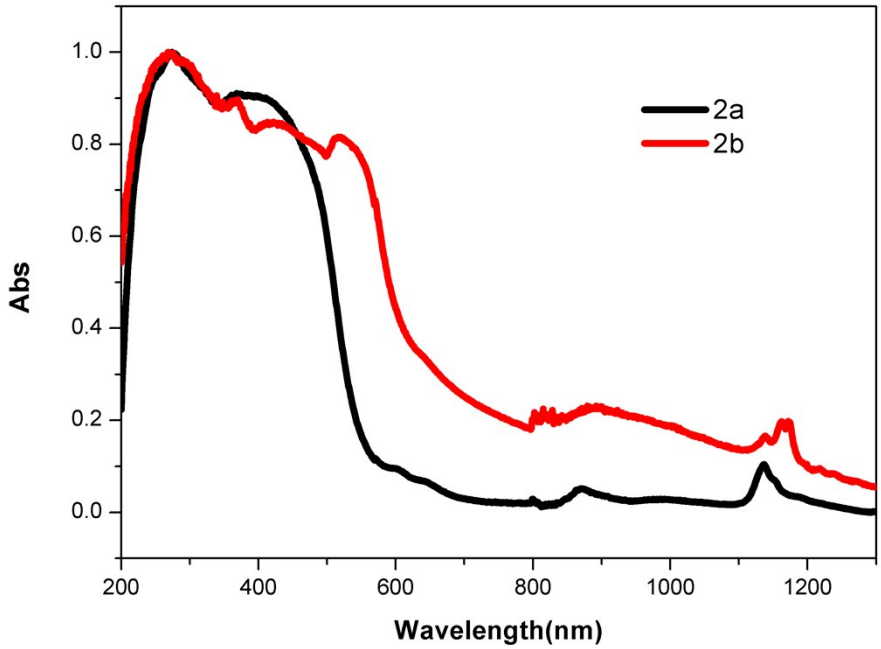


Figure S22. Diffuse reflectance spectra of solid **2a** and **2b**

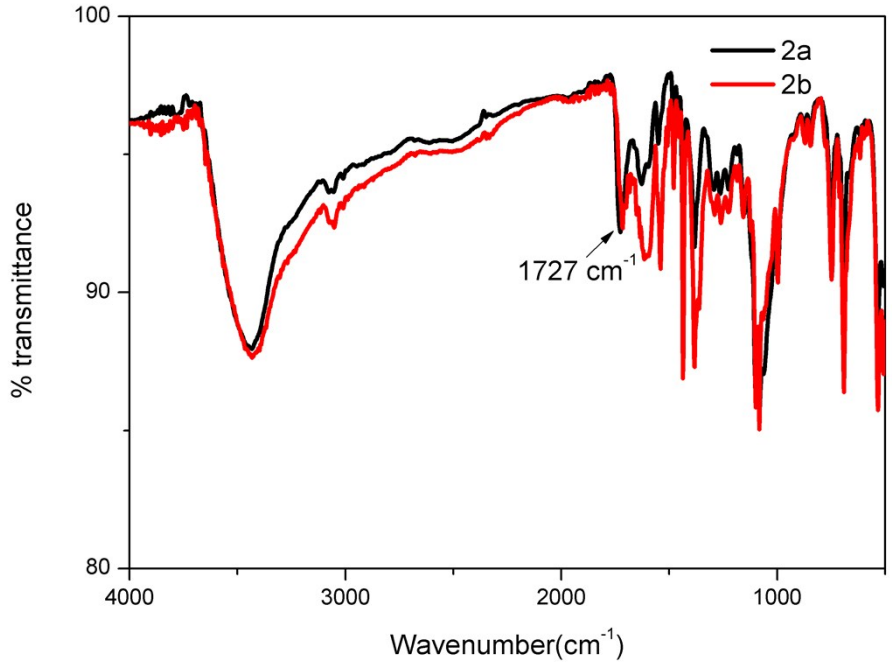


Figure S23. IR spectra of **2a** and **2b**

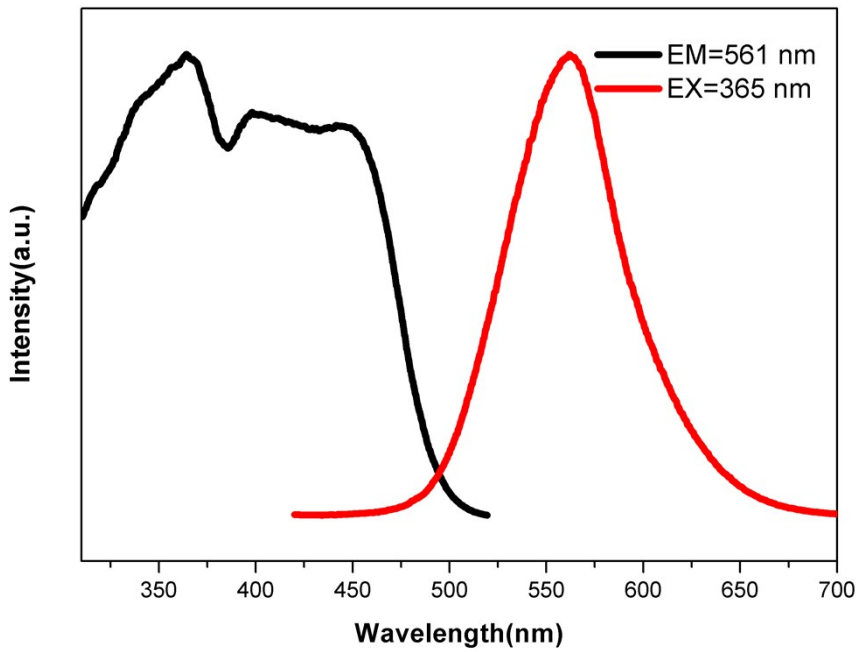


Figure S24. Excitation and emission spectra of **2a** in the solid state at room temperature

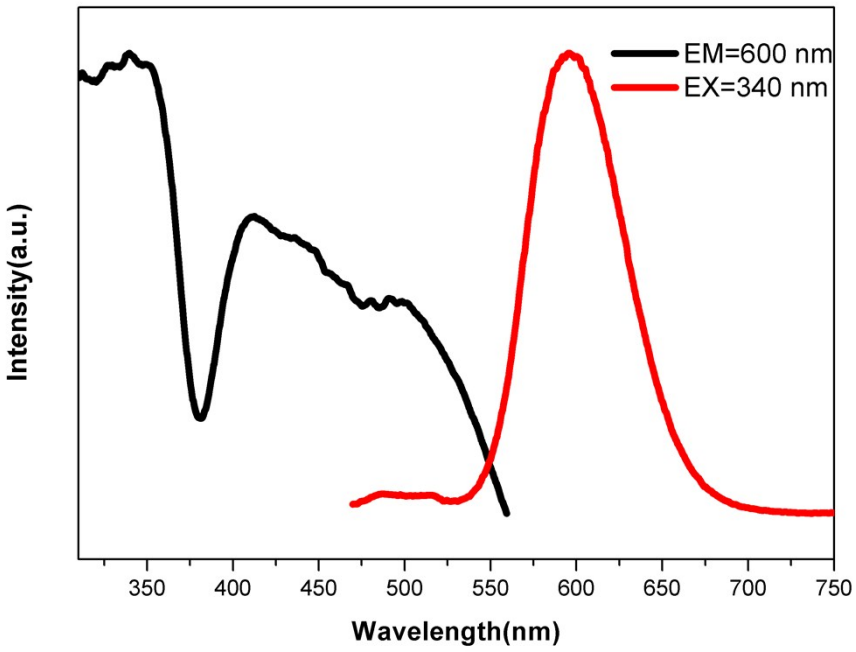


Figure S25. Excitation and emission spectra of **2b** in the solid state at room temperature

