

Supporting Information

Synergistic Interfacial Engineering and Orbital Hybridization in Polyoxometalates@Porous Aromatic Framework Catalyst for Efficient Ethanol Oxidative Esterification

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Materials. $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ (10213-10-2) was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. Hexane (110-54-3) was purchased from Sigma Aldrich Co., Ltd. Na_2HPO_4 (7558-79-4), acetone (67-64-1), ethanol (64-17-5), methanol (67-56-1), 1,4-diethynylbenzene (935-14-8), tetrakis (triphenylphosphine) palladium (14221-01-3), copper iodide (7681-65-4), N, N-dimethylformamide (68-12-2), triethylamine, chloroform (121-44-8), tetrahydrofuran (109-99-9) and $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10026-22-9) were purchased from Shanghai Macklin Biochemical Co., Ltd. All chemicals and solvents used in this work were of Analytical Reagent (AR) grade without further purification.

Syntheses of $\text{K}_5\text{PW}_{11}\text{CoO}_{39}$ (PW_{11}Co) and iPAF-2 followed the previous reports^[1, 2].

Preparation of $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ hybrids. To synthesize $\text{PW}_{11}\text{Co}(35\%)@i\text{PAF-2}$, 1.20 g of PW_{11}Co and 2.24 g of iPAF-2 were mixed in 100 mL of distilled water and stirred vigorously at room temperature for 48 h. Subsequently, the resultant solid was washed repeatedly with distilled water for 0.5 h to remove PW_{11}Co that was adsorbed on the surface of iPAF-2. The final product, $\text{PW}_{11}\text{Co}@i\text{PAF-2}$, was then dried, achieving a yield of 87.9%.

Physical measurements. Elemental analysis was performed using an inductively coupled plasma emission spectroscopy (ICP-ES) and a P-E 2400 CHN elemental analyzer. Fourier Transform Infrared Spectroscopy (FTIR) spectra ($400\text{-}4000\text{ cm}^{-1}$) were recorded in KBr disks on a Nicolet Magna 560 IR spectrometer. Transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HR-TEM) were recorded on a Hitachi H-600 transmission electron microscope, and Energy-dispersive X-ray (EDAX) spectroscopy and mapping were performed using an XL30 ESEM FEG at 25 kV (PhilipsXL-30). Acid and alkali quantities were obtained via a Zdj-4b automatic potentiometric titrator. The samples' Brunauer-Emmett-Teller (BET) surface areas were measured by N_2 adsorption desorption on Micromeritics ASAP 2020 at $196\text{ }^\circ\text{C}$. Before the analysis, the samples were degassed at $200\text{ }^\circ\text{C}$ for 3 h. The total pore volumes and the average pore sizes of the samples were determined by the Barrett-Joyner-Halenda (BJH) method. X-ray photoelectron spectroscopy (XPS)

was used to analyze the elemental state of the sample at ESCALAB 250 X, equipped with a microfocus monochromatic Al K X-ray source. ^1H nuclear magnetic resonance (NMR) was recorded with Bruker Avance III model 400 MHz NMR spectrometer. Gas Chromatography-Mass Spectrometry (GC-MS) was carried out using a TSQ8000evo instrument. Electrochemical analysis was carried out using a Shanghai Chenhua Instrument Company Limited CHI600E. *In-situ* Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectroscopy was utilized to analyze ethanol and O_2 adsorption on the surface of the catalyst. Measurements were conducted over the $400\text{--}4000\text{ cm}^{-1}$ with a 4 cm^{-1} resolution using a VERTEX70 infrared spectrometer equipped with an MCT detector. Catalysts were placed in a stainless steel *in-situ* cell with a zinc selenide window, allowing precise temperature control. Conducted in O_2 atmosphere, no pretreatment was applied to the catalysts. The experimental sequence for *in-situ* DRIFT spectroscopy measurement process included the following steps: The *in-situ* cell was purged with N_2 at 1.0 MPa and $20\text{ mL}\cdot\text{min}^{-1}$, followed by O_2 exposure over the catalyst at the same rate (O_2 adsorption). N_2 (1.0 MPa , $20\text{ mL}\cdot\text{min}^{-1}$) was passed through catalyst to remove adsorbates, then vaporized ethanol at $50\text{ }^\circ\text{C}$ was introduced with N_2 through the catalysts *in-situ* cell to complete ethanol adsorption.

Adsorption experiment. Adsorption of ethanol over $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ was done as follows: 0.1 g of $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ was added to 5 mL of ethanol, which was stirred at 600 rpm for 12 h at room temperature. Separated solid was characterized using FTIR spectroscopy to determine the chemical state changes upon ethanol adsorption on $\text{PW}_{11}\text{Co}@i\text{PAF-2}$.

Pyridine adsorption infrared spectroscopy (Py-FTIR): The samples were placed in a pyridine environment, baked under vacuum at $200\text{ }^\circ\text{C}$ for 12 h , and subjected to FTIR spectroscopy. The Brønsted (B) acidity and Lewis (L) acidity were determined from the peak positions of the samples at 1540 cm^{-1} and 1450 cm^{-1} , respectively.

Reaction performance evaluation. The gas chromatographic conditions were as follows: inlet temperature: $240\text{ }^\circ\text{C}$; detector temperature: $250\text{ }^\circ\text{C}$; column temperature: $100\text{ }^\circ\text{C}$ for 10 min , warming up to $210\text{ }^\circ\text{C}$ at $10\text{ }^\circ\text{C}\cdot\text{min}^{-1}$ for 10 min . The substrate and product contents in the samples were determined using the external standard method to

calculate the conversion rates. Agilent Technologies 7820A, HP-5 gas chromatography column, flame ionization detector.

Calculation of ethanol conversion efficiency, acetaldehyde, acetic acid, ethyl acetate (EA), and diethyl ether yield were done:

$$\text{Ethanol conversion} = \frac{M_1 - M_2}{M_1} \times 100 \%$$

$$\text{Yield of acetaldehyde} = \frac{M_{\text{acetaldehyde}}}{M_1} \times 100 \%$$

$$\text{Yield of acetic acid} = \frac{M_{\text{acetic acid}}}{M_1} \times 100 \%$$

$$\text{Yield of EA} = \frac{2M_{EA}}{M_1} \times 100 \%$$

$$\text{Yield of diethyl ether} = \frac{2M_{\text{diethyl ether}}}{M_1} \times 100 \%$$

M_1 : initial molar amount of ethanol (65.41 μmol); M_2 : molar amount of ethanol after reaction; $M_{\text{acetaldehyde}}$: molar amount of resulting acetaldehyde; $M_{\text{acetic acid}}$: molar amount of resulting acetic acid; M_{EA} : molar amount of resulting EA; $M_{\text{diethyl ether}}$: molar amount of resulting diethyl ether.

Computational methods.

The DMol³ module in Materials Studio (MS) 2023 was used to optimize the geometric structures of PW₁₁Co anionic clusters. The calculations employed the B3LYP hybrid functional in combination with the double numerical plus polarization (DNP) basis set for all-electron calculations. The B3LYP functional has gained widespread adoption due to its excellent performance in describing the electronic structure, geometric configurations, and reaction energies of transition metal systems. For the transition metal Co, B3LYP has reliably predicted its electronic spin states and bonding properties. This makes it suitable for analyzing the interactions between the PW₁₁Co cluster and the iPAF-2^[3]. The convergence criteria for structure optimization were established as follows: the total energy change must be less than 1.0×10^{-5} Ha, the maximum atomic force should be less than $0.002 \text{ Ha} \cdot \text{\AA}^{-1}$, and the maximum atomic

displacement must be less than 0.005 Å. The real-space orbital cutoff radius was set to 5.0 Å. To accurately account for long-range van der Waals interactions, the DFT-D3 dispersion correction method was applied in all calculations.

The calculations for the geometric and electronic structures of iPAF-2 and PW₁₁Co@iPAF-2 were performed using the CASTEP module. Norm-conserving pseudopotentials were employed to represent the ionic cores, and the wavefunctions were expanded using a plane-wave basis set with a kinetic energy cutoff of 571.4 eV. We performed Brillouin zone integration with a Monkhorst-Pack k-point grid of 2 × 2 × 1 for the iPAF-2 model structures. For all calculations, the generalized gradient approximation (GGA) was employed with the Perdew-Burke-Ernzerhof (PBE) functional. To incorporate van der Waals interactions, we utilized the DFT-D3 empirical correction method. The geometry optimizations were considered converged when the total energy change between successive steps was less than 1.0 × 10⁻⁵ eV · atom⁻¹, the maximum residual force on any atom was below 0.03 eV · Å⁻¹, the maximum atomic displacement was less than 0.001 Å, and the maximum stress component was under 0.05 GPa. The convergence threshold for the electronic energy was set to 2.0 × 10⁻⁶ eV · atom⁻¹. The Cartesian coordinates (XYZ files) of the optimized key structures, which include the pristine PW₁₁Co, iPAF-2, and PW₁₁Co@iPAF-2, along with the most stable adsorption configurations of reactants and intermediates.

The adsorption energies (ΔE_{ads}) were calculated by the following Eq. 1:

$$\Delta E_{\text{ads}} = E_{\text{ad/sub}} - E_{\text{ad}} - E_{\text{sub}} \quad (1)$$

Where $E_{\text{ad/sub}}$, E_{ad} , and E_{sub} are the total energies of the optimized adsorbate/substrate system, the adsorbate in the structure, and the clean substrate, respectively.

The adsorption capacities and heats of various molecules on the catalysts were calculated using the Sorption module. Simulations were conducted using the Monte Carlo method at 120 °C and 1000 kPa to replicate the experimental reaction conditions. The optimized molecular potentials for atomistic simulation studies used the Universal force field to describe interatomic and intermolecular interactions. During the simulations, the iPAF-2 were held fixed, while the adsorbate molecules were allowed

to rotate and translate freely. For each system, 1×10^7 steps were performed for equilibration, followed by 2×10^7 steps for production runs to obtain statistically reliable averages.

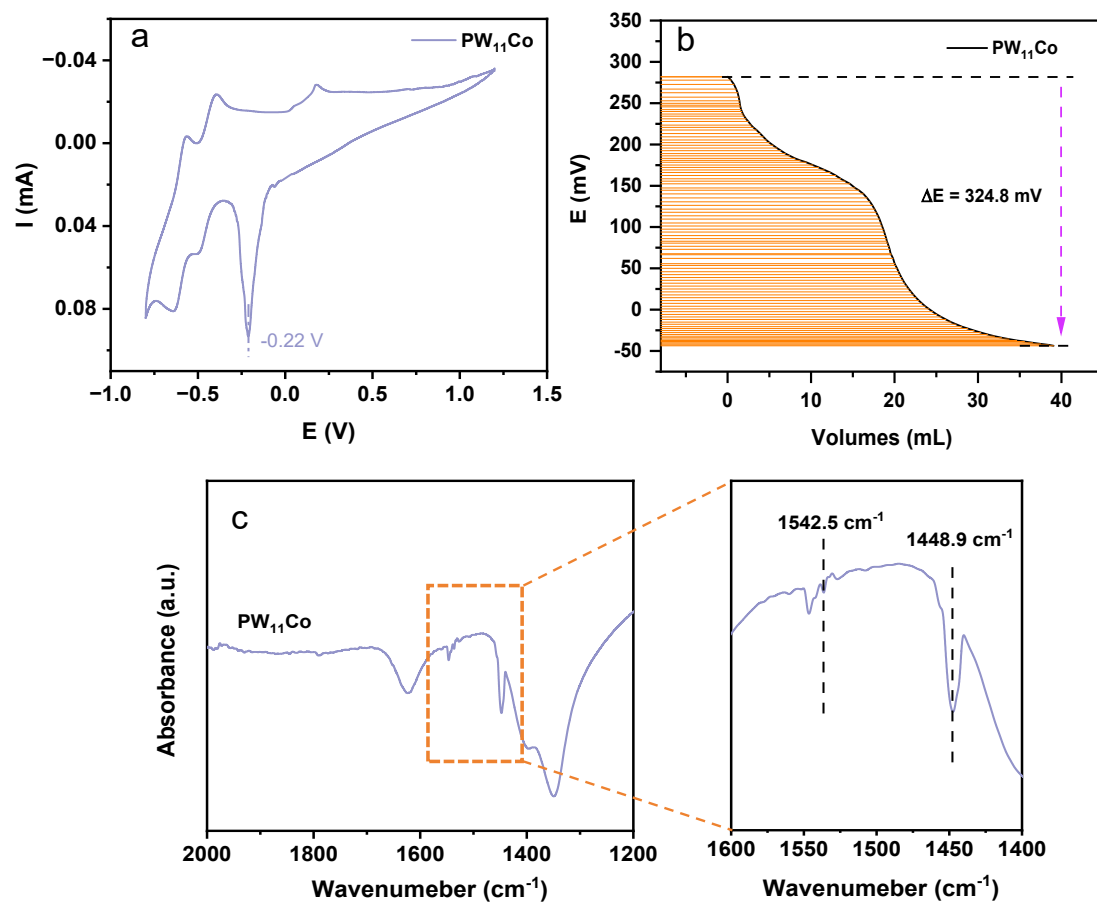


Fig. S1. Basic properties of $PW_{11}Co$. (a) Cyclic voltammetry (CV) curve, (b) potentiometric titration, and (c) Py-FTIR spectrum.

