

A General Strategy to Prepare Atomically Dispersed Biomimetic Catalysts Based on Host-guest Chemistry

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1. Materials and Methods

Materials

The purity and source of the transition metal precursors used for preparing atomically dispersed catalysts (M_1 /CDP) were listed in Supplementary Table 1. β -cyclodextrin (CD), sodium borohydride (98%) and chloroplatinic acid ($H_2PtCl_6 \cdot 6H_2O$, Pt 37% min) were purchased from Sinopharm Chemical Reagent Co., Ltd. (China). Tetrafluoroterephthalonitrile (98%) was obtained from Adamas Reagent Co., Ltd. (China). Bis(pinacolato)diboron (B_2pin_2 , 99%) and bis(neopentylglycolate)diboron (B_2neop_2 , 98%) were supplied by TCI. Alkynes used for catalytic test (highest purity available) were purchased from J&K Scientific Ltd. (China). Other reagents used in this work were of analytical grade and used without further purification.

Synthesis

Preparation of β -cyclodextrin polymer (CDP)

CDP was synthesized by an established method,^[1] with some modifications. In a typical synthesis of CDP, 2 g of β -cyclodextrin, 1 g of tetrafluoroterephthalonitrile, 3.2 g of K_2CO_3 , 8 mL of DMF and 72 mL of THF were sealed in a 150 mL pressure-resistant flask. The mixture was stirred for 72 h in an oil bath at 120 °C. After being cooled and filtered, the residual K_2CO_3 in the precipitate was removed by washing with 1 mol·L⁻¹ HCl until no CO_2 evolved. The solid was then soaked in H_2O (2×100 mL) for 15 min, THF (2×100 mL) for 30 min and CH_2Cl_2 (1×150 mL) for 15 min. Finally, a yellow powder product was obtained after being dried under high vacuum at 120 °C for 12 h, where the yield of CDP was 61%.

Preparation of CDP supported atomically dispersed catalysts (M_1 /CDP)

In a typical experiment, 0.1g of CDP and a certain amount of transition metal precursor (see Supplementary Table 1, the amount of precursor was determined for loading 1 wt% metal) were mixed with 13 mL of water. The mixture was stirred for 24 h to generate the corresponding inclusion complexes. Then, 4 mL of aqueous $NaBH_4$ solution (4 mg·mL⁻¹) was then added into the mixture. To reduce the metal precursor, the mixture was stirred for 10 min. The precipitate was collected by filtration and then washed with water. The powder catalyst was obtained after being dried in a vacuum oven at 60 °C for 3 h.

Preparation of inclusion complexes of CD with transition metal precursors

The inclusion complexes for comparison was prepared by a classic grinding method.^[2] In a typical experiment, 0.1g of CD and a certain amount of transition metal precursor (see Supplementary Table 1, the amount of precursor was determined for loading 1 wt% metal) were

fully grind for an hour. During the grinding process, a small amount of ethanol was added to improve the formation of inclusion complexes.

Preparation of nitrogen-doped carbon (CN) supported atomically dispersed Pt catalysts (Pt₁/CN)

CN was obtained by pyrolyzing the polydopamine at 900 °C for 2 h under an Ar atmosphere.^[3] Pt₁/CN was prepared by reported methods,^[4] with some modifications. In a typical synthesis, 53 mL of aqueous H₂PtCl₆ solution (0.1g·mL⁻¹) was added into 50 mL of aqueous CN dispersion (4 mg·mL⁻¹) and stirring for 12 h. After being washed with water, the resulting product was dried in a vacuum oven at 50 °C overnight, followed by annealing at 200 °C in a 5% H₂-95% Ar (v/v) atmosphere for 2 h.