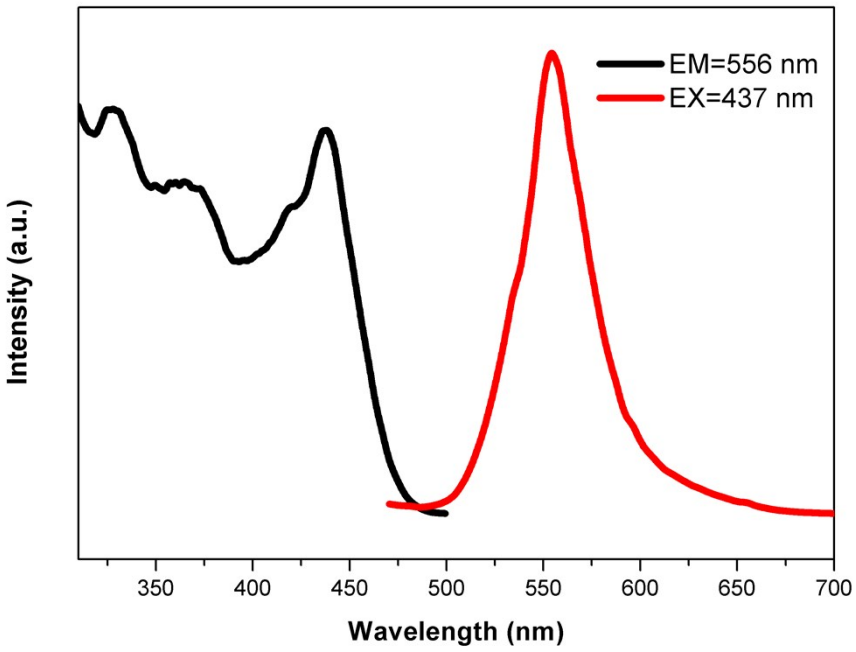


Figure S26. Excitation and emission spectra of **2a** in the solid state at 77K

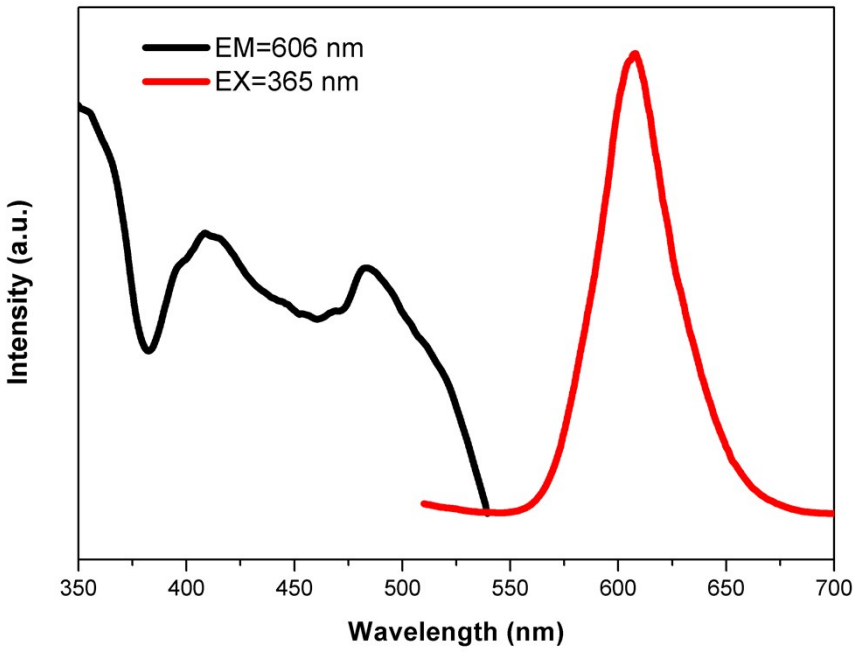


Figure S27. Excitation and emission spectra of **2b** in the solid state at 77K

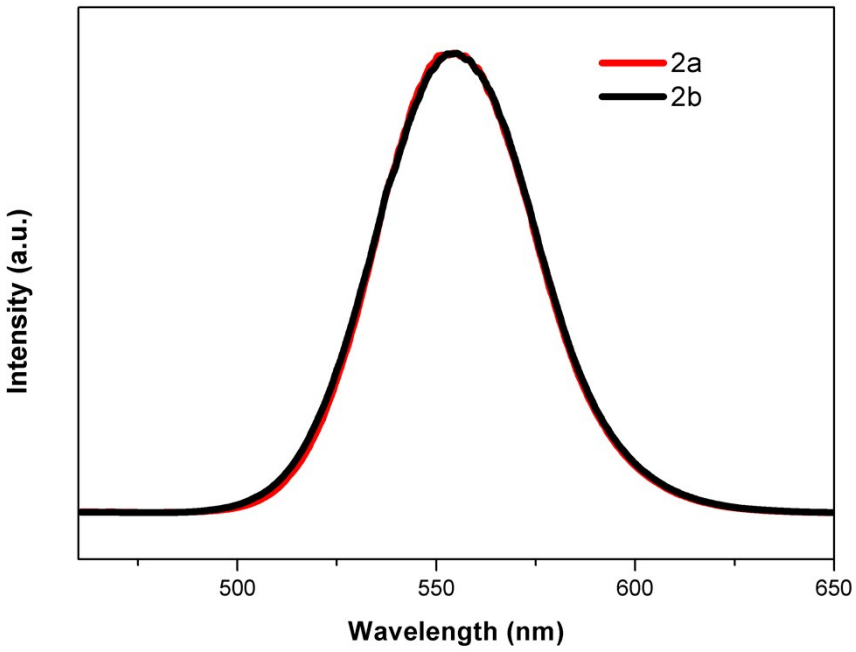


Figure S28. Emission spectra of **2a** and **2b** solution (V_{MeOH}:V_{EtOH}=9:1, frozen glass) at 77K (420 nm excitation)

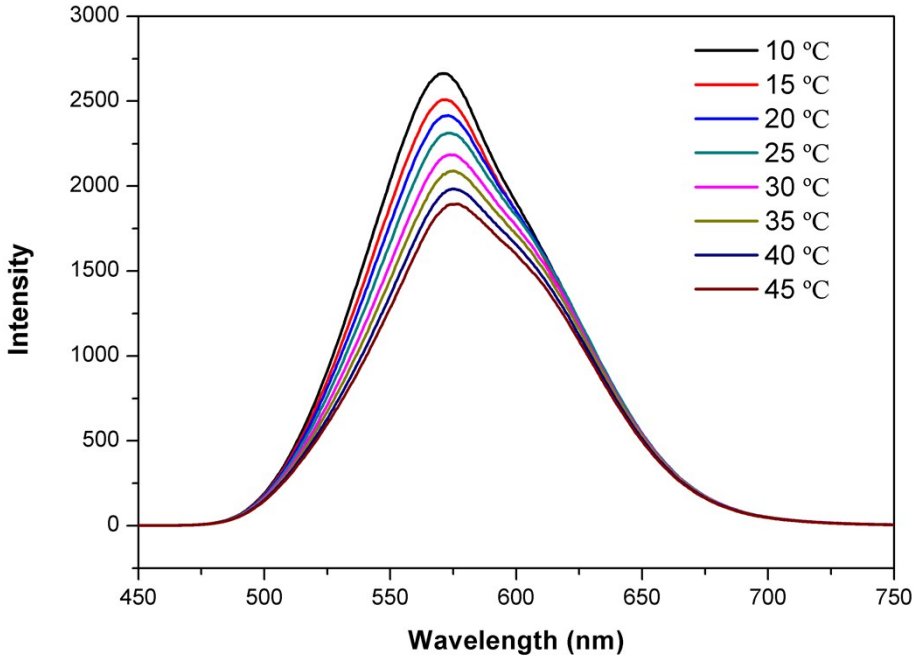


Figure S29. Emission spectra in MeOH (2.0×10^{-3} M) at different temperature (excited by 420 nm).

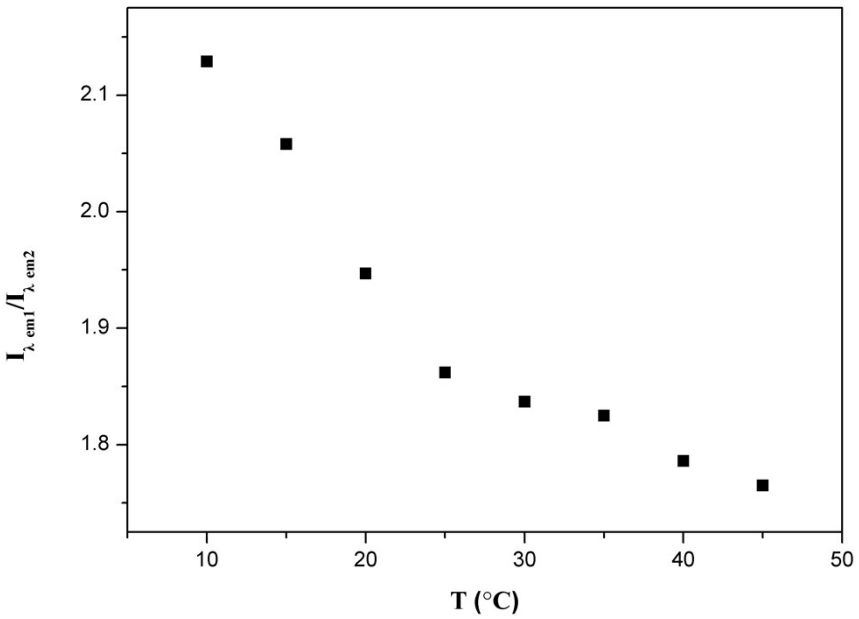


Figure S30. The radio of two isomers in MeOH solution (2.0×10^{-3} M) at different temperature

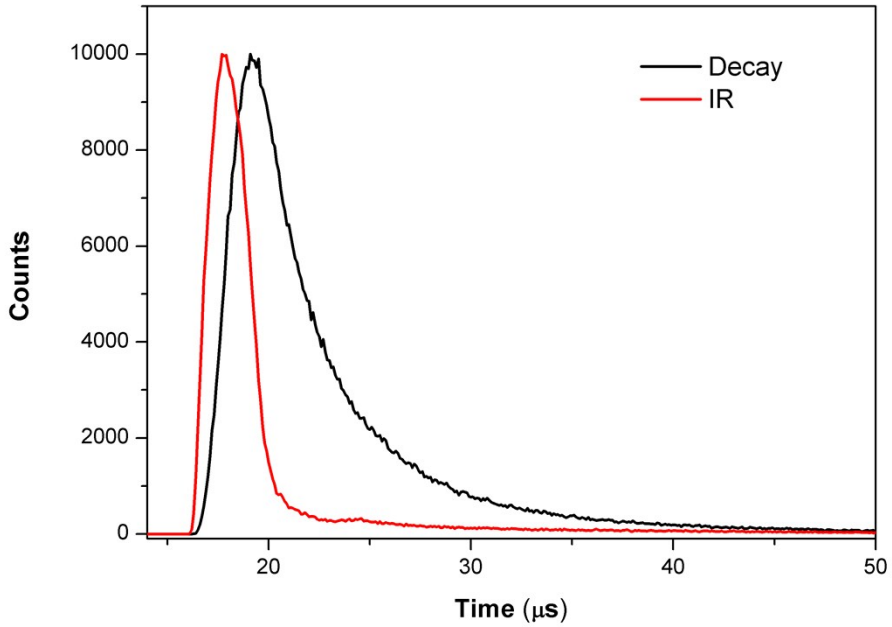


Figure S31. Luminescence decay profiles of **2a** in solid state at room temperature: the final lifetime was measured from the sample decay curve(black line) after deducting the instrument response time scan (red line)

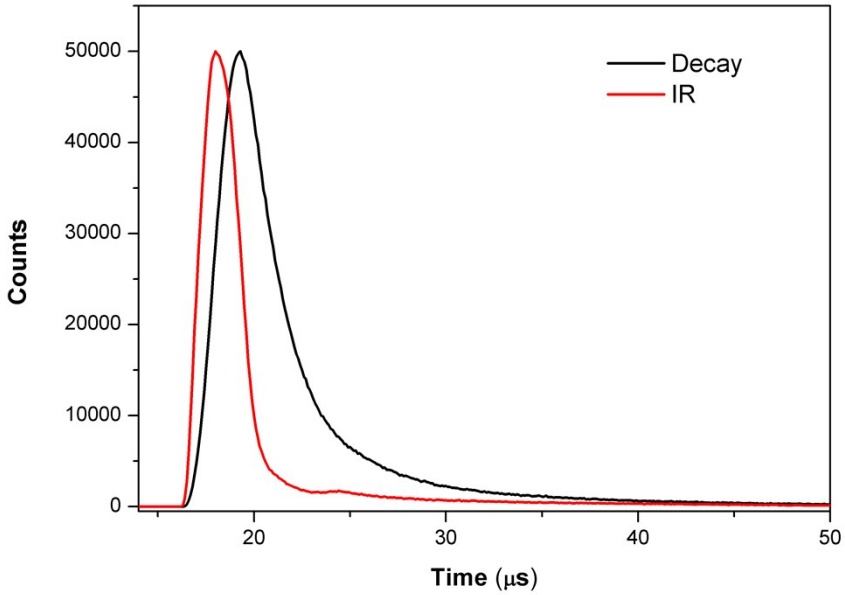


Figure S32. Luminescence decay profiles of **2b** in solid state at room temperature: the final lifetime was measured from the sample decay curve(black line) after deducting the instrument response time scan (red line)

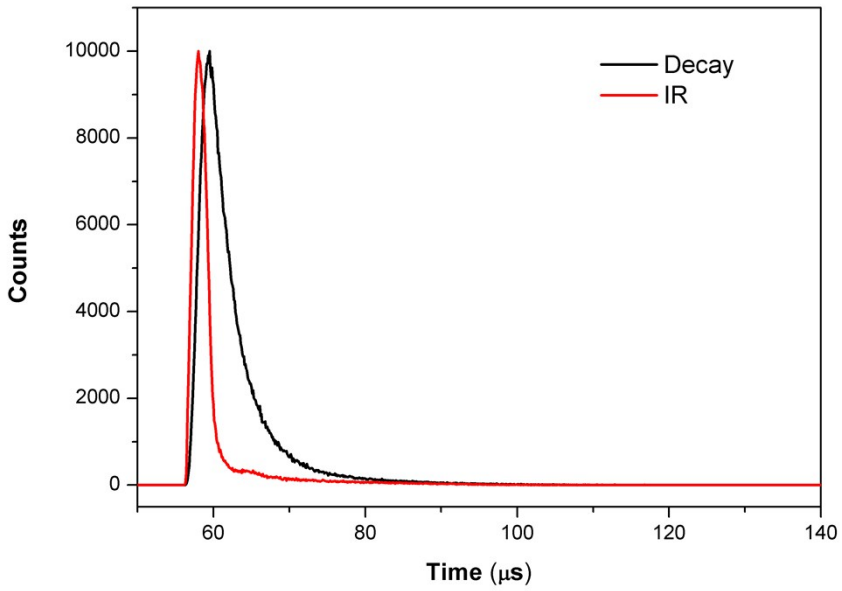


Figure S33. Luminescence decay profiles of **2a** in MeOH at room temperature: the final lifetime was measured from the sample decay curve(black line) after deducting the instrument response time scan (red line)