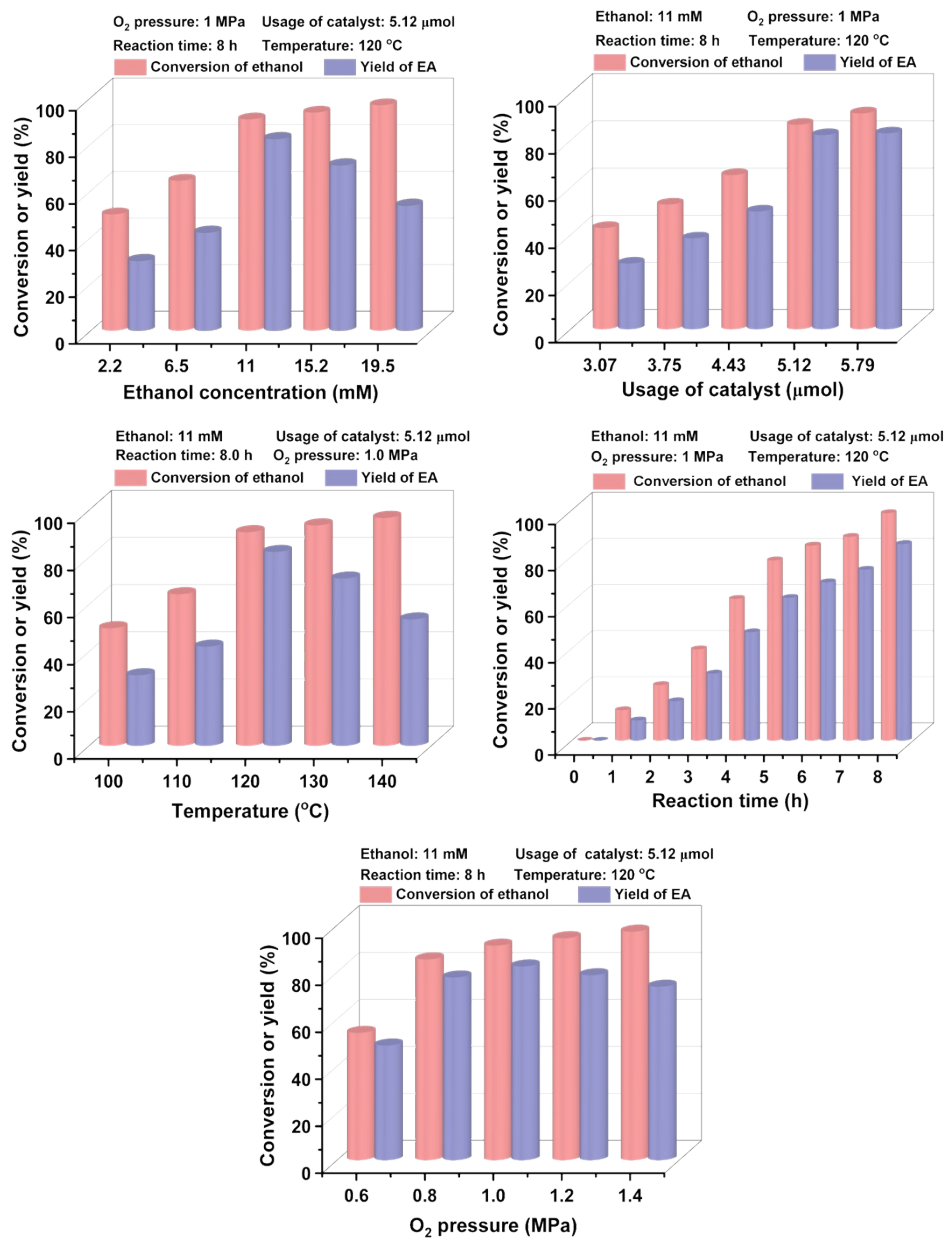


Fig. S2. The optimization results of the aerobic oxidation of ethanol catalyzed by $PW_{11}Co$.

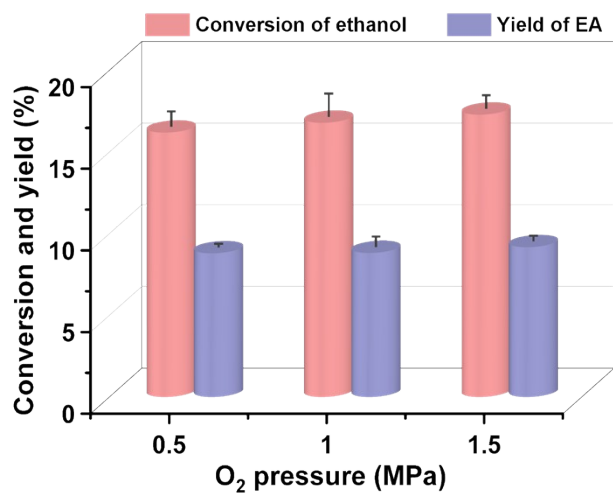


Fig. S3. Catalytic performance under different O₂ pressures with 5.12 μ mol of PW₁₁Co, 6 mL of hexane with 11 mM of ethanol, 120 °C and 1 h.

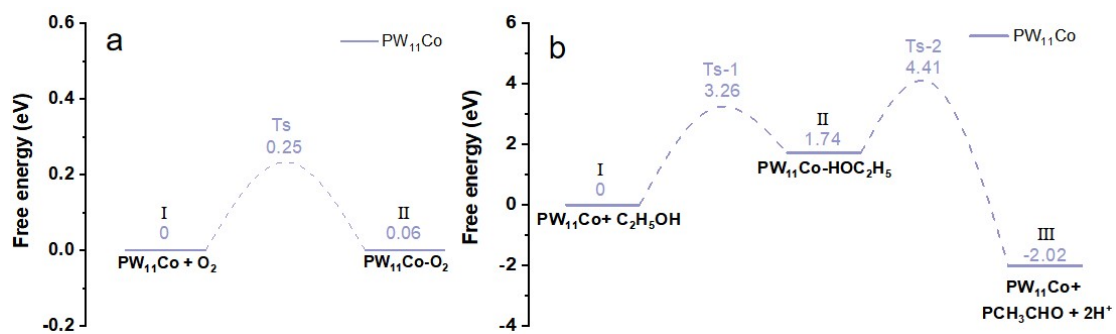


Fig. S4. The adsorption free energy of O₂ and ethanol at the Co²⁺ site.

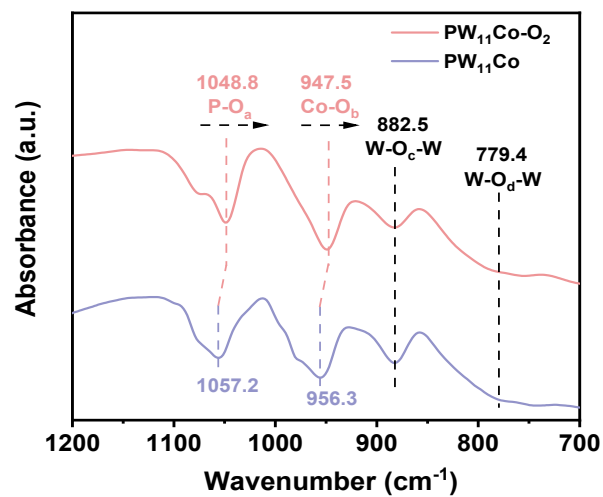


Fig. S5. FTIR spectra of POMs before and after adsorbing O₂.

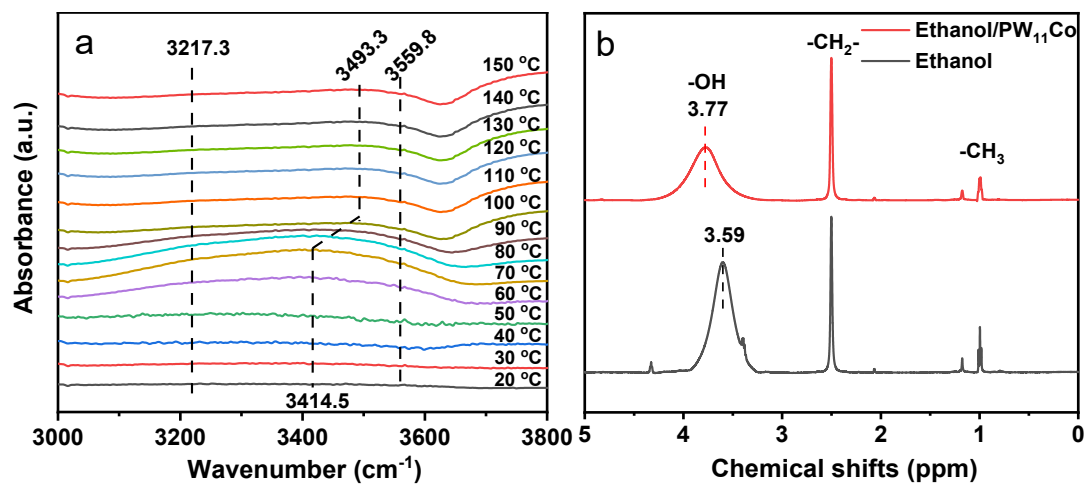


Fig. S6. (a) -OH adsorption *in-situ* DRIFT spectra and (b) ethanol adsorption 1H NMR on $PW_{11}Co$.

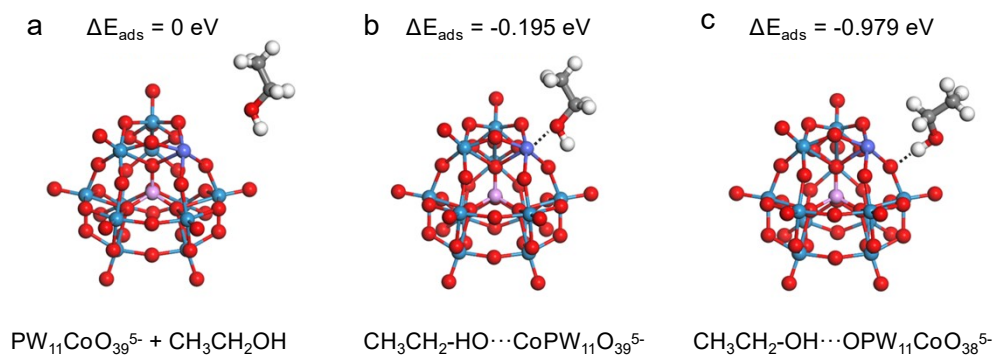


Fig. S7. Density functional theory (DFT) simulation for ΔE_{ads} between -OH group of ethanol and $\text{PW}_{11}\text{CoO}_{39}^{5-}$. (a) Initial stage; (b) Interaction of O in -OH with Co in POMs; (c) Interaction of H in -OH with O_b/O_c in POMs.

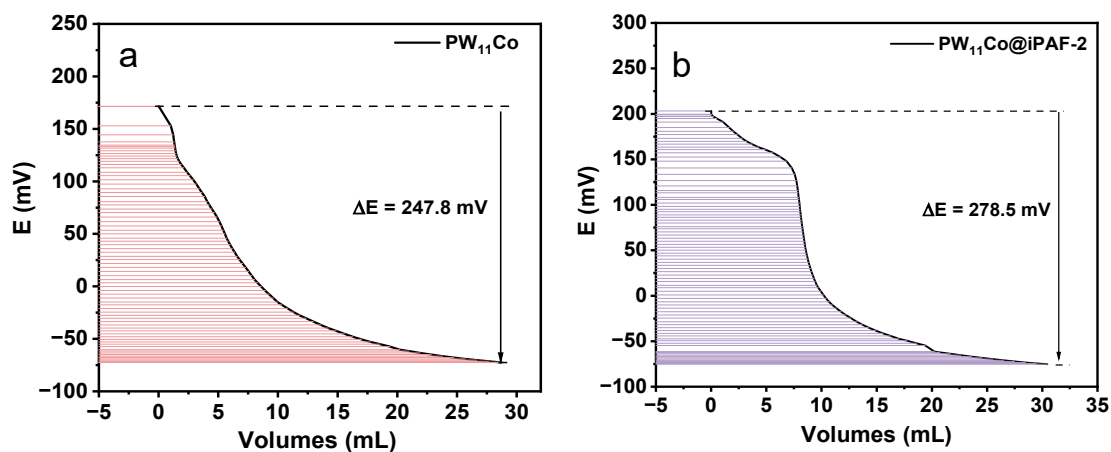


Fig. S8. The acidic contents being tested by potentiometric titration with n-Butylamine of the reaction mixture for ethanol dehydrogenation over (a) $PW_{11}Co$ and (b) $PW_{11}Co@iPAF-2$ with N_2 at 120 °C for 8 h.

In an N_2 atmosphere, the $PW_{11}Co$ achieved an ethanol conversion of 17.2%. However, when using the $PW_{11}Co@iPAF-2$ catalyst, the conversion improved to 21.3%. Notably, the product selectivity was predominantly toward acetaldehyde, with no detection of other products, such as acetic acid or EA.

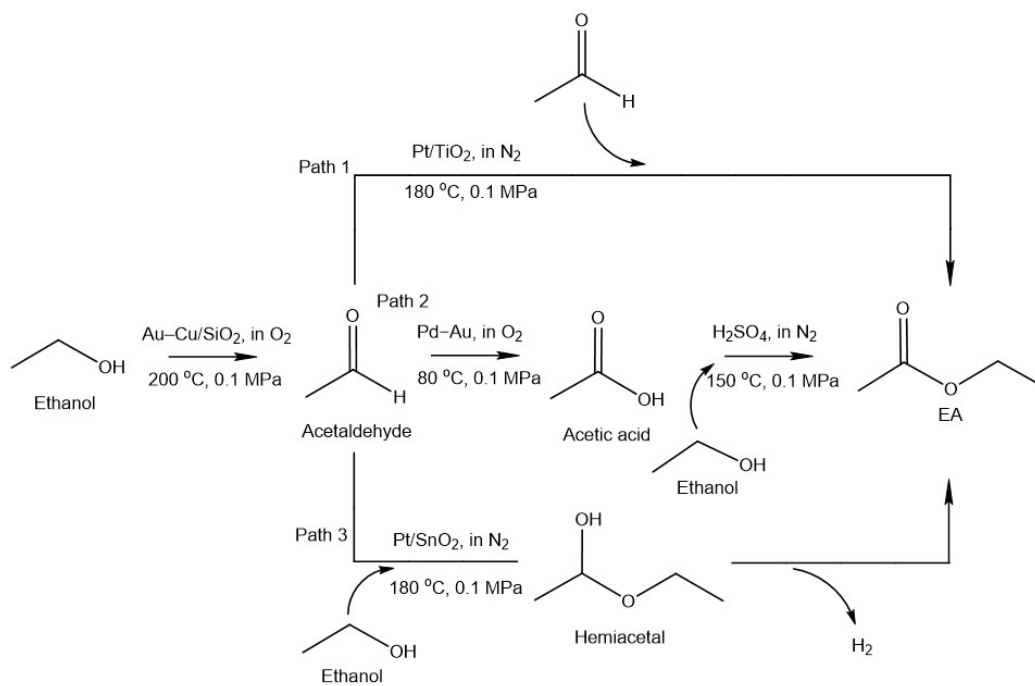


Fig. S9. Three possible reaction pathways for the conversion of ethanol to ethyl acetate by dehydrogenation and the corresponding catalysts.