Preparation of Pt nanocrystals

Pt nanocrystals, used to prepare supported Pt nanocrystal catalysts for comparison, were synthesized by a reported method,^[5] with some modifications. In a typical synthesis, 5 mL of NaOH glycol solution (0.26 M) was mixed with 5 mL of H₂PtCl₆·6H₂O glycol solution (20 g/L). The mixture was then stirred for 3 h at 160 °C under argon atmosphere. After cooling down to room temperature, a dark-brown colloidal solution of Pt nanocrystals (3.7 g/L) was obtained.

Preparation of activated carbon supported Pt nanocrystals (Pt_{nano}/C)

2.7 ml of colloidal solution of Pt nanocrystals (3.7 g/L) was added dropwise into a suspension containing 1 g of activated carbon and 100 ml of water under stirring. After stirring vigorously for an hour, the precipitate collected by filtration and then washed with water. The powder catalyst was obtained after being dried in a vacuum oven at 60 °C for 3 h.

Preparation of CDP supported Pt nanocrystals (Pt_{nano}/CDP)

1.1 ml of colloidal solution of Pt nanocrystals (3.7 g/L) was added dropwise into a suspension containing 0.4 g of CDP and 100 ml of dilute hydrochloric acid (1 M) under stirring. After stirring vigorously for an hour, the precipitate collected by filtration and then washed with water. The powder catalyst was obtained after being dried in a vacuum oven at 60 °C for 3 h.

Characterizations

Aberration-corrected High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images were recorded using a 200 kV JEOL JEM-ARM200F transmission electron microscope equipped with a probe spherical-aberration corrector. HAADF-STEM image and energydispersive X-ray spectroscopy (EDS) elemental mapping images were taken on a 200 kV JEOL JEM-2100F field-emission transmission electron microscope equipped with a JEOL EDS

detector system. Transmission electron microscopy (TEM) images of the nanocrystal catalysts were recorded by a Hitachi HT-7700 transmission electron microscope working at 100 kV. X-ray photoelectron spectroscopy (XPS) measurements were conducted on a Thermo fisher ESCALAB 250Xi spectrometer equipped with a monochromatic Al X-ray source. The binding energy scales for the samples were referenced by setting the C 1s binding energy of the aromatic sp^2 carbon in CDP to 284.6 eV. Fourier transform-infrared (FT-IR) spectrum was recorded using a PerkinElmer Spectrum 400 FT-IR/FT-NIR spectrometer equipped with an attenuated total reflectance (ATR) accessory in the range of 4,000-550 cm^{-1} with a resolution of 4 cm^{-1} . The powder X-ray diffraction (XRD) patterns were acquired using a Bruker D8-advance X-ray powder diffractometer with Cu $K\alpha$ ($\lambda = 1.5406 \text{ \AA}$) at an accelerating potential of 40 kV and a tube current of 40 mA. To determine the final metal loading, the prepared catalysts were digested in concentrated nitric acid at 140 $^{\circ}C$. The metal contents of the as-obtained solution samples were measured by a Leeman Prodigy 7 inductively coupled plasma-atomic emission spectrometer, which were further used to calculate the metal loading contents of the catalysts (see Supplementary Table 2). 1H and ^{13}C nuclear magnetic resonance (NMR) spectra of the diboration products were recorded in $CDCl_3$ on a Bruker Avance 400 MHz Spectrometer with a 5 mm PABBO BB-1H/D Z-GRD Z108618/0394 multinuclear Probe at 298 K. High resolution mass spectra (HRMS) were obtained on an APEXM Fourier transform mass spectrometry Agilent 6220 LC/MS-TOF System (APCI).

X-ray absorption fine structure (XAFS) measurements and data processing

We collected the XAFS spectra data at 1W1B station in Beijing Synchrotron Radiation Facility (BSRF, operated at 2.5 GeV with a maximum current of 250 mA, Pt L_3 -edge, Co K-edge, Ni K-edge, Cu K-edge and Ir L_3 -edge) and BL14W1 station in Shanghai Synchrotron Radiation Facility (SSRF, operated at 3.5 GeV with a maximum current of 250 mA, Ru K-edge and Rh K-edge), respectively. All samples were pelletized as disks of 13 mm diameter with 1mm thickness. The XAFS data of M_1 /CDP samples were collected at room temperature in fluorescence excitation mode using a Lytle detector and all the references were recorded in transmission mode using ionization chamber. The acquired XAFS data was processed according to the standard procedures using the ATHENA module implemented in the IFEFFIT software packages. The EXAFS spectra were Fourier-transformed (FT) in a k range from 2.0 to 12.0 $\text{\AA}^{-1}$ to evaluate the contribution of each bond pair to the FT peak.