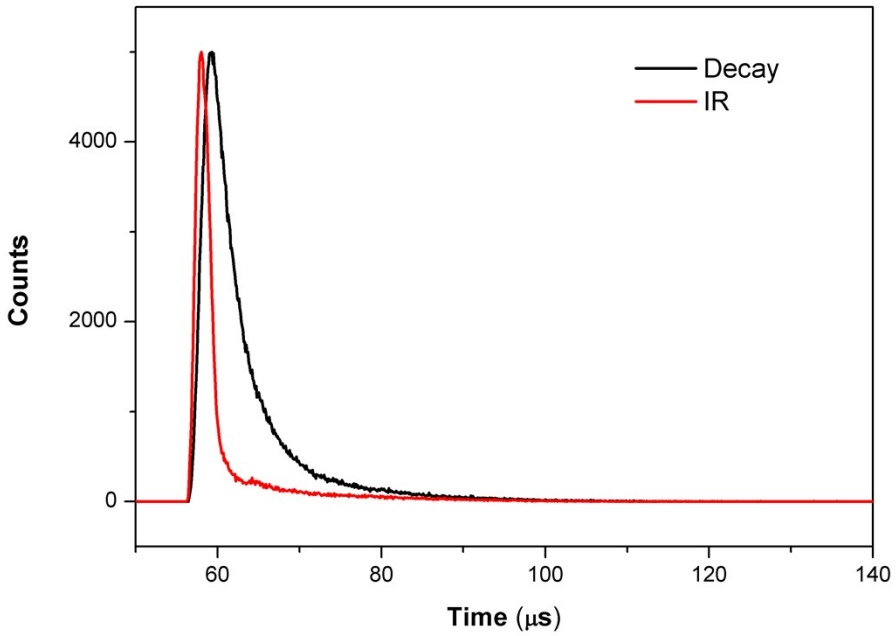


Figure S34. Luminescence decay profiles of **2b** in MeOH at room temperature: the final lifetime was measured from the sample decay curve(black line) after deducting the instrument response time scan (red line)

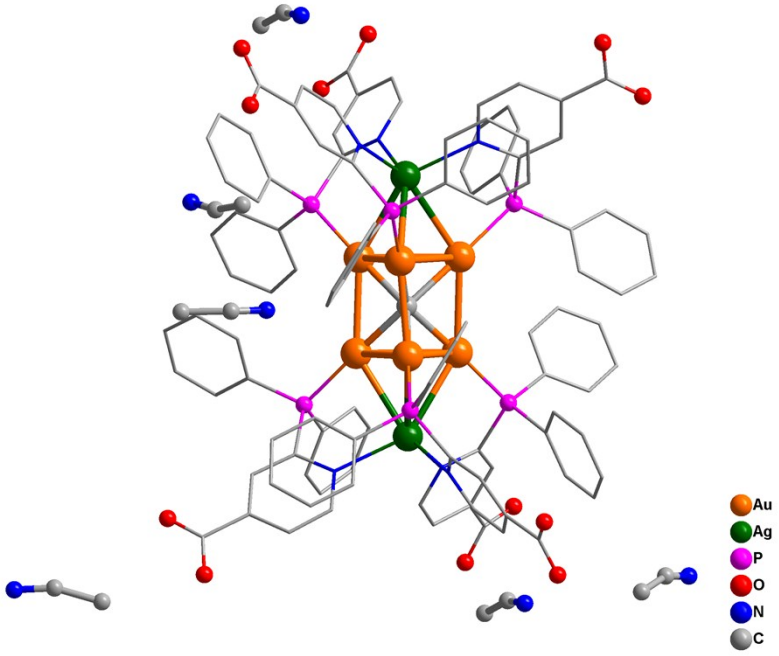


Figure S35. Molecular structure of **2b** and solvent moleculars

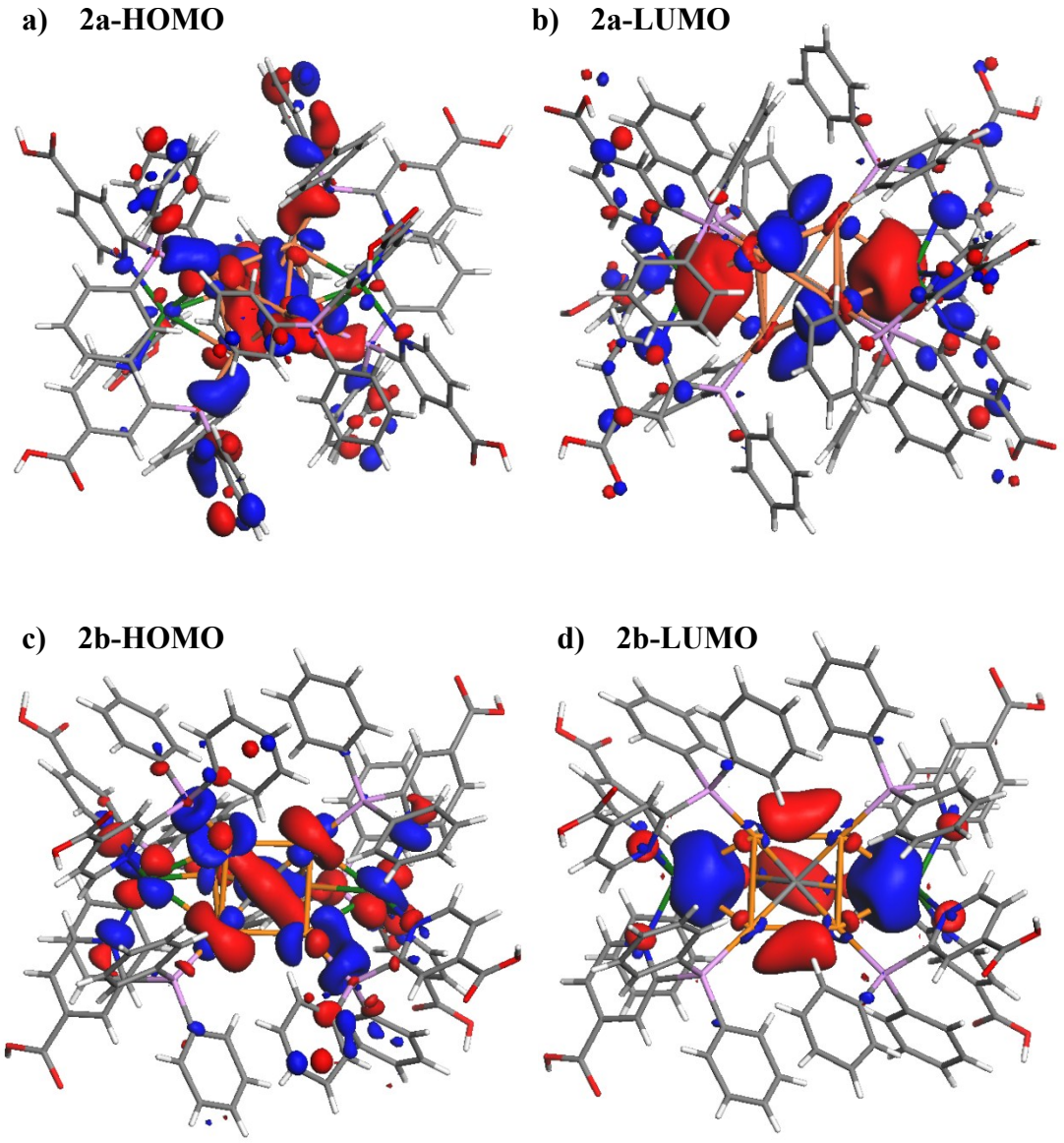


Figure S36. HOMOs and LUMOs of **2a** and **2b**

Table S1. Luminescence data of two isomers at different temperature

T (°C)	λ_{em} (nm)	I_{566} (Relative Intensity of 566 nm)	I_{608} (Relative Intensity of 608 nm)	I_{566}/I_{608}	Fitted Curves		
					$I_{\lambda em1}$ (Relative Intensity of Peak1)	$I_{\lambda em2}$ (Relative Intensity of Peak2)	$I_{\lambda em1}/I_{\lambda em2}$
10	571	0.9812	0.6335	1.549	0.7629	0.3583	2.129
15	572	0.9679	0.6668	1.452	0.7619	0.3702	2.058
20	573	0.9642	0.6960	1.385	0.7569	0.3888	1.947
25	575	0.9509	0.7305	1.302	0.7525	0.4041	1.862
30	574	0.9505	0.7356	1.292	0.7470	0.4067	1.837
35	575	0.9439	0.7507	1.257	0.7474	0.4095	1.825
40	575	0.9375	0.7644	1.226	0.7387	0.4137	1.786
45	577	0.9361	0.7760	1.206	0.7340	0.4158	1.765

Table S2. Coordinate file of **2a**

ATOM	X	Y	Z	ATOM	X	Y	Z
H	4.160262	-7.35594	-2.00938	C	-5.15329	-1.45848	-1.24763
C	3.754897	-6.63563	-1.29773	C	-3.91215	-3.97962	-0.39137
C	2.991186	-7.07706	-0.21483	C	-3.3772	-2.88984	-3.04742
C	4.009503	-5.26825	-1.46444	N	-2.79584	-1.96643	-3.85348
C	0	0	0	N	-3.63989	1.756199	-3.24358
Au	-1.74232	-1.21096	-0.54429	N	-0.40442	0.899278	-5.05972
Au	1.742319	1.210963	0.544288	C	5.153294	1.458475	1.247627
Au	1.024072	-1.75518	0.806159	C	3.912152	3.979616	0.391371
Au	-1.02407	1.755175	-0.80616	C	3.377204	2.889836	3.047416
Au	0.862441	-0.36669	-1.976	N	2.795843	1.966428	3.853478
Au	-0.86244	0.36669	1.975998	N	3.639886	-1.7562	3.243583
P	-3.59992	-2.41444	-1.26981	N	0.404423	-0.89928	5.059722
Ag	-1.80714	0.149931	-3.17644	C	-5.15329	-1.45848	-1.24763
P	3.599916	2.414436	1.269813	C	-3.91215	-3.97962	-0.39137
Ag	1.807135	-0.14993	3.17644	C	-3.3772	-2.88984	-3.04742
P	2.169619	-3.54643	1.758428	N	-2.79584	-1.96643	-3.85348