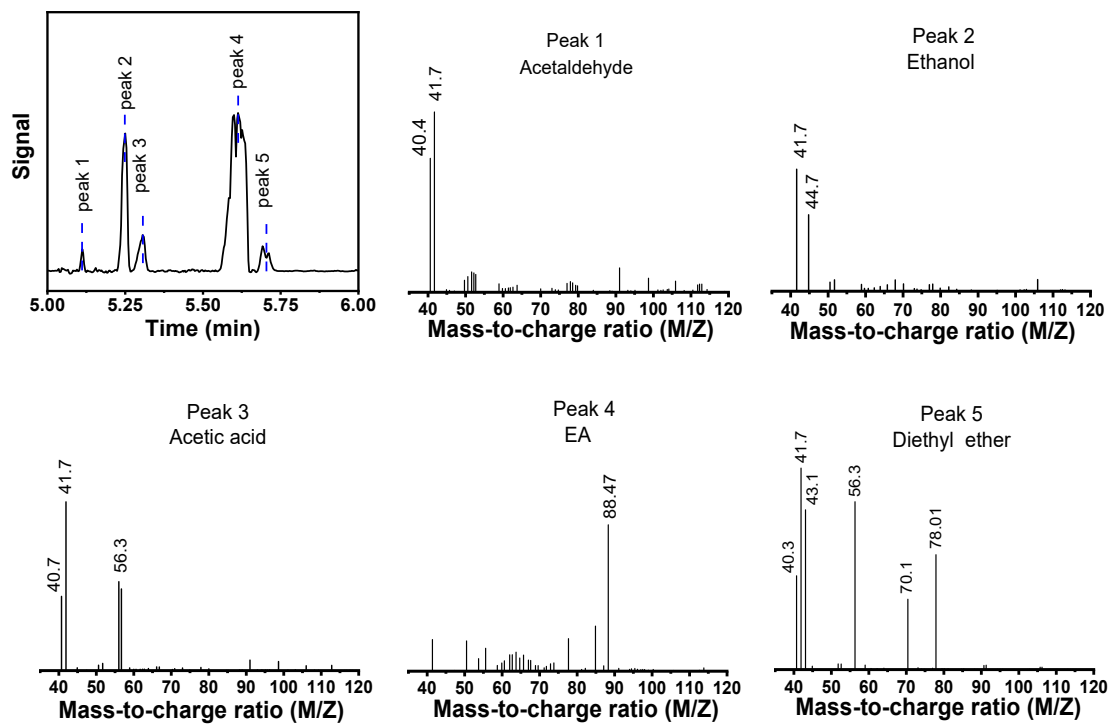


Fig. S10. Production distribution in ethanol conversion over $PW_{11}Co$ by GC-MS.

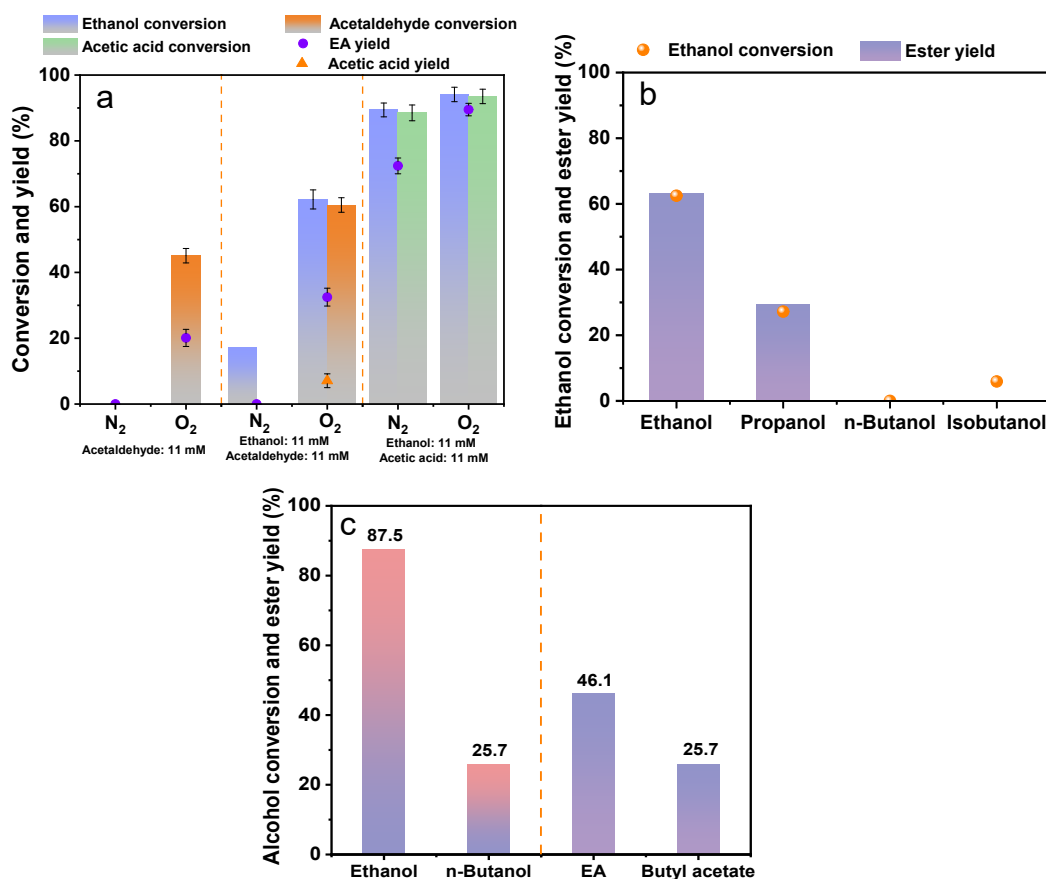


Fig. S11. (a) The catalytic activity of $PW_{11}Co$ under different substrates of ethanol (11 mM), acetaldehyde (11 mM) or acetic acid (11 mM) with different ratios and atmosphere with 5.12 μmol of $PW_{11}Co$, 1 MPa of N_2 or O_2 at 120 °C for 8 h in 6 mL of hexane as solvent. (b) The catalytic activity of $PW_{11}Co$ for various alcohols with 5.12 μmol of $PW_{11}Co$, 1 MPa of O_2 , at 120 °C, 8 h and 6 mL of hexane with 11 mM of alcohol. (c) The catalytic activity of $PW_{11}Co$ for ethanol and n-butanol with 5.12 μmol of $PW_{11}Co$, 1 MPa of O_2 , at 120 °C, 8 h and 6 mL of hexane with 11 mM of ethanol and n-butanol.

To investigate the pathway for ethanol conversion over $PW_{11}Co$, a series of controlled experiments was conducted using various substrates in N_2 and O_2 atmospheres (Figure S10a). The results showed that $PW_{11}Co$ effectively catalyzed the conversion of acetaldehyde to EA in the presence of O_2 , achieving a yield of 20.1% with a conversion of 45.1%. No conversion of acetaldehyde was observed in an N_2 atmosphere, indicating that acetaldehyde was oxidized to acetic acid and subsequently to EA. The results showed a consistent formation of ethanol and acetaldehyde when mixed in N_2 . However, in the presence of O_2 , both the conversion of ethanol and the

yield of acetaldehyde increased. This enhancement can be attributed to the acylating effect of acetaldehyde, which facilitates the conversion of ethanol to acetic acid in the presence of POMs^[4]. The esterification of ethanol and acetic acid was carried out under N₂ and O₂, with PW₁₁Co showing higher efficiency under O₂ compared to N₂ due to its acidity. We proposed that a hydrogen atom in the hydroxyl group was abstracted and then oxidized to H⁺ during the oxidation of ethanol, which assisted the L acidic site in PW₁₁Co to promote the esterification to EA. Inert alcohols such as propanol, n-butanol, and isobutanol were selected to perform the esterification reaction using 5.12 μmol of PW₁₁Co, 6 mL of hexane, 11 mM of alcohol, and 1 MPa of O₂ (Figure S10b). Only ethanol and propanol can be converted into their corresponding esters. During the aerobic oxidation of ethanol and n-butanol at 120 °C for 8 h, a conversion of 85.7% for ethanol was achieved, resulting in selectivity of 46.1% for EA and 25.7% for butyl acetate (Figure S10c). This clarified that the main pathway for oxidizing ethanol to acetic acid occurs in the presence of PW₁₁Co and O₂. Based on the above results, ethanol was rapidly oxidized to aldehyde, then acetic acid, and finally esterified to EA.

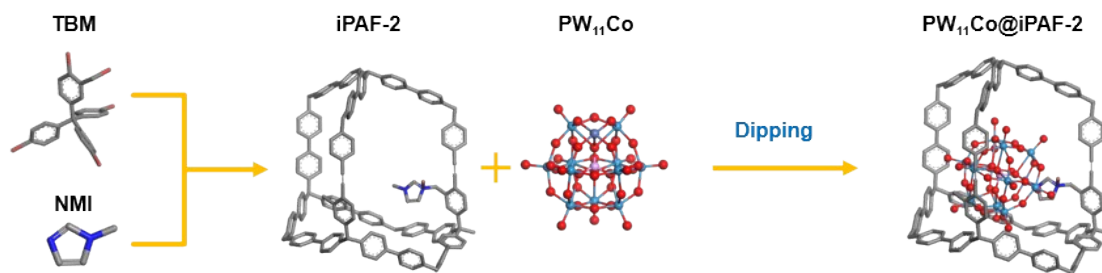


Fig. S12. Schematics for synthetic process of PW₁₁Co@iPAF-2.

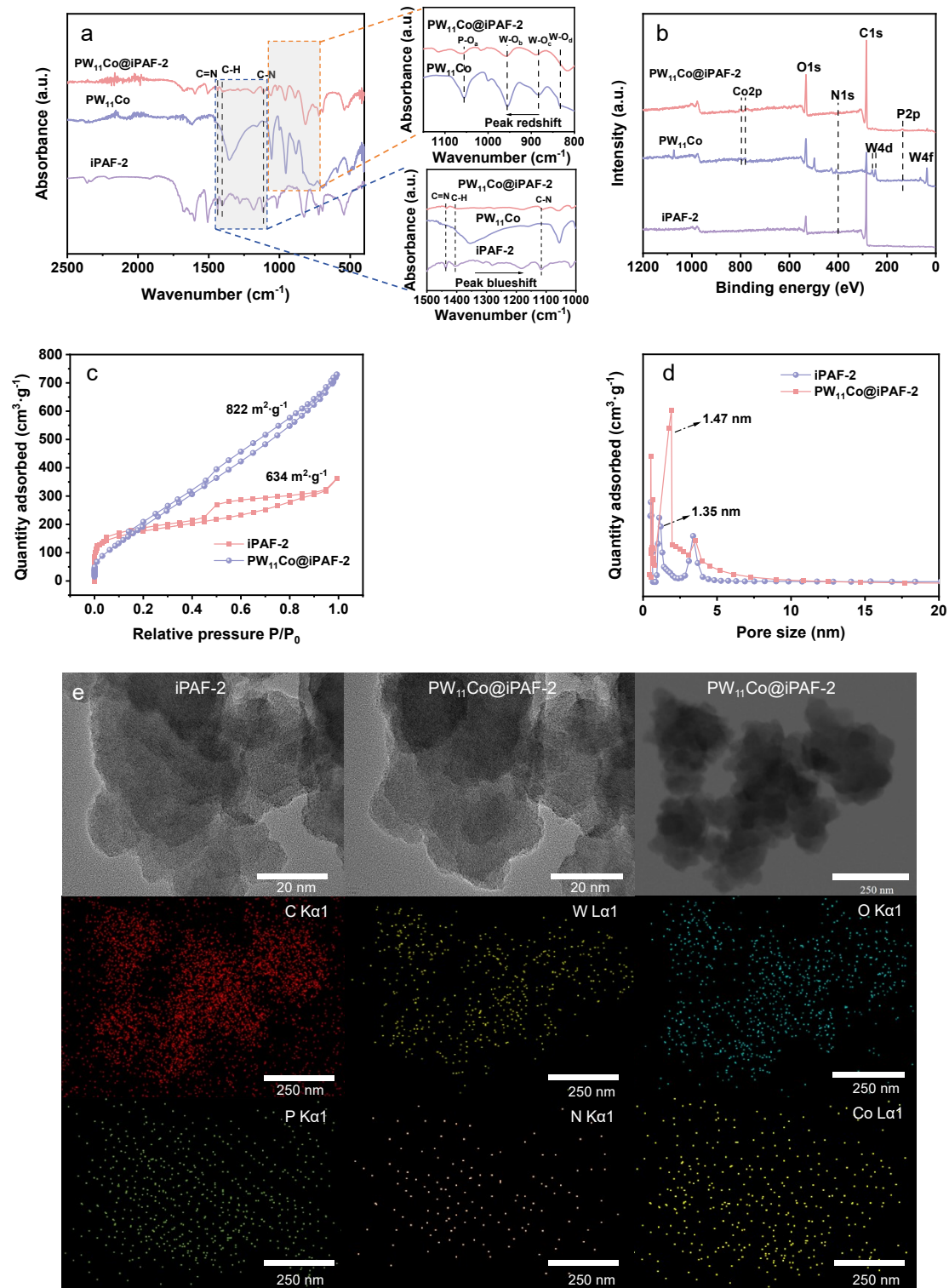


Fig. S13. (a) FTIR spectra. (b) XPS full spectra. (c) N_2 adsorption desorption isotherms and (d) pore size distribution curves for iPAF-2 and $PW_{11}Co@iPAF-2$. (e) HR-TEM images of iPAF-2 and $PW_{11}Co@iPAF-2$, TEM image of $PW_{11}Co@iPAF-2$ and its mapping of C, W, O, P, N, and Co elements.