2. Catalytic evaluation

Diboration of alkynes

In a typical experiment, 0.5 mmol of alkyne with the Pt₁/CDP catalyst (0.1 mol% of alkyne based on Pt) and 0.55 mmol of B₂pin₂ or B₂neop₂ were placed in a 10 mL flask with 2 mL of solvent. The reaction was performed in an oil bath at a specified temperature. After stirring the result mixture for a certain time, the catalyst was removed through centrifugation and the liquid sample was analyzed by GC and GC-MS to determine the conversion and selectivity. To obtain isolated products, the liquid samples was concentrated under reduced pressure to get a crude product which was then purified by silica gel column chromatography with a mixture of petroleum ether and ethyl acetate (v/v: 10:1) as the eluent.

Recovery and reuse test

The Pt₁/CDP catalyst after diboration of phenylacetylene was recovered by centrifugation at 10000 rpm. The recovered catalyst was washed with ethanol for three times, and then directly used for the next run.

Density functional theory (DFT) calculation.

We implemented the DFT calculations in the Gaussian 16 suite of programs.^[6] Molecular geometries of M₁/CDs (M=Pt, Co, Ni, Cu, Ru, Rh, Ir) were optimized using the B3LYP method, in combination with the LANL2DZ basis set for metal atom and the 6-31G(d,p) basis set for rest atoms. For each supported metal, the geometrical optimization have been performed for all the possible multiplicity values, where the geometry with the lowest energy was specified as the final optimized structure. The calculations involving Pt-catalyzed diboration of phenylacetylene were carried out in the SMD continuum solvent for toluene at the PBE0-D3(BJ)/def2-TZVPP//B3LYP-D3(BJ)/6-31G(d,p)+LANL2DZ level. All the optimized geometries were checked by means of frequency calculations to ensure that all ground state geometries contain only real frequencies and that the transition state geometries contain one imaginary frequency, and intrinsic reaction coordinates (IRC) calculations were carried out to ensure that the transition states connect to their corresponding reactant complex and product complex. The thermal corrections to the free energies were calculated at 1.0 atm and 373.15 K using the computed harmonic frequencies scaled with scaling factors (0.9838 for zero-point vibrational energies, 1.0033 for thermal contributions to entropy and 1.0003 for thermal contributions to enthalpy).^[7]

3. Supporting Figures, Tables, and Videos

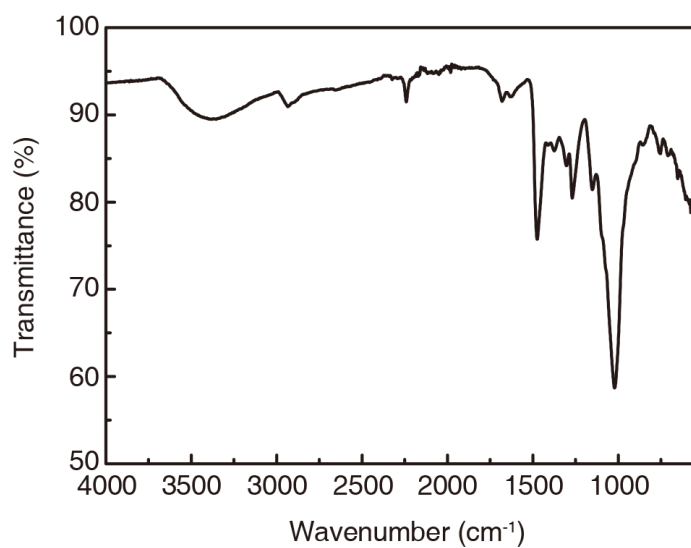


Figure S1. FT-IR spectrum of the CDP support.