P	-2.16962	3.546428	-1.75843	N	-3.63989	1.756199	-3.24358
P	1.667919	-0.63798	-4.14242	N	-0.40442	0.899278	-5.05972
P	-1.66792	0.637983	4.142416	C	5.153294	1.458475	1.247627
C	-5.15329	-1.45848	-1.24763	C	3.505672	-4.34539	-0.54665
C	-3.91215	-3.97962	-0.39137	C	4.873963	-3.71969	2.594416
C	-3.3772	-2.88984	-3.04742	C	0.167577	4.374058	-3.02469
N	-2.79584	-1.96643	-3.85348	C	-1.88487	5.220508	-4.01757
N	-3.63989	1.756199	-3.24358	C	-2.49298	6.160027	-0.7177
N	-0.40442	0.899278	-5.05972	C	-3.50567	4.34539	0.546653
C	5.153294	1.458475	1.247627	C	-4.87396	3.719692	-2.59442
C	3.912152	3.979616	0.391371	C	4.087408	0.631698	-3.62457
C	3.377204	2.889836	3.047416	C	4.24305	-1.25181	-5.15494
N	2.795843	1.966428	3.853478	C	1.03609	-2.29472	-6.34109
N	3.639886	-1.7562	3.243583	C	1.180467	-3.3793	-4.16921
N	0.404423	-0.89928	5.059722	C	1.695401	1.388881	-6.139
C	1.23719	-4.43183	3.048062	C	-4.08741	-0.6317	3.624567
C	2.760067	-4.78992	0.562885	C	-4.24305	1.251809	5.154939
C	3.709319	-2.95092	2.604914	C	-1.03609	2.294721	6.34109
C	-1.23719	4.431832	-3.04806	C	-1.18047	3.379302	4.169207
C	-2.76007	4.789916	-0.56289	C	-1.6954	-1.38888	6.139004
C	-3.70932	2.950921	-2.60491	H	-4.41512	-0.08505	0.257888
C	3.467657	-0.41968	-4.32864	C	-6.47376	0.32603	-0.25898
C	1.235839	-2.21172	-4.95177	C	-7.45487	-1.11221	-1.94438
C	0.917927	0.669139	-5.225	H	-6.1878	-2.65777	-2.74422
C	-3.46766	0.41968	4.328643	H	-1.82173	-4.56489	-0.50966
C	-1.23584	2.211715	4.951773	C	-3.01929	-6.06536	0.474135
C	-0.91793	-0.66914	5.224997	C	-5.37652	-5.56078	0.721935
C	-5.26862	-0.37504	-0.35908	H	-6.04177	-3.67627	-0.08726
C	-6.2539	-1.81979	-2.0475	H	-4.26271	-4.87119	-2.86776
C	-2.82232	-4.84349	-0.17012	C	-3.65488	-4.42822	-4.88485
C	-5.19037	-4.33918	0.067937	C	-3.05818	-3.47917	-5.71672
C	-3.80824	-4.12776	-3.5246	H	-2.15917	-1.51035	-5.77203
C	-2.64437	-2.26923	-5.15535	C	-5.93748	2.033497	-3.93853
C	-4.73754	1.320422	-3.88939	H	-4.65223	0.349496	-4.38107
C	-0.97792	1.852739	-5.82089	C	-0.2715	2.637787	-6.72948
C	5.26862	0.375039	0.359079	H	-2.04565	2.013589	-5.66544
C	6.253895	1.819789	2.047502	H	4.415122	0.085049	-0.25789
C	2.822321	4.843492	0.170116	C	6.473756	-0.32603	0.258982
C	5.190366	4.339178	-0.06794	C	7.454868	1.112207	1.944376
C	3.808244	4.127756	3.524603	H	6.187796	2.657767	2.744219
C	2.644372	2.269233	5.155345	H	1.821734	4.564893	0.509664
C	4.737536	-1.32042	3.889389	C	3.019292	6.06536	-0.47414
C	0.977915	-1.85274	5.820887	C	5.376518	5.560778	-0.72194

C	-0.16758	-4.37406	3.024691	H	6.041768	3.676265	0.087263
C	1.884871	-5.22051	4.017565	H	4.262705	4.871189	2.867763
C	2.492979	-6.16003	0.717697	C	3.65488	4.428217	4.884851
C	3.058175	3.47917	5.716715	C	-1.09775	-2.40801	6.895278
H	2.159171	1.510352	5.772033	H	-6.56196	1.156842	0.443656
C	5.937475	-2.0335	3.938534	C	-7.56762	-0.04215	-1.04869
H	4.652234	-0.3495	4.381074	H	-8.30829	-1.40706	-2.55731
C	0.271496	-2.63779	6.729478	H	-2.17612	-6.74002	0.628566
H	2.045649	-2.01359	5.665437	C	-4.29661	-6.42507	0.920721
H	-0.67291	-3.75894	2.276301	H	-6.37264	-5.84106	1.066529
C	-0.91512	-5.10263	3.954266	C	-4.14485	-5.76667	-5.36958
C	1.129221	-5.94275	4.945618	H	-2.9174	-3.67406	-6.77884
H	2.973969	-5.28149	4.053683	H	-6.79493	1.637231	-4.48076
H	1.907556	-6.51735	1.565924	H	-0.76792	3.434265	-7.283
H	3.708531	-3.28026	-0.68177	H	6.561962	-1.15684	-0.44366
H	4.926862	-4.67283	2.066113	C	7.567619	0.042154	1.048691
C	6.008557	-3.25918	3.273881	H	8.308286	1.407055	2.557305
H	0.672906	3.758942	-2.2763	H	2.176118	6.74002	-0.62857
C	0.915124	5.102634	-3.95427	C	4.296607	6.425074	-0.92072
C	-1.12922	5.942748	-4.94562	H	6.372641	5.841055	-1.06653
H	-2.97397	5.281493	-4.05368	C	4.144845	5.76667	5.369582
H	-1.90756	6.517348	-1.56592	H	2.9174	3.674058	6.778837
C	-2.99119	7.077061	0.214826	H	6.794925	-1.63723	4.480763
C	-4.0095	5.268245	1.464442	H	0.767921	-3.43427	7.283
H	-3.70853	3.28026	0.681768	H	-2.00511	-5.06041	3.926939
H	-4.92686	4.672831	-2.06611	C	-0.26866	-5.88759	4.914493
C	-6.00856	3.259177	-3.27388	H	1.634134	-6.55822	5.692189
H	3.497245	1.272839	-2.96512	H	2.790306	-8.14096	-0.08368
C	5.454971	0.86628	-3.77699	H	4.609668	-4.92293	-2.3081
C	5.615018	-1.01592	-5.29277	C	7.241621	-4.12233	3.244354
H	3.780773	-2.07973	-5.69399	H	2.005106	5.060411	-3.92694
H	1.074854	-1.39855	-6.96301	C	0.268664	5.887591	-4.91449
C	0.795832	-3.53417	-6.94084	H	-1.63413	6.558223	-5.69219
C	0.948117	-4.61595	-4.77705	H	-2.79031	8.140956	0.083679
H	1.326036	-3.322	-3.08818	C	-3.7549	6.635626	1.297725
H	2.764888	1.186787	-6.21678	H	-4.60967	4.922927	2.308095
C	1.097745	2.408009	-6.89528	C	-7.24162	4.122334	-3.24435
H	-3.49725	-1.27284	2.965116	H	5.926863	1.689704	-3.23887
C	-5.45497	-0.86628	3.776994	C	6.221276	0.044455	-4.61296
C	-5.61502	1.015924	5.292773	H	6.208947	-1.66311	-5.93963
H	-3.78077	2.079731	5.693992	H	0.654185	-3.59412	-8.02117
H	-1.07485	1.398549	6.963005	C	0.758727	-4.69529	-6.16059
C	-0.79583	3.534171	6.940838	H	0.920807	-5.52094	-4.16805

C	-0.94812	4.615947	4.777049	C	1.897264	3.359853	-7.75487
H	-1.32604	3.321998	3.088178	H	-5.92686	-1.6897	3.238871
H	-2.76489	-1.18679	6.216781	C	-6.22128	-0.04446	4.612963
H	-6.20895	1.663106	5.939625	H	-4.16026	7.355937	2.009383
H	-0.65419	3.594123	8.021171	O	-8.2433	3.595977	-3.98318
C	-0.75873	4.695293	6.160585	O	-7.30048	5.162674	-2.62045
H	-0.92081	5.52094	4.168053	H	7.289135	0.231107	-4.73204
C	-1.89726	-3.35985	7.754873	H	0.587686	-5.66285	-6.63472
H	-8.51116	0.499306	-0.96446	O	2.873358	2.843461	-8.53467
H	-4.45166	-7.38242	1.419555	O	1.689936	4.551464	-7.69982
O	-4.63439	-6.59673	-4.63042	H	-7.28914	-0.23111	4.732042
O	-3.9657	-5.91566	-6.70075	H	-0.58769	5.662854	6.634715
H	8.511159	-0.49931	0.964457	O	-2.87336	-2.84346	8.534672
H	4.451663	7.382423	-1.41956	O	-1.68994	-4.55146	7.699819
O	4.634388	6.596732	4.630415	H	-4.32199	-6.79662	-6.948
O	3.965701	5.915656	6.700754	H	4.321989	6.796624	6.948003
H	-0.85366	-6.44321	5.648257	H	9.002955	-4.21626	3.934268
O	8.243301	-3.59598	3.983179	H	-9.00296	4.216255	-3.93427
O	7.30048	-5.16267	2.620451	H	2.819976	1.870365	-8.5802
H	0.853657	6.443211	-5.64826	H	-2.81998	-1.87037	8.580199

Table S3. Coordinate file of **2b**

ATOM	X	Y	Z	ATOM	X	Y	Z
C	-5.00255	-1.14344	-2.24603	H	-5.83967	-3.73201	-0.17971
C	-6.29186	-0.68689	-2.56327	C	-3.79158	2.383387	-3.04899
C	-4.84408	-2.23421	-1.37087	C	-4.64521	1.198092	-4.99154
P	-3.49968	-0.38643	-2.94758	C	-3.92459	-2.40871	-4.89754
H	-6.43315	0.167779	-3.22528	N	-1.77708	-1.31957	-4.85847
C	-7.41087	-1.33584	-2.03184	C	-0.0336	0.004544	0.00227
C	-5.96634	-2.8801	-0.84974	Au	-1.74555	0.177965	1.423007
H	-3.84214	-2.57907	-1.10539	H	-8.12611	-2.93664	-0.77111
C	-4.00266	1.178573	-3.7404	H	-3.28711	2.370874	-2.08028
C	-3.02904	-1.48189	-4.36256	C	-4.22423	3.591994	-3.60097
Au	-1.75404	-0.16789	-1.41092	C	-5.07534	2.410856	-5.53798
H	-8.4107	-0.98398	-2.28748	H	-4.81467	0.272584	-5.54433
C	-7.2501	-2.43303	-1.18113	H	-4.9223	-2.54882	-4.47851
C	-3.53707	-3.17752	-6.00312	C	4.387357	3.069194	1.385594
C	-1.41286	-2.06667	-5.91624	C	3.469402	3.76051	2.198675
Ag	-0.02533	0.012223	-3.84899	C	0.96034	4.03568	3.704867
Au	0.976667	-1.40388	-1.41204	C	2.788439	1.888859	4.325486
Au	0.687825	1.575009	-1.42635	C	0.436566	-5.315	1.424305