The FTIR spectra of samples (Figure S11a) showed the red-shifts for $\nu_{as}(P-O_a)$, $\nu_{as}(X-$

O_b), $\nu_{\text{as}}(\text{W-O}_c)$, and $\nu_{\text{as}}(\text{W-O}_d)$ from 1055.2 cm^{-1} , 954.6 cm^{-1} , 883.4 cm^{-1} and 831.5 cm^{-1} of PW_{11}Co to 1062.4 cm^{-1} , 956.9 cm^{-1} , 888.4 cm^{-1} and 816.2 cm^{-1} of $\text{PW}_{11}\text{Co}@i\text{PAF-2}$, respectively. All characteristic peaks of PW_{11}Co shifted to lower frequencies after being anchored into iPAF-2 pores. Meanwhile, the vibration peaks corresponding to C=N and C-N changed from 1439.8 and 1117.9 cm^{-1} to 1435.8 and 1112.3 cm^{-1} . The XPS full spectra (Figure S11b) further determined the existence of W, Co, P, O, K, N and C elements in $\text{PW}_{11}\text{Co}@i\text{PAF-2}$, demonstrating the successful embedding of PW_{11}Co inside iPAF-2. After loading PW_{11}Co , the specific surface area and pore sizes of iPAF-2 increased from 634.32 to 822.54 $\text{m}^2\cdot\text{g}^{-1}$ (Figure S11c) and from 1.35 to 1.47 nm (Figure S11d), respectively. The HR-TEM images of iPAF-2 and $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ show no aggregation of PW_{11}Co on the surface of iPAF-2. Additionally, elemental mapping of $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ demonstrated a uniform distribution of W, P, and Co elements throughout the material's surface. The elemental analysis results for $\text{PW}_{11}\text{Co}@i\text{PAF-2}$ were as follows: C was measured at 35.7 wt%; N at 2.44 wt%; P at 0.65 wt%; W at 43.42 wt%; and Co at 1.27 wt%. These results aligned well with the calculated values, which were: C, 35.5 wt%; N, 2.43 wt%; P, 0.67 wt%; W, 44.05 wt%; and Co, 1.28 wt%. The loading amount of PW_{11}Co was determined to be 35.2 wt%.

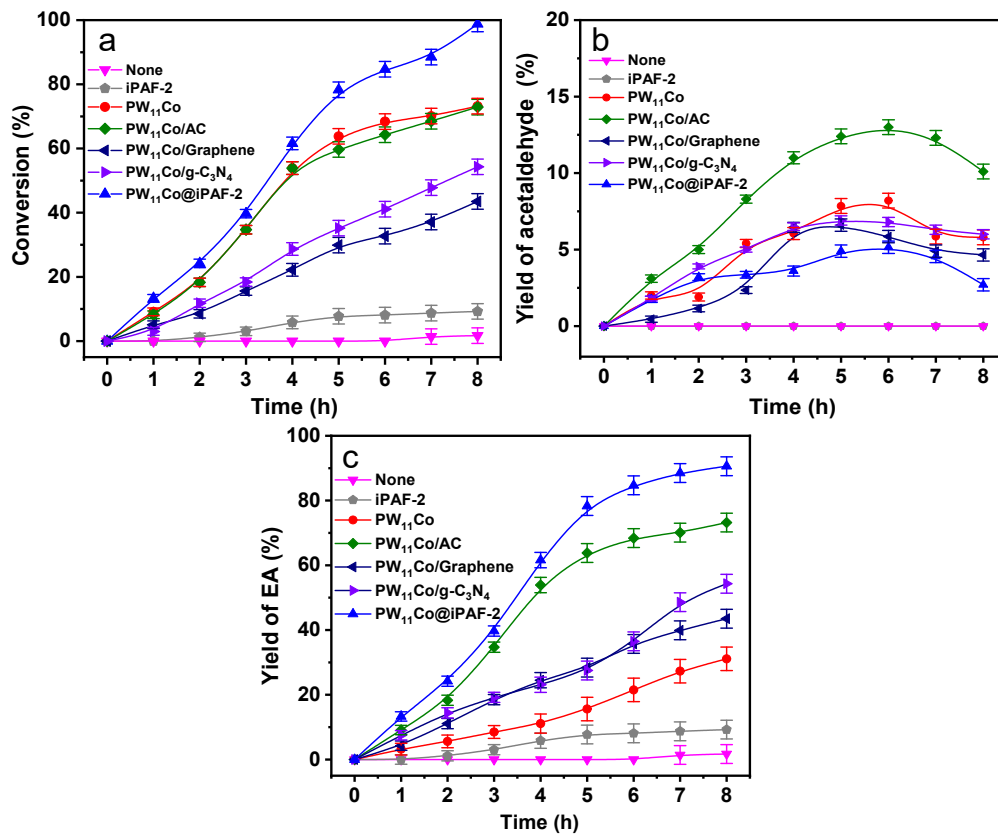


Fig. S14. The catalytic activity of various catalysts versus reaction time under reaction conditions as 5.12 μmol of catalyst, 6 mL of hexane with 11 mM of ethanol, 120 $^{\circ}\text{C}$ and 1 MPa of O_2 .

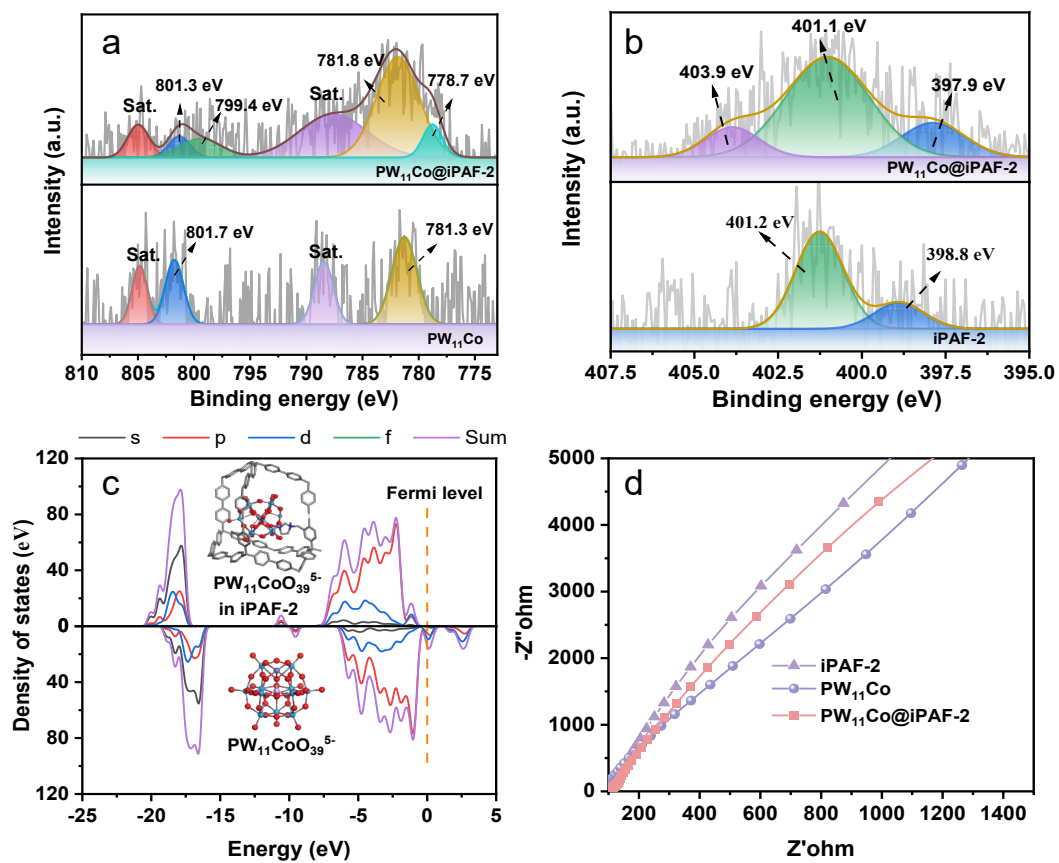


Fig. S15. (a) Co and (b) N elemental fine XPS spectra. (c) Partial density of states (PDOS) of $PW_{11}CoO_{39}^{5-}$ and $PW_{11}CoO_{39}^{5-}@iPAF-2$. (d) Electrochemical impedance spectra (EIS) of $iPAF-2$, $PW_{11}Co$ and $PW_{11}Co@iPAF-2$.

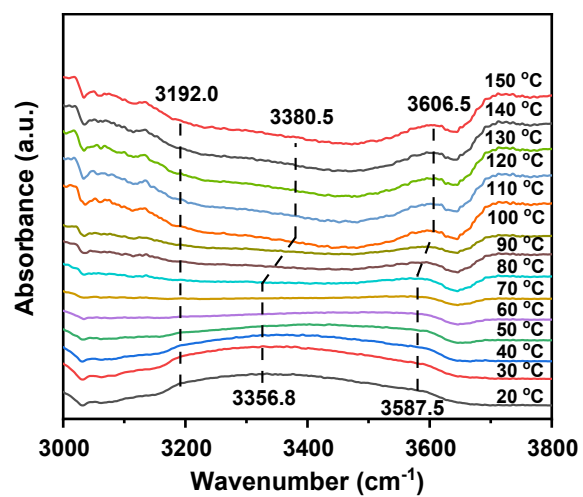


Fig. S16. *In-situ* -OH adsorption DRIFT spectra on $\text{PW}_{11}\text{Co@iPAF-2}$.

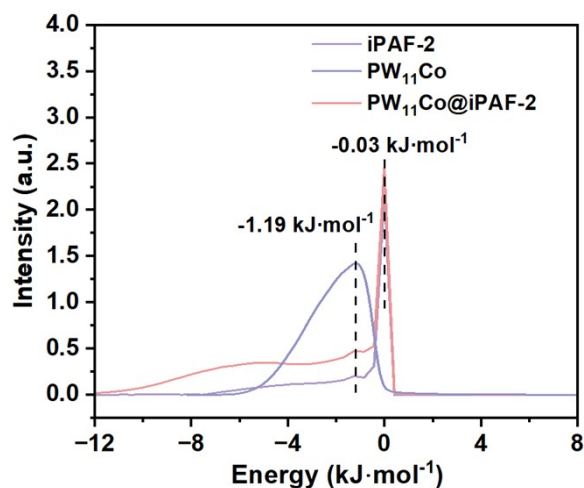


Fig. S17. The adsorption heat curves of water molecules by iPAF-2, PW_{11}Co $\text{PW}_{11}\text{Co@iPAF-2}$.

This curve was generated through simulation using the Sorption module, under constant temperature (120 °C) and constant pressure (1000 kPa). Throughout the simulation, the atomic coordinates of PW_{11}Co , iPAF-2, and $\text{PW}_{11}\text{Co@iPAF-2}$ were kept fixed. The original simulation data were not subjected to baseline correction or any further numerical processing.

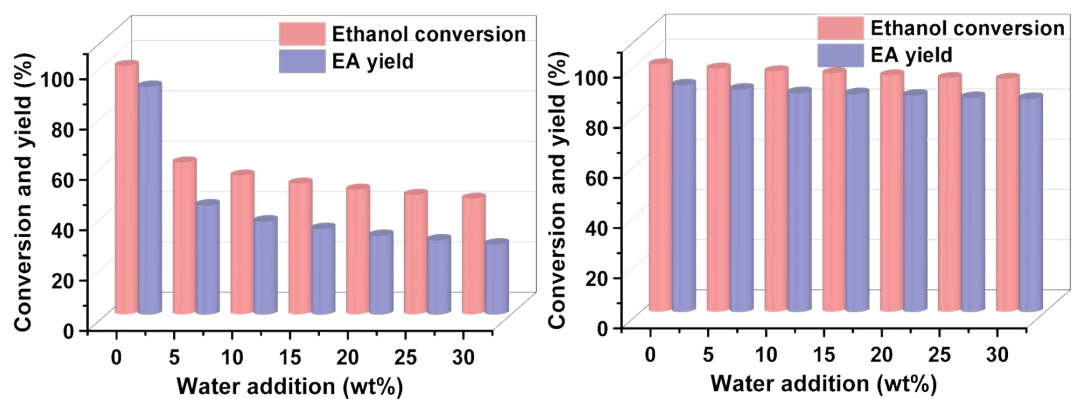


Fig. S18. The water-tolerance tests for PW₁₁Co (left) and PW₁₁Co@iPAF-2 (right). Reaction conditions: 5.12 μ mol of PW₁₁Co@iPAF-2, 6 mL of hexane with 11 mM of ethanol, 120 $^{\circ}$ C, 8 h and 1 MPa of O₂.

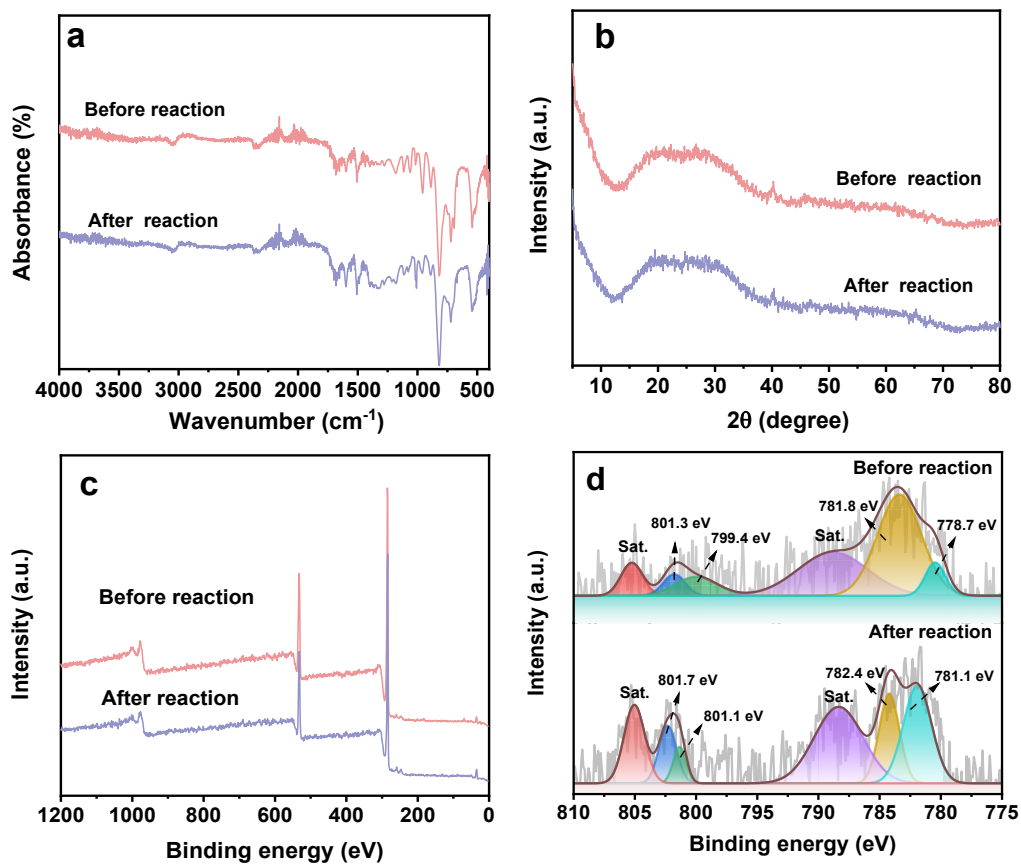


Fig. S19. The (a) FTIR spectra, (b) XRD, (c) XPS and (d) Co fine XPS spectra of $\text{PW}_{11}\text{Co}@i\text{PAF}-2$ before and after the reaction.