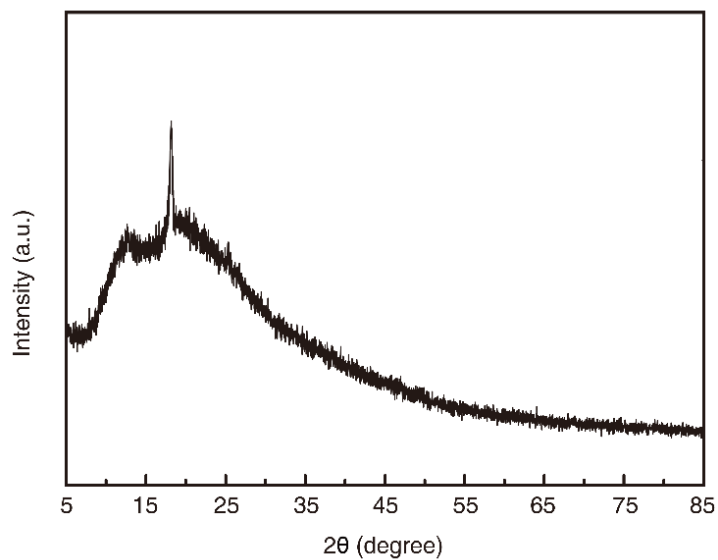


Figure S2. XRD pattern of the CDP support.

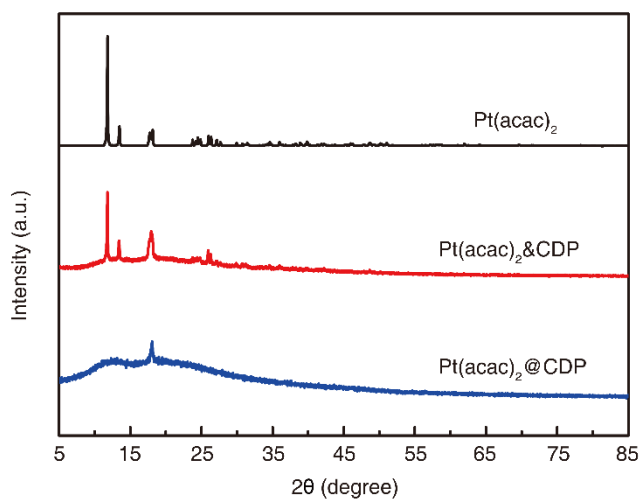


Figure S3. XRD patterns of the $\text{Pt}(\text{acac})_2$ precursor, mechanical mixture and inclusion complex of CDP with a certain amount of $\text{Pt}(\text{acac})_2$ (The amount of $\text{Pt}(\text{acac})_2$ was determined for loading 1 wt% Pt).