Au	0.997272	1.406982	1.396929	C	1.509868	-4.87105	2.220171
Au	0.691754	-1.57195	1.414758	C	3.024722	-2.85192	3.71312
H	-3.82932	2.592342	1.136328	C	0.244718	-3.35015	4.35561
P	-3.49269	0.388391	2.961786	C	-5.95233	2.889122	0.866047
H	-4.06314	4.52662	-3.06154	C	-6.28422	0.689843	2.571096
C	-4.86904	3.606545	-4.84218	C	-3.79216	-2.37985	3.049923
H	-5.58258	2.418116	-6.50423	C	-4.65387	-1.20267	4.993496
C	-2.25579	-2.99767	-6.52688	C	-3.91673	2.393894	4.931144
C	-4.52853	-4.16265	-6.5613	N	-1.76683	1.308935	4.877833
H	-0.39542	-1.91819	-6.28242	H	-4.74768	-5.40375	-7.975
N	2.017221	-0.86154	-4.84512	C	4.005896	-2.21744	-4.88119
N	-0.27376	2.206758	-4.86343	C	3.710861	-0.48836	-6.52526
H	4.191003	-2.00198	-1.1852	H	1.874807	0.632828	-6.2737
P	2.034231	-2.82162	-2.93095	C	-0.04499	4.602876	-4.92949
H	-0.40959	4.637385	-1.24487	C	-1.42974	3.491017	-6.5505
P	1.415929	3.189525	-2.94741	H	-1.51208	1.342993	-6.2818
H	4.228586	2.011791	1.158765	C	5.470986	-3.71741	-0.90312
P	2.069115	2.832185	2.899291	C	3.632132	-5.1175	-2.48746
H	-0.40686	-4.64929	1.225099	C	-0.24084	-4.43294	-3.06861
P	1.416003	-3.19536	2.927267	C	1.284585	-4.65041	-4.94735
C	-4.83267	2.246405	1.395701	C	0.447619	6.587979	-0.89379
C	-4.99329	1.151008	2.264894	C	2.611265	5.710794	-2.442
C	-3.99874	-1.17829	3.748996	C	3.955825	2.035189	-3.0425
C	-3.01912	1.47483	4.386149	C	3.397659	3.447533	-4.93989
H	-5.21727	4.549835	-5.26601	C	5.502309	3.7302	0.868674
H	-1.91306	-3.57342	-7.38582	C	3.664043	5.128241	2.45638
O	-4.04516	-4.79809	-7.65277	C	-0.23688	4.394179	3.062014
O	-5.62428	-4.34835	-6.07152	C	1.305911	4.65303	4.920707
C	2.763266	-1.87701	-4.34628	C	4.021622	2.238412	4.87598
C	2.493366	-0.18916	-5.90844	N	2.034363	0.880379	4.823804
C	0.252761	3.357977	-4.37636	C	0.445651	-6.60628	0.895812
C	-1.09397	2.286623	-5.92645	C	2.602828	-5.72282	2.449136
C	4.350108	-3.0592	-1.41159	C	3.952346	-2.0389	3.039227
C	3.433984	-3.75196	-2.22509	C	3.385458	-3.45233	4.93306
C	0.935932	-4.04011	-3.7286	C	-0.06964	-4.59319	4.903664
C	0.438974	5.299826	-1.43061	N	-0.26301	-2.19327	4.846336
C	1.514961	4.861134	-2.22556	C	-7.23734	2.435611	1.184683
C	3.031839	2.847812	-3.72082	H	-5.82361	3.744008	0.200265
H	-6.42743	-0.17023	3.225569	C	1.531087	-7.45703	1.137722
C	-7.40067	1.335846	2.031548	H	-0.39384	-6.953	0.290771
H	-3.28056	-2.36329	2.085033	H	3.449827	-5.38703	3.048214
C	-4.25375	-3.5873	3.580812	C	2.60727	-7.01274	1.909362
C	-5.11351	-2.41414	5.518459	H	3.670667	-1.56796	2.094714

H	-4.82199	-0.28032	5.552419	C	5.231684	-1.85136	3.568377
H	-4.91647	2.534371	4.517647	C	4.666508	-3.26126	5.456357
C	-3.52917	3.151638	6.045047	H	2.678412	-4.08506	5.472777
C	-1.40271	2.045765	5.943573	H	0.32815	-5.52057	4.488803
Ag	-0.00341	0.003801	3.841676	C	-0.91815	-4.65641	6.017456
H	4.611465	-3.01927	-4.45624	C	-1.08206	-2.2644	5.911779
C	4.488322	-1.52	-5.99552	H	-8.11186	2.940646	0.773535
H	4.046181	0.082385	-7.39061	H	-8.40164	0.980262	2.27805
H	0.369888	5.525243	-4.51913	H	-4.09679	-4.51874	3.034305
C	-0.89808	4.675847	-6.0387	C	-4.91746	-3.60539	4.811901
H	-2.09886	3.499751	-7.41004	H	-5.63127	-2.42491	6.479107
C	5.675648	-5.07364	-1.18363	C	-2.24659	2.969044	6.564308
H	6.188365	-3.17418	-0.28583	C	-4.52249	4.1278	6.615786
H	2.922646	-5.67331	-3.10066	H	-0.38377	1.897005	6.305297
C	4.754082	-5.77091	-1.96873	C	5.82939	-1.92497	-6.54694
H	-0.51942	-3.95432	-2.12692	C	-1.18831	6.03865	-6.60868
C	-1.04468	-5.44018	-3.60934	H	6.553154	-5.58629	-0.78844
C	0.476339	-5.65689	-5.48264	H	4.908919	-6.82815	-2.18792
H	2.191527	-4.3573	-5.47858	H	-1.9532	-5.74835	-3.08909
C	1.535128	7.438348	-1.12547	C	-0.68546	-6.056	-4.81306
H	-0.39418	6.931319	-0.29004	H	0.76366	-6.13735	-6.4196
H	3.459368	5.379933	-3.04229	H	1.540228	8.442976	-0.70107
C	2.61512	6.997565	-1.89375	H	3.465794	7.655927	-2.07258
H	3.66828	1.56025	-2.10154	H	5.955097	1.216999	-3.03583
C	5.235608	1.841165	-3.56884	C	5.599642	2.450212	-4.77464
C	4.678966	3.249418	-5.46055	H	4.962473	3.730571	-6.39832
H	2.692327	4.076213	-5.48585	H	6.578342	5.602339	0.746998
C	5.700828	5.089276	1.141346	H	4.932545	6.842814	2.145059
H	6.220074	3.188498	0.250427	H	-1.99004	5.654259	3.110397
H	2.951135	5.683348	3.066428	C	-0.70943	5.995465	4.818358
C	4.779945	5.784454	1.929117	H	0.757685	6.118162	6.405068
H	-0.5081	3.914588	2.11887	C	3.701531	0.526569	6.533557
C	-1.06486	5.373422	3.617027	C	5.805875	1.978983	6.591415
C	0.475352	5.633787	5.468778	H	1.871753	-0.60113	6.263954
H	2.230256	4.38852	5.437377	H	1.532606	-8.46774	0.728158
H	4.632046	3.03836	4.454929	H	3.454503	-7.67284	2.099084
C	4.485151	1.55519	6.007705	H	5.954282	-1.22793	3.038389
C	2.495076	0.218005	5.90105	C	5.591877	-2.46495	4.772802
H	4.94586	-3.74279	6.394995	H	-1.35805	6.757024	5.254159
C	-1.43065	-3.46556	6.534328	H	4.020828	-0.03112	7.413383
C	-1.22084	-6.01631	6.587967	O	6.10045	1.296804	7.7204
H	-1.48723	-1.31597	6.268904	O	6.505732	2.834264	6.087334
H	-5.27865	-4.54853	5.225118	H	6.594009	-2.32384	5.180696

H	-1.90387	3.536071	7.429212	H	-2.09567	-3.46705	7.397397
O	-4.03603	4.757037	7.709683	O	-2.03927	-5.94212	7.661333
O	-5.62139	4.312907	6.133044	O	-0.76918	-7.04206	6.120037
O	6.147664	-1.23072	-7.66153	H	-4.74028	5.355215	8.041971
O	6.523225	-2.77807	-6.03083	H	7.017833	-1.56081	-7.97453
O	-2.01983	5.974909	-7.67235	H	-2.14682	6.891363	-8.00114
O	-0.71652	7.058376	-6.14729	H	6.957641	1.639141	8.055225
H	-1.30586	-6.85265	-5.22698	H	-2.17328	-6.85698	7.991736
H	6.605622	2.313641	-5.1745				

Table S4. Coordinate file of **2a** with MeOH

ATOM	X	Y	Z	ATOM	X	Y	Z
H	13.81368	8.787239	12.35309	C	15.29147	17.78761	15.70863
C	13.52588	9.536238	13.09229	C	14.03383	20.30225	14.84891
C	12.74393	9.171591	14.19204	C	13.47902	19.20066	17.5018
C	13.93658	10.86642	12.9362	N	12.87625	18.26881	18.27957
C	10.16337	16.33436	14.44656	N	13.77603	14.52398	17.62161
Au	8.423734	15.1419	13.90186	N	10.63216	15.40864	19.4956
Au	11.8949	17.53642	14.99636	C	11.31335	11.94902	17.48303
Au	11.17897	14.5641	15.20383	C	12.79129	11.46129	14.99267
Au	9.157177	18.11505	13.69666	C	13.8289	13.32364	16.99415
Au	11.01753	16.03739	12.46232	C	9.012647	20.73534	11.42008
Au	9.297228	16.62109	16.429	C	7.560707	21.22273	13.92609
P	6.5738	13.94648	13.18062	C	6.497164	19.36832	11.93259
Ag	8.342387	16.54171	11.31641	C	13.60193	16.22147	10.14188
P	13.73701	18.73618	15.73015	C	11.52657	14.21785	9.530207
Ag	11.96865	16.13993	17.59234	C	10.98451	17.05733	9.188147
P	12.27463	12.75874	16.16295	C	6.696758	16.40369	18.71723
P	8.062293	19.92622	12.74826	C	8.740799	18.44929	19.34303
P	11.82753	15.83919	10.30079	C	9.312635	15.61376	19.70929
P	8.466141	16.81861	18.58352	C	4.918504	15.98473	14.10694
C	5.01929	14.89396	13.22529	C	3.916863	14.53607	12.4278
C	6.296116	12.37803	14.06407	C	7.383225	11.49188	14.19251
C	6.803726	13.48822	11.40387	C	5.068318	12.07056	14.67096
N	7.374878	14.42981	10.61341	C	6.411359	12.24339	10.91526
N	6.537983	18.16743	11.30554	C	7.553671	14.14258	9.312983
N	9.672949	17.29175	9.421371	C	5.430555	17.7437	10.6716
C	9.0327	18.16902	8.626434	C	9.659767	18.85316	7.586112
C	15.40275	16.69183	14.83478	H	7.975935	18.33532	8.837361
C	16.38534	18.15257	16.5143	H	14.55295	16.39632	14.21565