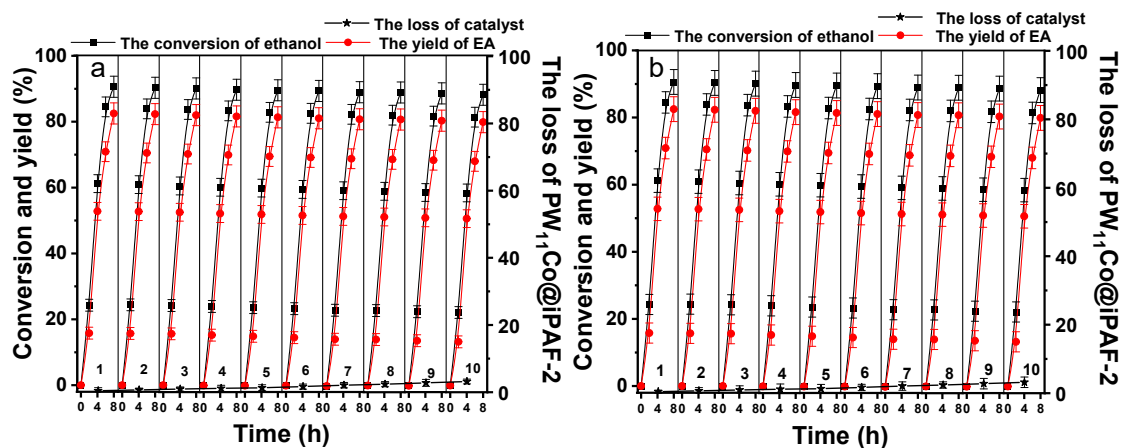


Fig. S20. Stability experiments of $PW_{11}Co@iPAF-2$. (a) Washed with acetone. (b) Unwashed with acetone. Reaction conditions: 5.12 μmol of $PW_{11}Co@iPAF-2$, 6 mL of hexane with 11 mM of ethanol, 120 $^{\circ}\text{C}$, 8 h, 1 MPa of O_2 .

The catalytic activity of reused $PW_{11}Co@iPAF-2$ showed less variation between treatments with or without acetone, indicating that no products or intermediates were attached to the solid catalyst.

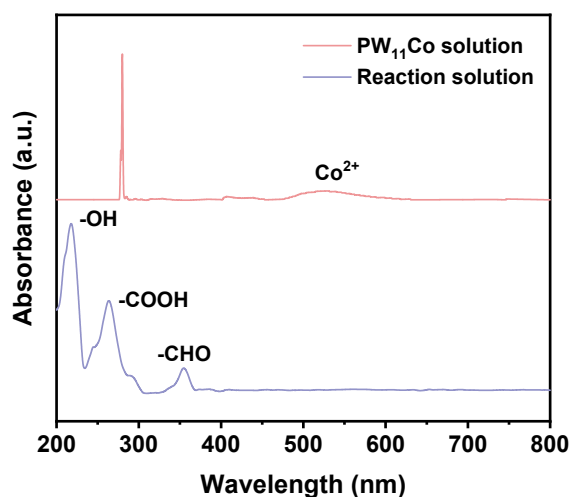


Fig. S21. UV-vis spectrum of the reaction solution after separating PW₁₁Co@iPAF-2. Reaction conditions: 5.12 μmol of PW₁₁Co@iPAF-2, 6 mL of hexane with 11 mM of ethanol, 120 $^{\circ}\text{C}$, 8 h, 1 MPa of O₂.

No characteristic diffraction peaks attributable to PW₁₁Co were observed in the post-reaction catalyst, indicating the absence of PW₁₁Co leaching from the iPAF-2 support during catalysis.

Table S1. Summary of catalysts used for oxidation-esterification of ethanol to EA.

| Catalysts | Solvents | Reaction conditions | Conversion (%) | Products | Yield (%) | Ref. |
|--|--|--|----------------|--|------------------------------|------|
| Rh/Ru pincer complex | C ₂ H ₅ ONa (1.3%, 2.2 mmol) | 90 °C, 2 h 10 mL of ethanol 4.2 μmol of catalyst | - | EA | 81.0 | [4] |
| Co ₃ O ₄ -N/TiO ₂ complex | N-heptane (8 mL) | 90 °C, 24 h 2 mmol of ethanol 0.12 g of catalyst 0.1 MPa of O ₂ | - | EA | 65.0 | [5] |
| CuO-Cr ₂ O ₃ | No | 300 °C 0.15 g·h ⁻¹ of ethanol 0.05 g of catalyst | 94.9 | EA Acetaldehyde | 88.2 4.6 | [6] |
| Ni _{0.1} Zn _{0.7} Al _{0.3} InO _x | No | 250 °C 3.1 h ⁻¹ of ethanol 1.5 g of catalyst | 46.2 | EA Ethyl ether Acetaldehyde | 1.8 2.1 38.4 | [7] |
| PdO/SiO ₂ | No | 200 °C 48,000 h ⁻¹ of ethanol 0.025 g of catalyst | 35.9 | EA Acetaldehyde Acetic acid CO ₂ | 22.5 21.4 20.9 19.7 | [8] |
| CuCeZrO _x | No | 240 °C 0.10 mL·min ⁻¹ of ethanol 0.004 g of catalyst | 97.4 | EA Other liquid products | 14.5 72.1 | [9] |
| Au/ZSM-5 | No | 250 °C 0.012 mL·min ⁻¹ of ethanol 0.1 g of catalyst 4.5 mL·min ⁻¹ of O ₂ | 43.5 | EA Ethylene Acetaldehyde | 4.1 19.8 2.6 | [10] |

Table S2. Brief review for POMs@PAFs in catalytic reactions.

| POMs | PAFs | Catalytic reactions | Reaction conditions | Conversion (%) | Ref. |
|---|---------|--|--|----------------|------|
| $(\text{NH}_4)_5\text{H}_6\text{PV}_8\text{Mo}_4\text{O}_{40}$ | PAF-1 | Aerobic oxidative desulfurization | Decalin 80 °C, 5 h O ₂ (1 atm) | 100 | [11] |
| $\text{Na}_5[\text{IMo}_6\text{O}_{24}]$ | PAF-1 | Aerobic oxidative desulfurization | Decalin 100 °C, 6 h O ₂ (1 atm) | 100 | [12] |
| $(\text{NH}_4)_5\text{H}_6\text{PV}_8\text{Mo}_4\text{O}_{40}$ | PAF-270 | Esterification of oleic acids, oxidative desulfurization | N-octane 110 °C, 10 h | 99.6 98.2 | [13] |
| $(\text{NH}_4)_3[\text{Co}(\text{OH})_6\text{Mo}_6\text{O}_{18}]$ | PAF-30 | Aerobic oxidative desulfurization | Decalin 130 °C, 1 h air (1 atm) | 100 | [14] |

Table S3. The atomic charges of each atom in the $PW_{11}Co$ anionic clusters.

| Number | Atoms | Charge |
|--------|-------|--------|
| 1 | W | 1.977 |
| 2 | W | 1.966 |
| 3 | W | 2.078 |
| 4 | Co | 0.83 |
| 5 | W | 2.056 |
| 6 | W | 2.022 |
| 7 | W | 2.017 |
| 8 | W | 2.038 |
| 9 | W | 2.061 |
| 10 | W | 2.042 |
| 11 | W | 2.042 |
| 12 | W | 2.096 |
| 13 | P | 1.886 |
| 14 | O | -0.789 |
| 15 | O | -0.718 |
| 16 | O | -0.788 |
| 17 | O | -0.798 |
| 18 | O | -0.676 |
| 19 | O | -0.696 |
| 20 | O | -0.776 |
| 21 | O | -0.597 |
| 22 | O | -0.768 |
| 23 | O | -0.769 |
| 24 | O | -0.773 |
| 25 | O | -0.574 |
| 26 | O | -0.76 |
| 27 | O | -0.775 |
| 28 | O | -0.801 |
| 29 | O | -0.795 |
| 30 | O | -0.713 |
| 31 | O | -0.559 |
| 32 | O | -0.705 |
| 33 | O | -0.71 |
| 34 | O | -0.718 |
| 35 | O | -0.555 |
| 36 | O | -0.684 |
| 37 | O | -0.684 |
| 38 | O | -0.687 |
| 39 | O | -0.694 |
| 40 | O | -0.705 |

| | | |
|----|---|--------|
| 41 | O | -0.715 |
| 42 | O | -0.463 |
| 43 | O | -0.461 |
| 44 | O | -0.468 |
| 45 | O | -0.464 |
| 46 | O | -0.462 |
| 47 | O | -0.472 |
| 48 | O | -0.466 |
| 49 | O | -0.468 |
| 50 | O | -0.465 |
| 51 | O | -0.465 |
| 52 | O | -0.475 |

The total charge of the cluster is 0.

Table S4. The atomic charges of each atom in the PW₁₁Co anionic clusters in iPAF-2

pore.

| Number | Atoms | Charge |
|--------|-------|--------|
| 1 | W | 1.564 |
| 2 | W | 1.545 |
| 3 | W | 1.693 |
| 4 | Co | 0.759 |
| 5 | W | 1.652 |
| 6 | W | 1.68 |
| 7 | W | 1.642 |
| 8 | W | 1.665 |
| 9 | W | 1.674 |
| 10 | W | 1.667 |
| 11 | W | 1.657 |
| 12 | W | 1.665 |
| 13 | P | 1.735 |
| 14 | O | -0.801 |
| 15 | O | -0.768 |
| 16 | O | -0.795 |
| 17 | O | -0.8 |
| 18 | O | -0.562 |
| 19 | O | -0.569 |
| 20 | O | -0.645 |
| 21 | O | -0.537 |
| 22 | O | -0.639 |
| 23 | O | -0.665 |
| 24 | O | -0.64 |
| 25 | O | -0.529 |
| 26 | O | -0.638 |
| 27 | O | -0.629 |
| 28 | O | -0.682 |
| 29 | O | -0.685 |
| 30 | O | -0.631 |
| 31 | O | -0.544 |
| 32 | O | -0.643 |
| 33 | O | -0.633 |
| 34 | O | -0.606 |
| 35 | O | -0.518 |
| 36 | O | -0.593 |
| 37 | O | -0.584 |
| 38 | O | -0.584 |

| | | |
|----|---|--------|
| 39 | O | -0.584 |
| 40 | O | -0.615 |
| 41 | O | -0.616 |
| 42 | O | -0.495 |
| 43 | O | -0.512 |
| 44 | O | -0.53 |
| 45 | O | -0.483 |
| 46 | O | -0.471 |
| 47 | O | -0.514 |
| 48 | O | -0.561 |
| 49 | O | -0.491 |
| 50 | O | -0.499 |
| 51 | O | -0.497 |
| 52 | O | -0.499 |

The total charge of the cluster is -2.689.

Table S5. The atomic coordinates of $PW_{11}Co$.

| Number | Atoms | x | y | z |
|--------|-------|-------------|-------------|-------------|
| 1 | W | 13.05762958 | 17.18790948 | 21.6989692 |
| 2 | W | 15.88176858 | 20.01408939 | 25.70140914 |
| 3 | W | 13.23212689 | 19.92035897 | 15.91803242 |
| 4 | Co | 18.88594179 | 25.35351056 | 23.84607603 |
| 5 | W | 22.25398177 | 20.15166145 | 25.03301301 |
| 6 | W | 16.60706436 | 14.68732939 | 17.02484502 |
| 7 | W | 15.56590086 | 26.11412532 | 17.84173583 |
| 8 | W | 22.63854103 | 15.12500886 | 20.34535838 |
| 9 | W | 18.63158465 | 23.20980524 | 13.1878884 |
| 10 | W | 21.83030517 | 26.34372705 | 17.6556167 |
| 11 | W | 25.59293886 | 20.48217455 | 18.98910194 |
| 12 | W | 22.42160047 | 17.37595613 | 14.49213958 |
| 13 | P | 18.88006474 | 20.51940216 | 19.30959949 |
| 14 | O | 16.40992814 | 18.82395877 | 18.67674911 |
| 15 | O | 18.98891297 | 21.26376528 | 22.26324142 |
| 16 | O | 18.81496368 | 23.06883167 | 17.61364588 |
| 17 | O | 21.47711536 | 18.96963776 | 18.54405254 |
| 18 | O | 13.31912988 | 20.57231449 | 23.11569688 |
| 19 | O | 15.80863618 | 16.75351814 | 23.98194733 |
| 20 | O | 13.53692082 | 23.09679962 | 17.52921292 |
| 21 | O | 16.28229603 | 25.79438366 | 21.32234679 |
| 22 | O | 21.96957798 | 16.90654816 | 23.39046306 |
| 23 | O | 19.29013531 | 14.25934422 | 19.49082423 |
| 24 | O | 15.89826589 | 20.96159807 | 13.73314998 |
| 25 | O | 21.3726135 | 26.12659751 | 21.22049055 |
| 26 | O | 24.42187558 | 21.15151554 | 22.37756985 |
| 27 | O | 19.12818578 | 16.0672263 | 14.79069741 |
| 28 | O | 20.90263861 | 20.46176551 | 13.40721001 |
| 29 | O | 24.12877905 | 23.61760814 | 18.01288832 |
| 30 | O | 11.41793312 | 18.6326618 | 18.86405876 |
| 31 | O | 16.38989704 | 23.55411334 | 25.92269606 |
| 32 | O | 19.2219162 | 19.18922394 | 26.85414207 |
| 33 | O | 14.24197763 | 14.34816134 | 19.81680198 |
| 34 | O | 14.02921337 | 16.47004032 | 15.22240534 |
| 35 | O | 21.50546125 | 23.60570286 | 25.70972393 |
| 36 | O | 16.24712823 | 25.72181818 | 14.25271128 |
| 37 | O | 18.63870892 | 28.06262193 | 17.6307668 |
| 38 | O | 25.72484174 | 17.04296749 | 20.10517419 |
| 39 | O | 23.30107901 | 14.75356429 | 16.77326578 |
| 40 | O | 21.31611069 | 25.5360581 | 14.1463008 |
| 41 | O | 25.36541583 | 19.18147606 | 15.58954133 |

| | | | | |
|----|---|-------------|-------------|-------------|
| 42 | O | 10.5438592 | 15.9533892 | 23.36230614 |
| 43 | O | 14.17519471 | 19.54543731 | 28.35911996 |
| 44 | O | 10.72703035 | 20.42189229 | 14.04597524 |
| 45 | O | 24.31264941 | 19.54335861 | 27.35888792 |
| 46 | O | 16.27097657 | 11.71239024 | 15.83671751 |
| 47 | O | 13.45331933 | 28.45190551 | 17.75675484 |
| 48 | O | 23.78541582 | 12.29676915 | 21.38943206 |
| 49 | O | 18.52267974 | 23.58926225 | 10.01311072 |
| 50 | O | 23.88103596 | 28.84988183 | 17.46777792 |
| 51 | O | 28.72270326 | 21.27642644 | 19.22664051 |
| 52 | O | 23.44224155 | 16.21549421 | 11.73438665 |