C	12.96589	21.21429	14.73825	C	16.6004	15.97485	14.75928
C	15.26064	20.58437	14.22765	C	17.57842	17.42893	16.43513
C	13.87531	20.44085	17.9991	H	16.31855	18.9975	17.20228
C	12.6576	18.56386	19.57208	H	12.00244	20.99823	15.2056
C	14.87545	14.95343	18.26564	C	13.13832	22.40662	14.03397
C	11.27969	14.54501	20.29941	C	15.42056	21.77632	13.51279
C	9.917839	12.11614	17.5019	H	16.09259	19.88237	14.29705
C	11.93425	11.1376	18.44995	H	14.35666	21.18097	17.35973
C	12.37576	10.1287	15.14327	C	13.64341	20.73993	19.34787
C	13.5637	11.83092	13.87382	C	13.01774	19.78351	20.14957
C	14.98112	12.53749	16.98823	H	12.17048	17.79459	20.1728
C	10.40818	20.5692	11.3897	C	16.06749	14.22792	18.31105
C	8.38242	21.54459	10.4576	H	14.80345	15.92202	18.76239
C	7.986936	22.55254	13.78202	C	10.64939	13.83681	21.32055
C	6.78755	20.85217	15.04417	H	12.34385	14.40649	20.10721
C	5.349392	20.16115	11.94809	H	9.43403	12.74855	16.75429
C	14.09279	17.35273	10.82092	C	9.147628	11.46863	18.47163
C	14.4774	15.42303	9.389206	C	11.15785	10.494	19.41719
C	11.2963	14.07469	8.151036	H	13.01639	10.99588	18.45402
C	11.54406	13.07977	10.35738	H	11.76514	9.830423	15.99602
C	11.68374	17.69237	8.157583	H	13.87737	12.86746	13.72437
C	6.258055	15.21978	18.09231	H	15.00552	11.5744	16.47812
C	5.772166	17.23075	19.37301	C	16.123	12.99645	17.65656
C	8.751946	18.63126	20.73773	H	10.89918	19.93862	12.13416
C	8.92592	19.55222	18.49132	C	11.16858	21.21457	10.4109
C	8.610216	14.95677	20.72405	C	9.149097	22.18569	9.481074
H	5.774456	16.27353	14.72067	H	7.300203	21.68544	10.46355
C	3.72321	16.70339	14.19931	H	8.597855	22.85102	12.92946
C	2.725947	15.26123	12.52394	C	7.628671	23.50571	14.74109
H	3.97548	13.6961	11.73313	C	6.424718	21.8124	15.98959
H	8.346812	11.72884	13.73551	H	6.463335	19.81692	15.17635
C	7.230129	10.30044	14.90271	H	5.334177	21.12455	12.45785
C	4.926726	10.8789	15.39042	C	4.19963	19.70862	11.28883
H	4.222053	12.75381	14.58746	H	13.42075	17.96982	11.42211
H	5.958041	11.49683	11.56728	C	15.44327	17.69096	10.72868
C	6.605765	11.95131	9.558827	C	15.83233	15.76292	9.31097
C	7.189358	12.92119	8.741675	H	14.11064	14.53856	8.866787
H	8.015892	14.91836	8.70099	H	11.27452	14.94378	7.491557
C	4.24287	18.47645	10.63501	C	11.09982	12.80149	7.607654
H	5.49228	16.77402	10.17558	C	11.35738	11.81058	9.805246
H	11.70594	13.18447	11.43193	C	6.84682	23.14	15.84059
H	12.74686	17.48628	8.027569	H	5.818078	21.52036	16.84833
C	11.01089	18.60676	7.336968	C	2.974994	20.57338	11.31566

H	6.968095	14.57924	17.56343	H	15.81798	18.57212	11.2518
C	4.912258	14.85868	18.14776	C	16.3148	16.8956	9.974204
C	4.421017	16.86706	19.41369	H	16.5098	15.13799	8.727322
H	6.096333	18.15875	19.84644	H	10.91826	12.69804	6.537059
H	8.620414	17.78642	21.41585	C	11.1298	11.67068	8.431498
C	8.933029	19.91156	21.26741	H	11.37709	10.9326	10.45342
C	9.10193	20.82938	19.02823	C	11.69306	19.35996	6.22995
H	8.933451	19.40931	17.40864	H	4.580598	13.93346	17.67279
H	7.541392	15.14275	20.83596	C	3.991498	15.68267	18.8069
C	9.287346	14.04584	21.54509	H	3.704285	17.51371	19.92289
H	3.652927	17.54802	14.88715	H	8.942462	20.05125	22.34962
C	2.627214	16.34256	13.40865	C	9.106217	21.00914	20.41577
H	1.873255	14.97746	11.90482	H	9.244519	21.68086	18.36114
H	8.073231	9.613299	14.99406	C	8.610322	13.24587	22.62407
C	6.003783	9.994135	15.50591	H	1.695768	16.90646	13.4777
H	3.970011	10.64601	15.86057	H	5.889634	9.066114	16.06825
C	6.181374	10.60472	9.053194	O	5.678595	9.747674	9.765124
H	7.368717	12.74417	7.682938	O	6.422294	10.45193	7.736532
H	3.378609	18.07868	10.10688	H	18.62102	15.77994	15.50157
H	9.100473	19.56368	6.97882	H	14.4959	23.61917	12.8641
H	16.67944	15.12613	14.07736	O	14.61869	22.92694	19.17072
C	17.68794	16.3427	15.55803	O	13.79362	22.23894	21.17252
H	18.42437	17.71845	17.06079	H	9.166347	10.15847	20.18998
H	12.31041	23.11389	13.95936	O	18.35552	12.66963	18.36644
C	14.36447	22.68861	13.41854	O	17.42793	11.08139	17.03166
H	16.37679	21.98872	13.03231	H	11.13298	22.51874	8.688424
C	14.07531	22.07954	19.86439	H	6.56733	23.88697	16.58487
H	12.80776	19.9667	21.20168	O	1.966194	20.05338	10.58992
H	16.92536	14.62983	18.8465	O	2.910585	21.62813	11.9299
H	11.21232	13.13232	21.93123	H	17.37219	17.15762	9.910223
H	8.064388	11.60178	18.48015	H	10.97258	10.67964	8.001877
C	9.767599	10.65842	19.42872	O	12.7405	18.76227	5.622636
H	11.64307	9.865559	20.1659	O	11.33599	20.47258	5.884656
H	12.41562	8.138149	14.31699	H	2.937713	15.40117	18.84027
H	14.54272	11.15847	12.07706	H	9.251356	22.00599	20.83599
C	17.35299	12.13922	17.63934	O	7.479514	13.74495	23.16512
H	12.25168	21.08199	10.39146	O	9.050705	12.17394	23.00225
C	10.53919	22.02148	9.457201	H	6.124316	9.551469	7.48184
H	8.65676	22.81144	8.734752	H	14.10164	23.1333	21.43645
H	7.964792	24.53725	14.62248	H	19.12317	12.05994	18.30738
H	1.202511	20.66733	10.6564	H	7.290682	14.64788	22.84098
H	12.85234	17.83811	5.922029				

Table S5. Coordinate file of **2b** with MeOH

ATOM	X	Y	Z	ATOM	X	Y	Z
C	7.013951	5.633083	1.939717	H	6.329867	9.32274	-2.22025
C	5.72621	6.174681	1.802242	C	9.712222	3.916736	-2.43006
C	7.202689	4.454405	2.685614	C	7.454944	2.746533	-2.49167
P	8.483191	6.430512	1.214701	H	11.56337	5.007585	-2.18304
H	5.568643	7.096962	1.242251	N	13.94396	6.018129	-0.74092
C	4.635494	5.53274	2.397418	N	11.62441	9.044649	-0.70387
C	6.107	3.813652	3.266175	H	16.22207	4.908897	2.90577
H	8.203627	4.036672	2.817987	P	14.04117	4.091756	1.1899
C	7.948303	8.010738	0.481682	H	11.40575	11.55754	2.883651
C	8.940624	5.378574	-0.23325	P	13.25995	10.11753	1.196456
Au	10.24258	6.653702	2.715039	H	16.23095	8.826779	5.323877
H	3.636844	5.959291	2.289288	P	14.05252	9.655327	7.037096
C	4.82234	4.351897	3.122046	H	11.43002	2.206168	5.324104
H	6.259124	2.896057	3.836861	P	13.27807	3.637257	7.02413
C	8.175823	9.196656	1.201538	C	7.208158	9.298561	5.5467
C	7.284199	8.061445	-0.75678	C	7.018219	8.119294	6.291402
C	8.041622	4.46977	-0.78969	C	7.947114	5.738619	7.74487
N	10.18932	5.556315	-0.72803	C	8.943984	8.367995	8.466644
C	11.95915	6.877014	4.113834	H	6.721543	11.42307	-0.9342
Au	10.24551	7.09765	5.515952	H	10.06628	3.364037	-3.29845
H	3.967331	3.854911	3.583522	O	7.949154	2.113879	-3.5742
H	8.698258	9.163179	2.16014	O	6.340056	2.551301	-2.03058
C	7.728851	10.4203	0.69574	C	14.7134	5.009259	-0.26717
C	6.842344	9.289212	-1.25728	C	14.36819	6.687483	-1.82668
H	7.106578	7.15413	-1.3363	C	12.08666	10.22602	-0.22811
H	7.044588	4.332836	-0.37131	C	10.80728	9.062521	-1.77081
C	8.431759	3.723938	-1.91012	C	16.37572	3.852878	2.67134
C	10.55356	4.840783	-1.80591	C	15.45843	3.162981	1.857577
Ag	11.94675	6.873081	0.301822	C	12.88182	2.884586	0.467013
Au	13.02235	5.518328	2.71562	C	12.24807	12.22561	2.6902
Au	12.59811	8.489785	2.716534	C	13.32524	11.79998	1.889663
Au	13.02613	8.233459	5.511528	C	14.86925	9.768287	0.415536
Au	12.60711	5.266339	5.51009	C	16.38773	9.883116	5.554761
H	8.209449	9.715689	5.415228	C	15.47327	10.57803	6.367506
P	8.48624	7.319471	7.016322	C	12.89499	10.86468	7.759338
H	7.90602	11.3371	1.260438	C	14.72057	8.735198	8.494688
C	7.062632	10.46677	-0.53397	C	12.27452	1.539128	5.511495
C	13.3496	1.960865	6.31692	H	7.104	6.592379	9.563697
C	14.88619	3.987368	7.806619	H	7.04763	9.412376	8.608734
C	12.09997	3.516933	8.443597	C	8.436934	10.02121	10.14548

C	6.113131	9.940441	4.966108	C	10.55897	8.905108	10.03762
C	5.730013	7.578468	6.427639	Ag	11.94884	6.873315	7.927886
C	8.172325	4.554195	7.021911	H	16.54273	3.856011	-0.44982
C	7.280059	5.686308	8.981749	C	16.36562	5.364489	-1.98455
C	8.045266	9.275432	9.025627	H	15.85515	6.969001	-3.36063
N	10.1935	8.190319	8.959632	H	12.08956	12.39044	-0.3849
H	7.261194	1.491172	-3.89601	C	10.87037	11.45877	-1.90308
C	15.93053	4.663231	-0.85295	H	9.744462	10.19451	-3.26626
C	15.56544	6.393308	-2.48354	C	17.68483	1.829165	2.908368
H	13.72835	7.496419	-2.18086	H	18.20267	3.730287	3.810175
C	11.72275	11.44824	-0.79189	H	14.9368	1.247005	0.974638
C	10.40728	10.24111	-2.40377	C	16.76423	1.137433	2.115391
H	10.45407	8.095805	-2.13122	H	11.5472	3.002323	2.17287
C	17.49088	3.188285	3.185256	C	10.84277	1.586258	0.700392
C	15.64938	1.797964	1.589299	C	12.2195	1.337281	-1.28113
C	11.73759	2.532849	1.20557	H	13.99412	2.553414	-1.3758
C	13.11824	2.284917	-0.78301	C	13.3356	14.36659	3.008743
C	12.25176	13.50967	3.237373	H	11.41167	13.83786	3.851895
C	14.41374	12.65794	1.668014	H	15.26035	12.33358	1.061521
C	15.79966	8.975416	1.109833	C	14.41423	13.93904	2.228981
C	15.19466	10.27477	-0.85533	H	15.54791	8.567506	2.091111
C	17.50361	10.54321	5.03655	C	17.0458	8.70042	0.541603
C	15.66855	11.94342	6.631093	C	16.44172	9.992896	-1.41868
C	11.75259	11.21903	7.019224	H	14.4837	10.88624	-1.41327
C	13.12956	11.46172	9.010941	C	17.70153	11.90274	5.308579
C	15.93606	9.080338	9.084272	H	18.21279	9.997329	4.412029
N	13.9508	7.72443	8.964336	H	14.95827	12.49841	7.244787
C	12.28333	0.260612	4.951667	C	16.7841	12.59937	6.100898
C	14.44109	1.104815	6.53101	H	11.56352	10.75141	6.050765
C	15.81741	4.779888	7.113051	C	10.85816	12.16621	7.523976
C	15.21085	3.479346	9.077029	C	12.23139	12.41017	9.508543
C	11.73144	2.289196	8.991236	H	14.00377	11.1909	9.605121
N	11.63142	4.693223	8.925878	H	16.54796	9.889642	8.685415
C	4.827955	9.403205	5.109513	C	16.36935	8.376333	10.21483
H	6.266113	10.85855	4.396481	C	14.37315	7.05265	10.04938
H	5.571541	6.655622	6.986415	C	13.37008	-0.59457	5.172805
C	4.639908	8.221929	5.833062	H	11.44497	-0.06459	4.333224
H	8.696758	4.588998	6.064471	H	15.28625	1.426468	7.140941
C	7.721202	3.330294	7.523433	C	14.44643	-0.17084	5.957818
C	6.835104	4.458103	9.478555	H	15.56606	5.189185	6.132229
C	17.06434	5.051811	7.681054	H	13.73283	6.242694	10.40028
C	16.4587	3.758199	9.640168	H	13.37805	-1.58939	4.725203
H	14.49902	2.868182	9.634227	H	15.29797	-0.83162	6.126121