Table S6. The atomic coordinates of iPAF-2.

| Number | Atoms | x | y | z |
|--------|-------|-------------|-------------|-------------|
| 1 | C | 28.71722306 | 47.64415301 | 44.85718492 |
| 2 | C | 26.79234803 | 45.84305504 | 44.49889285 |
| 3 | C | 26.84374858 | 43.52133752 | 45.75669455 |
| 4 | C | 28.82153594 | 42.93004222 | 47.41833074 |
| 5 | C | 30.72713577 | 44.73321889 | 47.81611809 |
| 6 | C | 30.67535727 | 47.05512538 | 46.55642665 |
| 7 | C | 28.87501519 | 40.46886291 | 48.76816211 |
| 8 | C | 30.81217344 | 39.92877919 | 50.49083644 |
| 9 | C | 30.81141755 | 37.66904469 | 51.85030542 |
| 10 | C | 28.87142471 | 35.87474973 | 51.54832718 |
| 11 | C | 26.978864 | 36.3876214 | 49.74855202 |
| 12 | C | 26.97584043 | 38.6549148 | 48.38492565 |
| 13 | C | 28.74840354 | 33.4413494 | 53.16744453 |
| 14 | C | 59.42130416 | 47.18683929 | 44.50607381 |
| 15 | C | 57.49642913 | 45.38574132 | 44.14778173 |
| 16 | C | 57.54782968 | 43.0640238 | 45.40558344 |
| 17 | C | 59.52561705 | 42.47272849 | 47.06721962 |
| 18 | C | 61.43121687 | 44.27609414 | 47.46500697 |
| 19 | C | 61.37943838 | 46.59800063 | 46.20531554 |
| 20 | C | 59.5790963 | 40.01173816 | 48.41705099 |
| 21 | C | 61.51625455 | 39.47165444 | 50.13972533 |
| 22 | C | 61.51549866 | 37.21191994 | 51.4991943 |
| 23 | C | 59.57550582 | 35.41762498 | 51.19721607 |
| 24 | C | 57.6829451 | 35.93049665 | 49.39725193 |
| 25 | C | 57.67992154 | 38.19779005 | 48.03381454 |
| 26 | C | 59.45248465 | 32.98403568 | 52.81633341 |
| 27 | C | 28.74575792 | 50.18696848 | 43.43270937 |
| 28 | C | 28.74840354 | 65.01508247 | 55.90112234 |
| 29 | C | 28.71363258 | 62.7468442 | 54.06695416 |
| 30 | C | 30.65967254 | 62.46111761 | 52.27757249 |
| 31 | C | 30.70105754 | 60.39545798 | 50.63218796 |
| 32 | C | 28.79432388 | 58.55259707 | 50.71798152 |
| 33 | C | 26.82541823 | 58.84739434 | 52.46711202 |
| 34 | C | 26.78535604 | 60.91456575 | 54.11192964 |
| 35 | C | 28.84232293 | 56.36429421 | 48.95959136 |
| 36 | C | 26.93521132 | 54.51916562 | 49.0125037 |
| 37 | C | 26.94182536 | 52.52021333 | 47.27830203 |
| 38 | C | 28.8445906 | 52.31839058 | 45.42826015 |
| 39 | C | 30.79119748 | 54.12988204 | 45.45282659 |
| 40 | C | 30.78836289 | 56.12184235 | 47.18041422 |
| 41 | C | 34.68214357 | 48.44067257 | 39.54894423 |

| | | | | |
|----|---|-------------|-------------|-------------|
| 42 | C | 32.68886046 | 48.28854962 | 41.2714296 |
| 43 | C | 31.03024784 | 50.3358789 | 41.62688708 |
| 44 | C | 31.39761059 | 52.51454415 | 40.14383002 |
| 45 | C | 33.39901953 | 52.67517087 | 38.43665144 |
| 46 | C | 54.70549262 | 48.71354902 | 37.67452489 |
| 47 | C | 56.7770104 | 48.43613723 | 39.28211491 |
| 48 | C | 57.08843726 | 50.0012084 | 41.40352145 |
| 49 | C | 55.13748401 | 51.96123234 | 41.8447725 |
| 50 | C | 53.08864295 | 52.16796838 | 40.20789173 |
| 51 | C | 59.44983903 | 49.72984373 | 43.08140928 |
| 52 | C | 59.45248465 | 64.55795772 | 55.55001123 |
| 53 | C | 59.41771369 | 62.28971945 | 53.71584305 |
| 54 | C | 61.36394262 | 62.00380389 | 51.92646138 |
| 55 | C | 61.40513865 | 59.93814426 | 50.28088787 |
| 56 | C | 59.49840499 | 58.09547232 | 50.36687041 |
| 57 | C | 57.52949934 | 58.39026959 | 52.11600091 |
| 58 | C | 57.48943715 | 60.45725203 | 53.76081853 |
| 59 | C | 59.54640403 | 55.90698049 | 48.60848025 |
| 60 | C | 57.63929243 | 54.0618519 | 48.66139258 |
| 61 | C | 57.64590647 | 52.06289961 | 46.92719092 |
| 62 | C | 59.54886068 | 51.86126583 | 45.07714904 |
| 63 | C | 61.49527859 | 53.67256832 | 45.10171548 |
| 64 | C | 61.492444 | 55.66452863 | 46.8293031 |
| 65 | C | 31.04536564 | 33.28941542 | 54.96249537 |
| 66 | C | 32.84608567 | 31.33506066 | 54.82284461 |
| 67 | C | 34.93706763 | 31.29084107 | 56.43931634 |
| 68 | C | 35.28118675 | 33.19927548 | 58.24589452 |
| 69 | C | 33.45986871 | 35.11394599 | 58.4392135 |
| 70 | C | 31.36945367 | 35.15003976 | 56.83483602 |
| 71 | C | 37.54281098 | 33.23650309 | 59.89827104 |
| 72 | C | 38.11426416 | 35.40307409 | 61.30895159 |
| 73 | C | 40.24133989 | 35.47450574 | 62.85909393 |
| 74 | C | 41.84949682 | 33.3716185 | 63.08340442 |
| 75 | C | 41.30034241 | 31.2167638 | 61.62132332 |
| 76 | C | 39.17118798 | 31.1477888 | 60.05247269 |
| 77 | C | 46.49236494 | 33.27410864 | 62.92391154 |
| 78 | C | 46.8058705 | 35.13511092 | 61.05100397 |
| 79 | C | 48.84337321 | 35.04308126 | 59.37670663 |
| 80 | C | 50.61499145 | 33.07474253 | 59.50804259 |
| 81 | C | 50.27616356 | 31.17670161 | 61.32728193 |
| 82 | C | 48.23866085 | 31.27099894 | 63.00384695 |
| 83 | C | 52.82162465 | 33.02712143 | 57.77951011 |
| 84 | C | 54.5766133 | 31.04101927 | 57.86549265 |
| 85 | C | 56.67515416 | 31.02892503 | 56.25998133 |

| | | | | |
|-----|---|-------------|-------------|-------------|
| 86 | C | 57.07653199 | 32.99669684 | 54.51330747 |
| 87 | C | 55.31776388 | 34.98960201 | 54.46115103 |
| 88 | C | 53.22092378 | 35.00226318 | 56.06023728 |
| 89 | C | 31.04536564 | 64.86314849 | 57.69617319 |
| 90 | C | 32.84608567 | 62.9089827 | 57.55633345 |
| 91 | C | 34.93706763 | 62.86457414 | 59.17280518 |
| 92 | C | 35.28118675 | 64.77300855 | 60.97957233 |
| 93 | C | 33.45986871 | 66.68767906 | 61.17289131 |
| 94 | C | 31.36945367 | 66.72377283 | 59.56832486 |
| 95 | C | 37.54281098 | 64.81042513 | 62.63175988 |
| 96 | C | 38.11426416 | 66.97680716 | 64.04244043 |
| 97 | C | 40.24133989 | 67.04823881 | 65.59258277 |
| 98 | C | 41.84949682 | 64.94535157 | 65.81708223 |
| 99 | C | 41.30034241 | 62.79068585 | 64.35481216 |
| 100 | C | 39.17118798 | 62.72171084 | 62.7861505 |
| 101 | C | 46.49236494 | 64.84803068 | 65.65758935 |
| 102 | C | 46.8058705 | 66.70903297 | 63.78468179 |
| 103 | C | 48.84337321 | 66.61681433 | 62.11019547 |
| 104 | C | 50.61499145 | 64.6484756 | 62.24172041 |
| 105 | C | 50.27616356 | 62.75062365 | 64.06077077 |
| 106 | C | 48.23866085 | 62.84492099 | 65.73752476 |
| 107 | C | 52.82162465 | 64.6008545 | 60.51318792 |
| 108 | C | 54.5766133 | 62.61475234 | 60.59917046 |
| 109 | C | 56.67515416 | 62.60284707 | 58.99365914 |
| 110 | C | 57.07653199 | 64.57061888 | 57.24698529 |
| 111 | C | 55.31776388 | 66.56352405 | 57.19482884 |
| 112 | C | 53.22092378 | 66.57599625 | 58.79391509 |
| 113 | C | 42.01144635 | 59.78356466 | 72.01670673 |
| 114 | C | 42.09081485 | 61.41005194 | 69.94103156 |
| 115 | C | 44.25681893 | 62.86287338 | 69.43552982 |
| 116 | C | 46.33419486 | 62.63081502 | 71.08091436 |
| 117 | C | 46.25425944 | 61.00602849 | 73.14959754 |
| 118 | C | 43.95654145 | 51.40092855 | 31.46904224 |
| 119 | C | 41.50424386 | 51.17019299 | 33.10233253 |
| 120 | C | 46.31718732 | 51.19532634 | 33.23253466 |
| 121 | C | 40.5489873 | 53.31219755 | 34.39792876 |
| 122 | C | 40.1929629 | 48.86416019 | 33.45004214 |
| 123 | C | 46.27806999 | 52.03360885 | 35.77346041 |
| 124 | C | 48.65156601 | 50.2531089 | 32.3077027 |
| 125 | C | 38.44307651 | 53.15138185 | 35.97339343 |
| 126 | C | 38.10972882 | 48.69899813 | 35.06462414 |
| 127 | C | 48.40117729 | 51.82706179 | 37.31585487 |
| 128 | C | 50.76427981 | 50.0191608 | 33.87560846 |
| 129 | C | 37.22136857 | 50.83457763 | 36.35417325 |

| | | | | |
|-----|----|-------------|-------------|-------------|
| 130 | C | 50.652597 | 50.79602721 | 36.40651866 |
| 131 | C | 35.06500208 | 50.64220351 | 38.1271143 |
| 132 | H | 41.50651153 | 55.22781292 | 34.16435861 |
| 133 | H | 44.46109832 | 52.89135554 | 36.55070476 |
| 134 | H | 48.83430252 | 49.66691585 | 30.24279896 |
| 135 | H | 37.70192592 | 54.9146853 | 36.96436581 |
| 136 | H | 37.13066171 | 46.79812262 | 35.32635121 |
| 137 | H | 52.59542443 | 49.19146076 | 33.09930897 |
| 138 | C | 52.85696252 | 50.56094528 | 38.11388621 |
| 139 | C | 44.00057207 | 57.88760244 | 75.88743275 |
| 140 | C | 46.35271417 | 57.09901973 | 77.16923399 |
| 141 | C | 41.72534181 | 56.85921348 | 76.75292732 |
| 142 | C | 46.28619582 | 55.17357778 | 78.95842668 |
| 143 | C | 41.71721599 | 54.96910941 | 78.58974111 |
| 144 | C | 43.98715501 | 53.99760121 | 79.64420829 |
| 145 | C | 43.95654145 | 51.40092855 | 81.03183418 |
| 146 | C | 44.05310645 | 49.26345933 | 78.98053648 |
| 147 | C | 43.64265794 | 49.75195353 | 76.37857257 |
| 148 | C | 44.71640032 | 46.76070605 | 79.6434524 |
| 149 | C | 43.94898254 | 47.89907706 | 74.51643645 |
| 150 | C | 44.92200253 | 44.86512177 | 77.81759902 |
| 151 | C | 44.53498662 | 45.41427618 | 75.26174443 |
| 152 | C | 43.53475458 | 48.6578021 | 71.76216062 |
| 153 | N | 45.79883545 | 49.8135586 | 70.56445221 |
| 154 | C | 45.17465891 | 50.80982221 | 68.26881291 |
| 155 | C | 46.65563727 | 51.90680823 | 71.80543535 |
| 156 | Br | 48.48734881 | 47.47313279 | 70.12660266 |
| 157 | N | 45.55524975 | 53.32032337 | 68.09628091 |
| 158 | C | 46.50389226 | 54.02726991 | 70.31973267 |
| 159 | C | 45.07223575 | 54.94945626 | 65.92876505 |
| 160 | C | 44.08012954 | 59.59175746 | 73.66473689 |
| 161 | C | 44.64742532 | 43.39812738 | 73.44288304 |
| 162 | H | 48.21655105 | 58.06769334 | 76.69170019 |
| 163 | H | 39.85224528 | 57.56502619 | 75.95640776 |
| 164 | H | 48.1078918 | 54.51614206 | 79.90177796 |
| 165 | H | 39.84941069 | 54.15539334 | 79.28988464 |
| 166 | H | 43.0405912 | 51.74523665 | 75.82601666 |
| 167 | H | 45.09566836 | 46.25652711 | 81.70325388 |
| 168 | H | 45.40955187 | 42.85690982 | 78.42609083 |
| 169 | H | 41.90599963 | 50.0647032 | 71.66786329 |
| 170 | H | 43.01375708 | 46.91509667 | 70.60791591 |
| 171 | H | 44.40875291 | 49.53236735 | 66.71243447 |
| 172 | H | 47.37637882 | 51.73975644 | 73.82876511 |
| 173 | H | 47.14299764 | 55.93324768 | 71.09433141 |

| | | | | |
|-----|---|-------------|-------------|-------------|
| 174 | H | 44.22885098 | 53.78179449 | 64.32684421 |
| 175 | H | 46.92152174 | 55.83876138 | 65.27265214 |
| 176 | H | 43.68876726 | 56.50186627 | 66.49133652 |
| 177 | C | 42.39090335 | 38.30210294 | 69.8185773 |
| 178 | C | 44.54953751 | 39.80065575 | 69.9973454 |
| 179 | C | 46.59214247 | 39.37130998 | 68.37936189 |
| 180 | C | 46.49444363 | 37.41053015 | 66.60849954 |
| 181 | C | 44.32106962 | 35.86473418 | 66.39798405 |
| 182 | C | 42.28318896 | 36.35001585 | 68.05924228 |
| 183 | C | 44.65328347 | 41.75217592 | 71.87516625 |
| 184 | H | 40.71074786 | 38.67475693 | 71.11417354 |
| 185 | H | 48.34335167 | 40.62022997 | 68.5006823 |
| 186 | H | 48.17705578 | 37.04297842 | 65.31441509 |
| 187 | H | 40.50911408 | 35.13095353 | 67.97250385 |
| 188 | C | 44.23792167 | 33.44531782 | 64.75297745 |
| 189 | C | 44.23792167 | 65.01923986 | 67.48646629 |
| 190 | H | 25.17247479 | 46.30471513 | 43.15586449 |
| 191 | H | 25.26828391 | 42.08741334 | 45.436197 |
| 192 | H | 32.34096188 | 44.3121879 | 49.17936651 |
| 193 | H | 32.23419235 | 48.5018997 | 46.89997886 |
| 194 | H | 32.39935441 | 41.35722316 | 50.77637406 |
| 195 | H | 32.40370078 | 37.2466909 | 53.23849823 |
| 196 | H | 25.41965097 | 34.94651626 | 49.38459077 |
| 197 | H | 25.42097378 | 39.04438736 | 46.94571023 |
| 198 | H | 28.74443511 | 31.72207657 | 51.86939165 |
| 199 | H | 26.94239228 | 33.45079803 | 54.34190931 |
| 200 | H | 55.8765559 | 45.84759038 | 42.8045644 |
| 201 | H | 55.97236501 | 41.63028859 | 45.08508589 |
| 202 | H | 63.04504298 | 43.85487418 | 48.8282554 |
| 203 | H | 62.93827346 | 48.04477495 | 46.54886775 |
| 204 | H | 63.10343552 | 40.89990944 | 50.42526295 |
| 205 | H | 63.10778189 | 36.78937717 | 52.88738711 |
| 206 | H | 56.12373208 | 34.48920253 | 49.03329068 |
| 207 | H | 56.12505488 | 38.58707364 | 46.59459912 |
| 208 | H | 61.21068583 | 32.86460498 | 54.05542683 |
| 209 | H | 59.37613971 | 31.26344004 | 51.52224896 |
| 210 | H | 26.92973112 | 50.3751852 | 42.28923609 |
| 211 | H | 26.93596721 | 65.01451555 | 57.06576055 |
| 212 | H | 28.8680232 | 66.84754989 | 54.77484557 |
| 213 | H | 32.21794071 | 63.94549748 | 52.18214133 |
| 214 | H | 32.29598639 | 60.19212345 | 49.19826377 |
| 215 | H | 25.23785932 | 57.39400598 | 52.55687402 |
| 216 | H | 25.1717189 | 61.13830932 | 55.52166533 |
| 217 | H | 25.37089604 | 54.66070611 | 50.48705699 |

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|-----|---|-------------|-------------|-------------|
| 218 | H | 25.391872 | 51.02581791 | 47.35124546 |
| 219 | H | 32.41333839 | 53.98720772 | 44.04233501 |
| 220 | H | 32.38045715 | 57.57296304 | 47.15376908 |
| 221 | H | 36.01307768 | 46.76637522 | 39.29080765 |
| 222 | H | 32.38744914 | 46.48688473 | 42.41358007 |
| 223 | H | 30.04777922 | 54.18336129 | 40.32807832 |
| 224 | H | 33.68795866 | 54.47022172 | 37.28127288 |
| 225 | H | 54.49006384 | 47.42362197 | 35.96262199 |
| 226 | H | 58.25364239 | 46.91887612 | 38.88394961 |
| 227 | H | 55.3149293 | 53.29878049 | 43.52398314 |
| 228 | H | 51.57289362 | 53.65726154 | 40.56202641 |
| 229 | H | 61.21257556 | 49.831511 | 41.84722915 |
| 230 | H | 59.52183759 | 66.38702363 | 54.41390788 |
| 231 | H | 61.19764672 | 64.43796011 | 56.80724602 |
| 232 | H | 62.92202181 | 63.48837273 | 51.83103021 |
| 233 | H | 63.0000675 | 59.73480973 | 48.84715266 |
| 234 | H | 55.94194042 | 56.93669226 | 52.2057629 |
| 235 | H | 55.87580001 | 60.6809956 | 55.17036525 |
| 236 | H | 56.07497714 | 54.20358136 | 50.13594588 |
| 237 | H | 56.0959531 | 50.56850419 | 47.00013435 |
| 238 | H | 63.11741949 | 53.529894 | 43.6912239 |
| 239 | H | 63.08453826 | 57.11583829 | 46.80265797 |
| 240 | H | 32.57944531 | 29.77301304 | 53.36340913 |
| 241 | H | 36.37722791 | 29.6953453 | 56.29380743 |
| 242 | H | 33.678699 | 36.66352141 | 59.91981392 |
| 243 | H | 29.88960915 | 36.70358361 | 57.02834397 |
| 244 | H | 36.81810101 | 37.11875644 | 61.17893843 |
| 245 | H | 40.70299998 | 37.25973001 | 63.97289851 |
| 246 | H | 42.59707247 | 29.49862481 | 61.70579408 |
| 247 | H | 38.74826728 | 29.38580816 | 58.88726756 |
| 248 | H | 45.36835584 | 36.73363025 | 60.91135321 |
| 249 | H | 49.08034486 | 36.57716093 | 57.8830671 |
| 250 | H | 51.66983657 | 29.53849803 | 61.44709057 |
| 251 | H | 47.97258741 | 29.70989619 | 64.46441627 |
| 252 | H | 54.27879246 | 29.42719316 | 59.26124436 |
| 253 | H | 58.09301567 | 29.40961871 | 56.35276688 |
| 254 | H | 55.59215212 | 36.63309682 | 53.09563493 |
| 255 | H | 51.81194398 | 36.62988429 | 55.97633344 |
| 256 | H | 32.57944531 | 61.34674611 | 56.09708694 |
| 257 | H | 36.37722791 | 61.26907837 | 59.02748524 |
| 258 | H | 33.678699 | 68.23725448 | 62.65330276 |
| 259 | H | 29.88960915 | 68.27750565 | 59.76202179 |
| 260 | H | 36.81810101 | 68.69267848 | 63.91242727 |
| 261 | H | 40.70299998 | 68.83346308 | 66.70657632 |

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|-----|---|-------------|-------------|-------------|
| 262 | H | 42.59707247 | 61.07235788 | 64.43928292 |
| 263 | H | 38.74826728 | 60.9597302 | 61.62094537 |
| 264 | H | 45.36835584 | 68.30755229 | 63.64503103 |
| 265 | H | 49.08034486 | 68.15108297 | 60.61655594 |
| 266 | H | 51.66983657 | 61.1122311 | 64.18076838 |
| 267 | H | 47.97258741 | 61.28381823 | 67.19790511 |
| 268 | H | 54.27879246 | 61.00111521 | 61.9947332 |
| 269 | H | 58.09301567 | 60.98354075 | 59.0864447 |
| 270 | H | 55.59215212 | 68.20682989 | 55.82912377 |
| 271 | H | 51.81194398 | 68.20361736 | 58.70982228 |
| 272 | H | 40.25362311 | 58.59436001 | 72.38671511 |
| 273 | H | 40.38647085 | 61.57143455 | 68.63315211 |
| 274 | H | 48.11979707 | 63.78373692 | 70.73055913 |
| 275 | H | 47.9691859 | 60.8197015 | 74.43990254 |
| 276 | H | 43.9741159 | 53.30501659 | 30.46144027 |
| 277 | H | 44.00076104 | 49.81469244 | 30.01187443 |
| 278 | H | 40.83131238 | 47.09348682 | 32.40237797 |
| 279 | H | 48.31859626 | 52.50622936 | 39.35864881 |
| 280 | H | 42.14864046 | 51.21649128 | 82.18853555 |
| 281 | H | 45.66844434 | 51.26146676 | 82.33215473 |
| 282 | H | 44.24718133 | 31.71924198 | 66.04195964 |
| 283 | H | 44.3142666 | 66.90594243 | 68.52335902 |

Table S7. The atomic coordinates of PW₁₁Co@iPAF-2.

| Number | Atoms | x | y | z |
|--------|-------|-------------|-------------|-------------|
| 1 | C | 28.71722306 | 47.64415301 | 44.85718492 |
| 2 | C | 26.79234803 | 45.84305504 | 44.49889285 |
| 3 | C | 26.84374858 | 43.52133752 | 45.75669455 |
| 4 | C | 28.82153594 | 42.93004222 | 47.41833074 |
| 5 | C | 30.72713577 | 44.73321889 | 47.81611809 |
| 6 | C | 30.67535727 | 47.05512538 | 46.55642665 |
| 7 | C | 28.87501519 | 40.46886291 | 48.76816211 |
| 8 | C | 30.81217344 | 39.92877919 | 50.49083644 |
| 9 | C | 30.81141755 | 37.66904469 | 51.85030542 |
| 10 | C | 28.87142471 | 35.87474973 | 51.54832718 |
| 11 | C | 26.978864 | 36.3876214 | 49.74855202 |
| 12 | C | 26.97584043 | 38.6549148 | 48.38492565 |
| 13 | C | 28.74840354 | 33.4413494 | 53.16744453 |
| 14 | C | 59.42130416 | 47.18683929 | 44.50607381 |
| 15 | C | 57.49642913 | 45.38574132 | 44.14778173 |
| 16 | C | 57.54782968 | 43.0640238 | 45.40558344 |
| 17 | C | 59.52561705 | 42.47272849 | 47.06721962 |
| 18 | C | 61.43121687 | 44.27609414 | 47.46500697 |
| 19 | C | 61.37943838 | 46.59800063 | 46.20531554 |
| 20 | C | 59.5790963 | 40.01173816 | 48.41705099 |
| 21 | C | 61.51625455 | 39.47165444 | 50.13972533 |
| 22 | C | 61.51549866 | 37.21191994 | 51.4991943 |
| 23 | C | 59.57550582 | 35.41762498 | 51.19721607 |
| 24 | C | 57.6829451 | 35.93049665 | 49.39725193 |
| 25 | C | 57.67992154 | 38.19779005 | 48.03381454 |
| 26 | C | 59.45248465 | 32.98403568 | 52.81633341 |
| 27 | C | 28.74575792 | 50.18696848 | 43.43270937 |
| 28 | C | 28.74840354 | 65.01508247 | 55.90112234 |
| 29 | C | 28.71363258 | 62.7468442 | 54.06695416 |
| 30 | C | 30.65967254 | 62.46111761 | 52.27757249 |
| 31 | C | 30.70105754 | 60.39545798 | 50.63218796 |
| 32 | C | 28.79432388 | 58.55259707 | 50.71798152 |
| 33 | C | 26.82541823 | 58.84739434 | 52.46711202 |
| 34 | C | 26.78535604 | 60.91456575 | 54.11192964 |
| 35 | C | 28.84232293 | 56.36429421 | 48.95959136 |
| 36 | C | 26.93521132 | 54.51916562 | 49.0125037 |
| 37 | C | 26.94182536 | 52.52021333 | 47.27830203 |
| 38 | C | 28.8445906 | 52.31839058 | 45.42826015 |
| 39 | C | 30.79119748 | 54.12988204 | 45.45282659 |
| 40 | C | 30.78836289 | 56.12184235 | 47.18041422 |
| 41 | C | 34.68214357 | 48.44067257 | 39.54894423 |