H	12.10536	1.351897	8.579483	H	17.78265	5.668588	7.138158
C	10.86044	2.2655	10.08757	C	17.38435	4.545127	8.945765
C	10.80268	4.663351	9.983526	H	16.70285	3.362688	10.62739
H	3.973518	9.901239	4.648137	C	10.39251	3.477739	10.59708
H	3.64091	7.796048	5.940527	C	10.46228	0.936204	10.65571
H	7.897458	2.414594	6.956682	H	10.44671	5.626259	10.35145
C	7.053209	3.282046	8.752116	H	6.709673	2.325393	9.149417
H	6.321731	4.423074	10.441	H	10.07367	10.38167	11.53104
C	9.718325	9.828843	10.66326	O	7.9561	11.63148	11.80987
C	7.460498	10.99816	10.72839	O	6.344809	11.19256	10.26886
H	11.5695	8.73866	10.41299	O	17.93383	5.675178	-3.72931
C	17.6733	4.974707	-2.60858	O	18.41184	4.118516	-2.1441
C	10.48959	12.77997	-2.50133	O	9.683276	12.64223	-3.57207
H	18.55268	1.309328	3.316502	O	10.86732	13.85466	-2.05818
H	16.9088	0.077155	1.902471	H	10.38292	0.250672	-0.93673
H	9.955788	1.319101	1.276743	H	18.33675	8.982292	-1.1712
C	11.08381	0.987516	-0.54105	H	10.39695	13.49975	9.162332
H	12.40536	0.875629	-2.25225	H	15.85691	6.768305	11.58603
H	13.33959	15.36575	3.446626	O	17.93558	8.060736	11.96052
H	15.26351	14.60123	2.05487	O	18.41495	9.622553	10.38079
H	17.76297	8.082533	1.084734	H	18.35569	4.7651	9.392739
C	17.36614	9.204844	-0.72392	H	9.716909	3.514819	11.44999
H	16.68616	10.38677	-2.40647	O	9.634589	1.059445	11.71169
H	18.56987	12.41907	4.897042	O	10.84267	-0.13249	10.20045
H	16.93158	13.65999	6.310019	H	7.268291	12.25385	12.13265
H	9.97272	12.43551	6.946276	H	18.79968	5.369479	-4.07761
C	11.09763	12.76262	8.76681	H	9.474684	13.54143	-3.9071
H	12.41591	12.87002	10.48077	H	18.80118	8.365275	12.31047
C	15.56874	7.345924	10.7097	H	9.413025	0.155504	12.02507
C	17.67594	8.764975	10.84197				

Table S6. Coordinate file of **2a** with MeCN

ATOM	X	Y	Z	ATOM	X	Y	Z
H	13.80262	8.751911	12.36588	Au	11.90317	17.5308	14.99617
C	13.50787	9.505731	13.09749	Au	11.16543	14.55922	15.19772
C	12.72477	9.146946	14.19831	Au	9.170819	18.13188	13.69189
C	13.91365	10.83619	12.93215	Au	11.02489	16.04635	12.45874
C	10.16655	16.34468	14.44461	Au	9.290516	16.62782	16.42695
Au	8.419338	15.16479	13.90592	P	6.568654	13.96712	13.19649
Ag	8.34872	16.55617	11.32385	C	13.88113	20.44412	17.97458

P	13.75468	18.71951	15.72166	C	12.67086	18.57514	19.56382
Ag	11.95705	16.13822	17.58356	C	14.85945	14.92432	18.2631
P	12.25249	12.74465	16.1515	C	11.27302	14.54574	20.29558
P	8.073925	19.94275	12.74165	C	9.902162	12.095	17.50251
P	11.8388	15.85903	10.2977	C	11.9267	11.12233	18.43873
P	8.450337	16.8097	18.57959	C	12.35341	10.1104	15.14189
C	5.00479	14.89818	13.24498	C	13.5356	11.80756	13.86089
C	6.314069	12.40861	14.1041	C	14.95707	12.51368	16.97522
C	6.797464	13.50392	11.42074	C	10.40755	20.5883	11.36053
N	7.36387	14.44896	10.6305	C	8.371365	21.56116	10.44919
N	6.540305	18.18091	11.3131	C	8.022943	22.56863	13.77952
N	9.674393	17.30081	9.421967	C	6.812657	20.87554	15.04137
C	15.30345	17.7631	15.69781	C	5.35747	20.17955	11.95076
C	14.0515	20.27852	14.82736	C	14.10077	17.38423	10.81361
C	13.49589	19.19519	17.48979	C	14.49199	15.44369	9.399297
N	12.89548	18.26743	18.27467	C	11.33629	14.09887	8.137314
N	13.7603	14.50435	17.61205	C	11.58696	13.09654	10.34018
N	10.62338	15.40658	19.49068	C	11.68143	17.71549	8.157032
C	11.29792	11.9325	17.47583	C	6.247087	15.19724	18.0953
C	12.76477	11.44342	14.98258	C	5.759213	17.20287	19.3837
C	13.80919	13.30623	16.98026	C	8.718684	18.60825	20.74899
C	9.011992	20.75112	11.40401	C	8.890482	19.54619	18.50958
C	7.584894	21.24231	13.92151	C	8.599927	14.93701	20.70952
C	6.503007	19.38329	11.93752	H	5.747632	16.28651	14.73895
C	13.61242	16.24823	10.14074	C	3.689121	16.68958	14.22495
C	11.55655	14.2383	9.51849	C	2.704052	15.2353	12.55295
C	10.98739	17.07477	9.187901	H	3.97198	13.68685	11.75694
C	6.683198	16.38421	18.71628	H	8.368294	11.77389	13.77126
C	8.712005	18.43591	19.35294	C	7.278344	10.36166	14.98291
C	9.301608	15.60201	19.69945	C	4.975367	10.92941	15.48354
C	4.893949	15.98764	14.12684	H	4.243528	12.77817	14.644
C	3.903917	14.52572	12.45201	H	5.965301	11.50675	11.58446
C	7.411292	11.53667	14.24173	C	6.608111	11.9674	9.574556
C	5.096592	12.10418	14.73316	C	7.184118	12.94201	8.757797
C	6.413004	12.25647	10.93199	H	7.999076	14.94381	8.717794
C	7.543771	14.16407	9.329959	C	4.247843	18.49677	10.63762
C	5.432427	17.75931	10.67872	H	5.491213	16.78801	10.18565
C	9.027259	18.17264	8.626433	C	9.648665	18.86143	7.586079
C	15.40883	16.67169	14.81746	H	7.969562	18.33183	8.83823
C	16.39974	18.1194	16.50395	H	14.55689	16.38369	14.19768
C	12.9756	21.17711	14.69187	C	16.60389	15.95149	14.73408
C	15.28308	20.56494	14.21769	C	17.59037	17.39244	16.41695
H	16.33664	18.96117	17.196	C	4.412569	16.82627	19.44323

H	12.00902	20.95661	15.1509	H	6.080532	18.13454	19.85167
C	13.14421	22.36206	13.97412	H	8.590814	17.75812	21.42122
C	15.43981	21.74975	13.49	C	8.888726	19.8862	21.28823
H	16.12089	19.87234	14.30886	C	9.056217	20.8208	19.05615
H	14.36098	21.17948	17.32875	H	8.903361	19.41165	17.42587
C	13.63817	20.75733	19.31787	H	7.527926	15.11301	20.80748
C	13.01665	19.80516	20.12775	C	9.279236	14.03173	21.5349
H	12.18436	17.81	20.17047	H	3.608825	17.53166	14.91483
C	16.04651	14.1908	18.31189	C	2.59454	16.31435	13.43879
H	14.79107	15.89094	18.76414	H	1.852649	14.93992	11.93745
C	10.64392	13.83415	21.31521	H	8.129349	9.685827	15.08442
H	12.33856	14.41344	20.10688	C	6.06245	10.05885	15.60878
H	9.412168	12.72554	16.75732	H	4.027203	10.70107	15.97269
C	9.139949	11.44602	18.47758	C	6.190289	10.62072	9.063693
C	11.15856	10.47749	19.41147	H	7.360983	12.76836	7.698112
H	13.00926	10.98415	18.43649	H	3.383915	18.10188	10.10687
H	11.74471	9.815516	15.99715	H	9.083488	19.56711	6.978632
H	13.8474	12.84332	13.70071	H	16.67794	15.10608	14.04755
H	14.97859	11.5531	16.46038	C	17.69466	16.31178	15.53206
C	16.09822	12.96231	17.65168	H	18.43928	17.67554	17.04157
H	10.90683	19.95664	12.09859	H	12.31043	23.05973	13.87728
C	11.15703	21.23817	10.37632	C	14.37455	22.64771	13.36886
C	9.127003	22.2058	9.466661	H	16.39942	21.96631	13.01799
H	7.289274	21.7016	10.46742	C	14.04618	22.11132	19.81795
H	8.633144	22.86428	12.92541	H	12.79285	20.00316	21.17465
C	7.677056	23.52187	14.74318	H	16.90363	14.58503	18.85433
C	6.462106	21.83594	15.99121	H	11.20944	13.13491	21.92941
H	6.475881	19.84377	15.16837	H	8.056136	11.57373	18.49196
H	5.344764	21.14347	12.45947	C	9.768036	10.63884	19.43179
C	4.207775	19.7303	11.28892	H	11.65013	9.851256	20.15794
H	13.42649	18.00756	11.40569	H	12.40038	8.113237	14.33152
C	15.45214	17.72019	10.72621	H	14.52264	11.12291	12.07324
C	15.84787	15.78075	9.326859	C	17.3228	12.09753	17.63619
H	14.12802	14.5551	8.882018	H	12.24024	21.10873	10.34603
H	11.30349	14.97082	7.482026	C	10.51734	22.04628	9.430635
C	11.15976	12.82572	7.586989	H	8.626471	22.83253	8.726601
C	11.41852	11.8277	9.781194	H	8.023226	24.55027	14.62742
H	11.74291	13.19818	11.41592	C	6.896325	23.15997	15.84476
H	12.74594	17.51721	8.02622	H	5.855583	21.54681	16.85099
C	11.0015	18.62489	7.336635	C	2.986162	20.59939	11.30974
H	6.956046	14.56192	17.55883	H	15.8241	18.60605	11.24335
C	4.905871	14.82251	18.17082	C	16.32791	16.91786	9.984153
H	16.52766	15.15012	8.752052	O	18.32251	12.61294	18.37778