| | | | | |
|----|---|-------------|-------------|-------------|
| 42 | C | 32.68886046 | 48.28854962 | 41.2714296 |
| 43 | C | 31.03024784 | 50.3358789 | 41.62688708 |
| 44 | C | 31.39761059 | 52.51454415 | 40.14383002 |
| 45 | C | 33.39901953 | 52.67517087 | 38.43665144 |
| 46 | C | 54.70549262 | 48.71354902 | 37.67452489 |
| 47 | C | 56.7770104 | 48.43613723 | 39.28211491 |
| 48 | C | 57.08843726 | 50.0012084 | 41.40352145 |
| 49 | C | 55.13748401 | 51.96123234 | 41.8447725 |
| 50 | C | 53.08864295 | 52.16796838 | 40.20789173 |
| 51 | C | 59.44983903 | 49.72984373 | 43.08140928 |
| 52 | C | 59.45248465 | 64.55795772 | 55.55001123 |
| 53 | C | 59.41771369 | 62.28971945 | 53.71584305 |
| 54 | C | 61.36394262 | 62.00380389 | 51.92646138 |
| 55 | C | 61.40513865 | 59.93814426 | 50.28088787 |
| 56 | C | 59.49840499 | 58.09547232 | 50.36687041 |
| 57 | C | 57.52949934 | 58.39026959 | 52.11600091 |
| 58 | C | 57.48943715 | 60.45725203 | 53.76081853 |
| 59 | C | 59.54640403 | 55.90698049 | 48.60848025 |
| 60 | C | 57.63929243 | 54.0618519 | 48.66139258 |
| 61 | C | 57.64590647 | 52.06289961 | 46.92719092 |
| 62 | C | 59.54886068 | 51.86126583 | 45.07714904 |
| 63 | C | 61.49527859 | 53.67256832 | 45.10171548 |
| 64 | C | 61.492444 | 55.66452863 | 46.8293031 |
| 65 | C | 31.04536564 | 33.28941542 | 54.96249537 |
| 66 | C | 32.84608567 | 31.33506066 | 54.82284461 |
| 67 | C | 34.93706763 | 31.29084107 | 56.43931634 |
| 68 | C | 35.28118675 | 33.19927548 | 58.24589452 |
| 69 | C | 33.45986871 | 35.11394599 | 58.4392135 |
| 70 | C | 31.36945367 | 35.15003976 | 56.83483602 |
| 71 | C | 37.54281098 | 33.23650309 | 59.89827104 |
| 72 | C | 38.11426416 | 35.40307409 | 61.30895159 |
| 73 | C | 40.24133989 | 35.47450574 | 62.85909393 |
| 74 | C | 41.84949682 | 33.3716185 | 63.08340442 |
| 75 | C | 41.30034241 | 31.2167638 | 61.62132332 |
| 76 | C | 39.17118798 | 31.1477888 | 60.05247269 |
| 77 | C | 46.49236494 | 33.27410864 | 62.92391154 |
| 78 | C | 46.8058705 | 35.13511092 | 61.05100397 |
| 79 | C | 48.84337321 | 35.04308126 | 59.37670663 |
| 80 | C | 50.61499145 | 33.07474253 | 59.50804259 |
| 81 | C | 50.27616356 | 31.17670161 | 61.32728193 |
| 82 | C | 48.23866085 | 31.27099894 | 63.00384695 |
| 83 | C | 52.82162465 | 33.02712143 | 57.77951011 |
| 84 | C | 54.5766133 | 31.04101927 | 57.86549265 |
| 85 | C | 56.67515416 | 31.02892503 | 56.25998133 |

| | | | | |
|-----|---|-------------|-------------|-------------|
| 86 | C | 57.07653199 | 32.99669684 | 54.51330747 |
| 87 | C | 55.31776388 | 34.98960201 | 54.46115103 |
| 88 | C | 53.22092378 | 35.00226318 | 56.06023728 |
| 89 | C | 31.04536564 | 64.86314849 | 57.69617319 |
| 90 | C | 32.84608567 | 62.9089827 | 57.55633345 |
| 91 | C | 34.93706763 | 62.86457414 | 59.17280518 |
| 92 | C | 35.28118675 | 64.77300855 | 60.97957233 |
| 93 | C | 33.45986871 | 66.68767906 | 61.17289131 |
| 94 | C | 31.36945367 | 66.72377283 | 59.56832486 |
| 95 | C | 37.54281098 | 64.81042513 | 62.63175988 |
| 96 | C | 38.11426416 | 66.97680716 | 64.04244043 |
| 97 | C | 40.24133989 | 67.04823881 | 65.59258277 |
| 98 | C | 41.84949682 | 64.94535157 | 65.81708223 |
| 99 | C | 41.30034241 | 62.79068585 | 64.35481216 |
| 100 | C | 39.17118798 | 62.72171084 | 62.7861505 |
| 101 | C | 46.49236494 | 64.84803068 | 65.65758935 |
| 102 | C | 46.8058705 | 66.70903297 | 63.78468179 |
| 103 | C | 48.84337321 | 66.61681433 | 62.11019547 |
| 104 | C | 50.61499145 | 64.6484756 | 62.24172041 |
| 105 | C | 50.27616356 | 62.75062365 | 64.06077077 |
| 106 | C | 48.23866085 | 62.84492099 | 65.73752476 |
| 107 | C | 52.82162465 | 64.6008545 | 60.51318792 |
| 108 | C | 54.5766133 | 62.61475234 | 60.59917046 |
| 109 | C | 56.67515416 | 62.60284707 | 58.99365914 |
| 110 | C | 57.07653199 | 64.57061888 | 57.24698529 |
| 111 | C | 55.31776388 | 66.56352405 | 57.19482884 |
| 112 | C | 53.22092378 | 66.57599625 | 58.79391509 |
| 113 | C | 42.01144635 | 59.78356466 | 72.01670673 |
| 114 | C | 42.09081485 | 61.41005194 | 69.94103156 |
| 115 | C | 44.25681893 | 62.86287338 | 69.43552982 |
| 116 | C | 46.33419486 | 62.63081502 | 71.08091436 |
| 117 | C | 46.25425944 | 61.00602849 | 73.14959754 |
| 118 | C | 43.95654145 | 51.40092855 | 31.46904224 |
| 119 | C | 41.50424386 | 51.17019299 | 33.10233253 |
| 120 | C | 46.31718732 | 51.19532634 | 33.23253466 |
| 121 | C | 40.5489873 | 53.31219755 | 34.39792876 |
| 122 | C | 40.1929629 | 48.86416019 | 33.45004214 |
| 123 | C | 46.27806999 | 52.03360885 | 35.77346041 |
| 124 | C | 48.65156601 | 50.2531089 | 32.3077027 |
| 125 | C | 38.44307651 | 53.15138185 | 35.97339343 |
| 126 | C | 38.10972882 | 48.69899813 | 35.06462414 |
| 127 | C | 48.40117729 | 51.82706179 | 37.31585487 |
| 128 | C | 50.76427981 | 50.0191608 | 33.87560846 |
| 129 | C | 37.22136857 | 50.83457763 | 36.35417325 |

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|-----|----|-------------|-------------|-------------|
| 130 | C | 50.652597 | 50.79602721 | 36.40651866 |
| 131 | C | 35.06500208 | 50.64220351 | 38.1271143 |
| 132 | H | 41.50651153 | 55.22781292 | 34.16435861 |
| 133 | H | 44.46109832 | 52.89135554 | 36.55070476 |
| 134 | H | 48.83430252 | 49.66691585 | 30.24279896 |
| 135 | H | 37.70192592 | 54.9146853 | 36.96436581 |
| 136 | H | 37.13066171 | 46.79812262 | 35.32635121 |
| 137 | H | 52.59542443 | 49.19146076 | 33.09930897 |
| 138 | C | 52.85696252 | 50.56094528 | 38.11388621 |
| 139 | C | 44.00057207 | 57.88760244 | 75.88743275 |
| 140 | C | 46.35271417 | 57.09901973 | 77.16923399 |
| 141 | C | 41.72534181 | 56.85921348 | 76.75292732 |
| 142 | C | 46.28619582 | 55.17357778 | 78.95842668 |
| 143 | C | 41.71721599 | 54.96910941 | 78.58974111 |
| 144 | C | 43.98715501 | 53.99760121 | 79.64420829 |
| 145 | C | 43.95654145 | 51.40092855 | 81.03183418 |
| 146 | C | 44.05310645 | 49.26345933 | 78.98053648 |
| 147 | C | 43.64265794 | 49.75195353 | 76.37857257 |
| 148 | C | 44.71640032 | 46.76070605 | 79.6434524 |
| 149 | C | 43.94898254 | 47.89907706 | 74.51643645 |
| 150 | C | 44.92200253 | 44.86512177 | 77.81759902 |
| 151 | C | 44.53498662 | 45.41427618 | 75.26174443 |
| 152 | C | 43.53475458 | 48.6578021 | 71.76216062 |
| 153 | N | 45.79883545 | 49.8135586 | 70.56445221 |
| 154 | C | 45.17465891 | 50.80982221 | 68.26881291 |
| 155 | C | 46.65563727 | 51.90680823 | 71.80543535 |
| 156 | Br | 48.48734881 | 47.47313279 | 70.12660266 |
| 157 | N | 45.55524975 | 53.32032337 | 68.09628091 |
| 158 | C | 46.50389226 | 54.02726991 | 70.31973267 |
| 159 | C | 45.07223575 | 54.94945626 | 65.92876505 |
| 160 | C | 44.08012954 | 59.59175746 | 73.66473689 |
| 161 | C | 44.64742532 | 43.39812738 | 73.44288304 |
| 162 | H | 48.21655105 | 58.06769334 | 76.69170019 |
| 163 | H | 39.85224528 | 57.56502619 | 75.95640776 |
| 164 | H | 48.1078918 | 54.51614206 | 79.90177796 |
| 165 | H | 39.84941069 | 54.15539334 | 79.28988464 |
| 166 | H | 43.0405912 | 51.74523665 | 75.82601666 |
| 167 | H | 45.09566836 | 46.25652711 | 81.70325388 |
| 168 | H | 45.40955187 | 42.85690982 | 78.42609083 |
| 169 | H | 41.90599963 | 50.0647032 | 71.66786329 |
| 170 | H | 43.01375708 | 46.91509667 | 70.60791591 |
| 171 | H | 44.40875291 | 49.53236735 | 66.71243447 |
| 172 | H | 47.37637882 | 51.73975644 | 73.82876511 |
| 173 | H | 47.14299764 | 55.93324768 | 71.09433141 |

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|-----|---|-------------|-------------|-------------|
| 174 | H | 44.22885098 | 53.78179449 | 64.32684421 |
| 175 | H | 46.92152174 | 55.83876138 | 65.27265214 |
| 176 | H | 43.68876726 | 56.50186627 | 66.49133652 |
| 177 | C | 42.39090335 | 38.30210294 | 69.8185773 |
| 178 | C | 44.54953751 | 39.80065575 | 69.9973454 |
| 179 | C | 46.59214247 | 39.37130998 | 68.37936189 |
| 180 | C | 46.49444363 | 37.41053015 | 66.60849954 |
| 181 | C | 44.32106962 | 35.86473418 | 66.39798405 |
| 182 | C | 42.28318896 | 36.35001585 | 68.05924228 |
| 183 | C | 44.65328347 | 41.75217592 | 71.87516625 |
| 184 | H | 40.71074786 | 38.67475693 | 71.11417354 |
| 185 | H | 48.34335167 | 40.62022997 | 68.5006823 |
| 186 | H | 48.17705578 | 37.04297842 | 65.31441509 |
| 187 | H | 40.50911408 | 35.13095353 | 67.97250385 |
| 188 | C | 44.23792167 | 33.44531782 | 64.75297745 |
| 189 | C | 44.23792167 | 65.01923986 | 67.48646629 |
| 190 | H | 25.17247479 | 46.30471513 | 43.15586449 |
| 191 | H | 25.26828391 | 42.08741334 | 45.436197 |
| 192 | H | 32.34096188 | 44.3121879 | 49.17936651 |
| 193 | H | 32.23419235 | 48.5018997 | 46.89997886 |
| 194 | H | 32.39935441 | 41.35722316 | 50.77637406 |
| 195 | H | 32.40370078 | 37.2466909 | 53.23849823 |
| 196 | H | 25.41965097 | 34.94651626 | 49.38459077 |
| 197 | H | 25.42097378 | 39.04438736 | 46.94571023 |
| 198 | H | 28.74443511 | 31.72207657 | 51.86939165 |
| 199 | H | 26.94239228 | 33.45079803 | 54.34190931 |
| 200 | H | 55.8765559 | 45.84759038 | 42.8045644 |
| 201 | H | 55.97236501 | 41.63028859 | 45.08508589 |
| 202 | H | 63.04504298 | 43.85487418 | 48.8282554 |
| 203 | H | 62.93827346 | 48.04477495 | 46.54886775 |
| 204 | H | 63.10343552 | 40.89990944 | 50.42526295 |
| 205 | H | 63.10778189 | 36.78937717 | 52.88738711 |
| 206 | H | 56.12373208 | 34.48920253 | 49.03329068 |
| 207 | H | 56.12505488 | 38.58707364 | 46.59459912 |
| 208 | H | 61.21068583 | 32.86460498 | 54.05542683 |
| 209 | H | 59.37613971 | 31.26344004 | 51.52224896 |
| 210 | H | 26.92973112 | 50.3751852 | 42.28923609 |
| 211 | H | 26.93596721 | 65.01451555 | 57.06576055 |
| 212 | H | 28.8680232 | 66.84754989 | 54.77484557 |
| 213 | H | 32.21794071 | 63.94549748 | 52.18214133 |
| 214 | H | 32.29598639 | 60.19212345 | 49.19826377 |
| 215 | H | 25.23785932 | 57.39400598 | 52.55687402 |
| 216 | H | 25.1717189 | 61.13830932 | 55.52166533 |
| 217 | H | 25.37089604 | 54.66070611 | 50.48705699 |

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|-----|---|-------------|-------------|-------------|
| 218 | H | 25.391872 | 51.02581791 | 47.35124546 |
| 219 | H | 32.41333839 | 53.98720772 | 44.04233501 |
| 220 | H | 32.38045715 | 57.57296304 | 47.15376908 |
| 221 | H | 36.01307768 | 46.76637522 | 39.29080765 |
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| 335 | O | 51.74317566 | 46.8443074 | 46.54540846 |

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