H	10.98586	12.72522	6.514786	O	17.39581	11.04621	17.01688
C	11.20079	11.69147	8.405601	H	11.10273	22.54597	8.657118
H	11.44777	10.94657	10.42466	H	6.627918	23.90712	16.59285
C	11.67708	19.38193	6.228209	O	1.982749	20.08835	10.57012
H	4.575528	13.89452	17.70054	O	2.919419	21.65101	11.92918
C	3.986446	15.63753	18.84278	H	17.38607	17.17802	9.925101
H	3.696735	17.46629	19.96197	H	11.06052	10.70048	7.970121
H	8.893279	20.01763	22.37155	O	12.72597	18.78961	5.618406
C	9.055453	20.99114	20.44482	O	11.31508	20.4936	5.884678
H	9.194496	21.67787	18.39536	H	2.936037	15.34589	18.89148
C	8.609443	13.23264	22.62019	H	9.192269	21.98588	20.87272
H	1.6551	16.86449	13.51331	O	7.423478	13.67257	23.08961
H	5.966734	9.145301	16.19723	O	9.10124	12.21151	23.06956
O	5.685459	9.760368	9.770081	H	6.149939	9.571519	7.487896
O	6.442987	10.47175	7.748732	H	14.06804	23.18097	21.37879
H	18.6262	15.74723	15.4691	H	19.08639	11.99849	18.31811
H	14.50126	23.57085	12.80102	H	1.221124	20.70536	10.63196
O	14.55482	22.96541	19.10644	H	12.84333	17.86597	5.917307
O	13.78191	22.27538	21.12861	H	7.179143	14.5407	22.71288
H	9.17231	10.13616	20.19572				

Table S7. Coordinate file of **2b** with MeCN

ATOM	X	Y	Z	ATOM	X	Y	Z
C	7.049735	5.53678	1.963437	C	8.046914	4.391506	-0.77916
C	5.755719	6.072845	1.87056	N	10.19827	5.471618	-0.73135
C	7.267194	4.352581	2.692972	C	11.96746	6.874779	4.103698
P	8.495785	6.356434	1.215241	Au	10.2582	7.136063	5.509259
H	5.578282	6.999378	1.323758	H	4.066783	3.732377	3.693678
C	4.687332	5.421722	2.496107	H	8.645431	9.098061	2.144873
C	6.194107	3.703572	3.304982	C	7.636285	10.32136	0.678477
H	8.273729	3.939296	2.791598	C	6.771423	9.159235	-1.26589
C	7.91708	7.918145	0.475189	H	7.087924	7.030438	-1.33268
C	8.951798	5.298981	-0.22931	H	7.053257	4.255823	-0.35234
Au	10.25606	6.621398	2.710491	C	8.426463	3.645009	-1.90243
H	3.684071	5.844657	2.423956	C	10.55267	4.75516	-1.81236
C	4.902884	4.237838	3.207387	Ag	11.97312	6.766824	0.278954
H	6.366597	2.780634	3.861022	Au	13.00776	5.454518	2.739052
C	8.117369	9.112387	1.188886	Au	12.64943	8.421064	2.653576
C	7.246073	7.945618	-0.76013	Au	12.98363	8.316923	5.461866

Au	12.64605	5.322232	5.545083	C	14.92242	4.025539	7.86444
H	8.287358	9.835953	5.475888	C	12.1055	3.62128	8.488705
P	8.490126	7.38089	6.997468	C	6.216697	10.07335	4.928174
H	7.79474	11.24588	1.235939	C	5.758814	7.682604	6.318035
C	6.964411	10.34512	-0.54851	C	8.113419	4.62352	6.956636
H	6.256095	9.175197	-2.2278	C	7.218215	5.744421	8.920842
C	9.70358	3.835428	-2.43199	C	8.027687	9.261488	9.071812
C	7.444373	2.667763	-2.47502	N	10.19922	8.228543	8.956027
H	11.56135	4.917002	-2.19479	H	7.238783	1.407861	-3.873
N	14.02324	5.924849	-0.68755	C	16.06933	4.655519	-0.64053
N	11.67276	8.937429	-0.76591	C	15.7793	6.409246	-2.26311
H	16.07387	4.728311	3.157382	H	13.86374	7.406703	-2.13065
P	14.03879	4.006345	1.241721	C	11.65485	11.34528	-0.79102
H	11.54313	11.3899	2.959273	C	10.32119	10.11708	-2.3726
P	13.30796	10.03345	1.117344	H	10.49126	7.971921	-2.17198
H	15.92386	9.226069	4.873225	C	17.25325	2.961711	3.535853
P	13.99784	9.775256	6.960735	C	15.57545	1.670659	1.696084
H	11.565	2.326651	5.230871	C	11.7138	2.488649	1.138212
P	13.30666	3.70901	7.086337	C	13.17379	2.240776	-0.79199
C	7.280511	9.418491	5.550124	C	12.36081	13.35757	3.297112
C	7.052935	8.222547	6.257538	C	14.41661	12.60559	1.546253
C	7.901181	5.802105	7.692734	C	15.85577	8.918484	0.999807
C	8.943864	8.396654	8.473921	C	15.25753	10.31101	-0.90365
H	6.599972	11.29141	-0.95243	C	17.07531	11.02895	4.577667
H	10.04946	3.282812	-3.30373	C	15.50413	12.14345	6.616522
O	7.929804	2.031407	-3.55929	C	11.69212	11.33234	7.133575
O	6.33276	2.47412	-2.00527	C	13.11901	11.38901	9.103508
C	14.79109	4.940688	-0.16217	C	16.07256	9.130421	8.797858
C	14.51002	6.628242	-1.72347	N	14.04526	7.831234	8.85976
C	12.10287	10.12765	-0.28112	C	12.39238	0.355931	4.932886
C	10.81258	8.944294	-1.79735	C	14.42326	1.138509	6.697889
C	16.22682	3.674364	2.91325	C	15.89935	4.7026	7.113884
C	15.38855	3.032856	1.98269	C	15.23348	3.549746	9.15019
C	12.89023	2.834003	0.451037	C	11.6654	2.406892	9.013564
C	12.34937	12.08733	2.718971	N	11.6657	4.813811	8.958802
C	13.37236	11.71	1.829324	C	4.925595	9.533773	4.991225
C	14.91728	9.71838	0.325425	H	6.396334	11.00472	4.389022
C	16.08765	10.25759	5.194143	H	5.57485	6.746887	6.8463
C	15.30224	10.81038	6.222009	C	4.699941	8.339695	5.682423
C	12.84585	10.90259	7.812976	H	8.651345	4.66031	6.00684
C	14.79296	8.830492	8.332957	C	7.637469	3.400693	7.437777
C	12.36939	1.634761	5.492183	C	6.74841	4.517333	9.397287
C	13.38044	2.026798	6.388706	H	7.049945	6.644538	9.513782

H	7.025747	9.392668	8.663121	C	16.51835	3.735812	9.66861
C	8.405916	9.968582	10.22048	H	14.484	3.033292	9.7527
C	10.55377	8.910477	10.05893	H	12.01958	1.456822	8.614111
Ag	11.99539	6.980278	7.919225	C	10.73875	2.416273	10.06498
H	16.67573	3.867645	-0.19393	C	10.79344	4.813548	9.979619
C	16.57867	5.409042	-1.70609	H	4.098284	10.04306	4.494257
H	16.12421	7.019459	-3.09603	H	3.698278	7.909363	5.724705
H	11.99676	12.29246	-0.37435	H	7.80533	2.490778	6.859381
C	10.74076	11.34234	-1.85302	C	6.955652	3.347	8.658589
H	9.618746	10.06001	-3.20219	H	6.222756	4.47861	10.35299
C	17.43833	1.604126	3.247874	C	9.69385	9.786246	10.72492
H	17.89868	3.46369	4.258869	C	7.410458	10.8912	10.85662
H	14.92419	1.156125	0.988615	H	11.57002	8.754311	10.42283
C	16.60216	0.962689	2.329057	C	17.96513	5.112226	-2.19477
H	11.4864	2.954902	2.099228	C	10.2471	12.65574	-2.37972
C	10.83357	1.550095	0.594027	H	18.23348	1.044547	3.74297
C	12.28837	1.301923	-1.33009	H	16.74156	-0.09573	2.103076
H	14.07505	2.5059	-1.34673	H	9.923061	1.285664	1.133628
C	13.39873	14.25144	3.006182	C	11.12286	0.954274	-0.63846
H	11.5624	13.64872	3.981763	H	12.51118	0.844406	-2.29553
H	15.22779	12.31725	0.877213	H	13.40952	15.24044	3.466567
C	14.42416	13.87346	2.134685	H	15.24129	14.56299	1.915234
H	15.59019	8.44396	1.946955	H	17.85706	8.112008	0.987882
C	17.13095	8.732399	0.459495	C	17.47209	9.33595	-0.75603
C	16.53482	10.12056	-1.43779	H	16.79524	10.58596	-2.38987
H	14.53685	10.92574	-1.44621	H	18.03783	12.96329	4.48213
C	17.27517	12.35651	4.973512	H	16.64329	13.94685	6.297939
H	17.68053	10.59459	3.78017	H	9.935768	12.58243	7.202154
H	14.88923	12.59362	7.39677	C	11.10919	12.74235	9.015843
C	16.49248	12.90983	5.991779	H	12.46535	12.68038	10.70167
H	11.47102	10.94994	6.13492	C	15.8225	7.367357	10.41661
C	10.82922	12.25236	7.734708	C	17.98486	8.702197	10.34116
C	12.24992	12.30736	9.699185	H	13.92511	6.334758	10.29188
H	14.00408	11.06061	9.650615	H	13.4483	-1.52489	4.800792
H	16.66184	9.929785	8.349024	H	15.25934	-0.82159	6.366717
C	16.60176	8.381626	9.857243	H	17.93779	5.400318	7.045058
C	14.55359	7.127886	9.885201	C	17.49348	4.394924	8.911959
C	13.42911	-0.53025	5.248699	H	16.75296	3.365542	10.66766
H	11.60472	0.05182	4.241704	C	10.29853	3.644715	10.55929
H	15.2234	1.439957	7.374427	C	10.25596	1.106545	10.60994
C	14.44311	-0.13747	6.127459	H	10.46589	5.788235	10.34207
H	15.65853	5.089225	6.121564	H	6.590968	2.390692	9.03768
C	17.18254	4.879452	7.63616	H	10.03834	10.30909	11.61522

O	7.902861	11.4926	11.95729	O	18.6936	9.562848	9.839831
O	6.284035	11.07449	10.41837	H	18.49587	4.537202	9.319656
O	18.3239	5.905749	-3.22235	H	9.582974	3.707742	11.3772
O	18.68475	4.253122	-1.7063	O	9.297815	1.265453	11.54357
O	9.380302	12.50181	-3.39939	O	10.6881	0.022399	10.24558
O	10.59405	13.73822	-1.92922	H	7.201809	12.07829	12.31764
H	10.43487	0.223011	-1.06584	H	19.24026	5.664373	-3.48004
H	18.46802	9.187998	-1.17767	H	9.099114	13.39602	-3.69159
H	10.43304	13.45974	9.48435	H	19.26584	8.187371	11.63598
H	16.18197	6.762186	11.24709	H	9.038097	0.373479	11.86133
O	18.35338	7.92905	11.381				