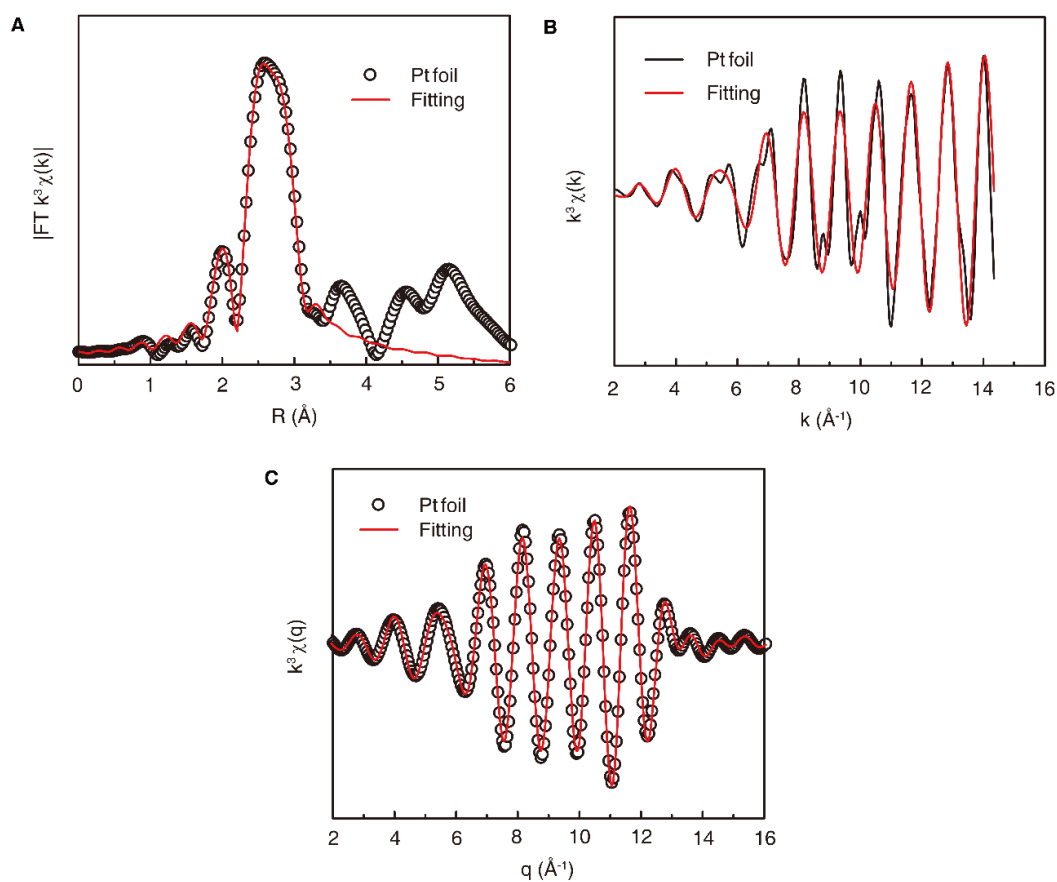


Figure S4. The corresponding EXAFS fitting curves of Pt foil at (A) R space, (B) k space and (C) q space.

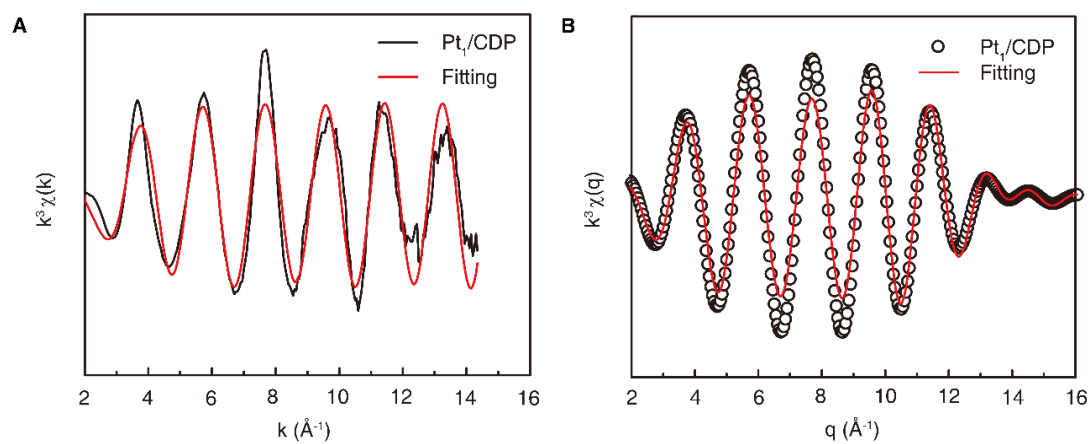


Figure S5. The corresponding EXAFS fitting curves of Pt₁/CDP at (A) k space and (B) q space.

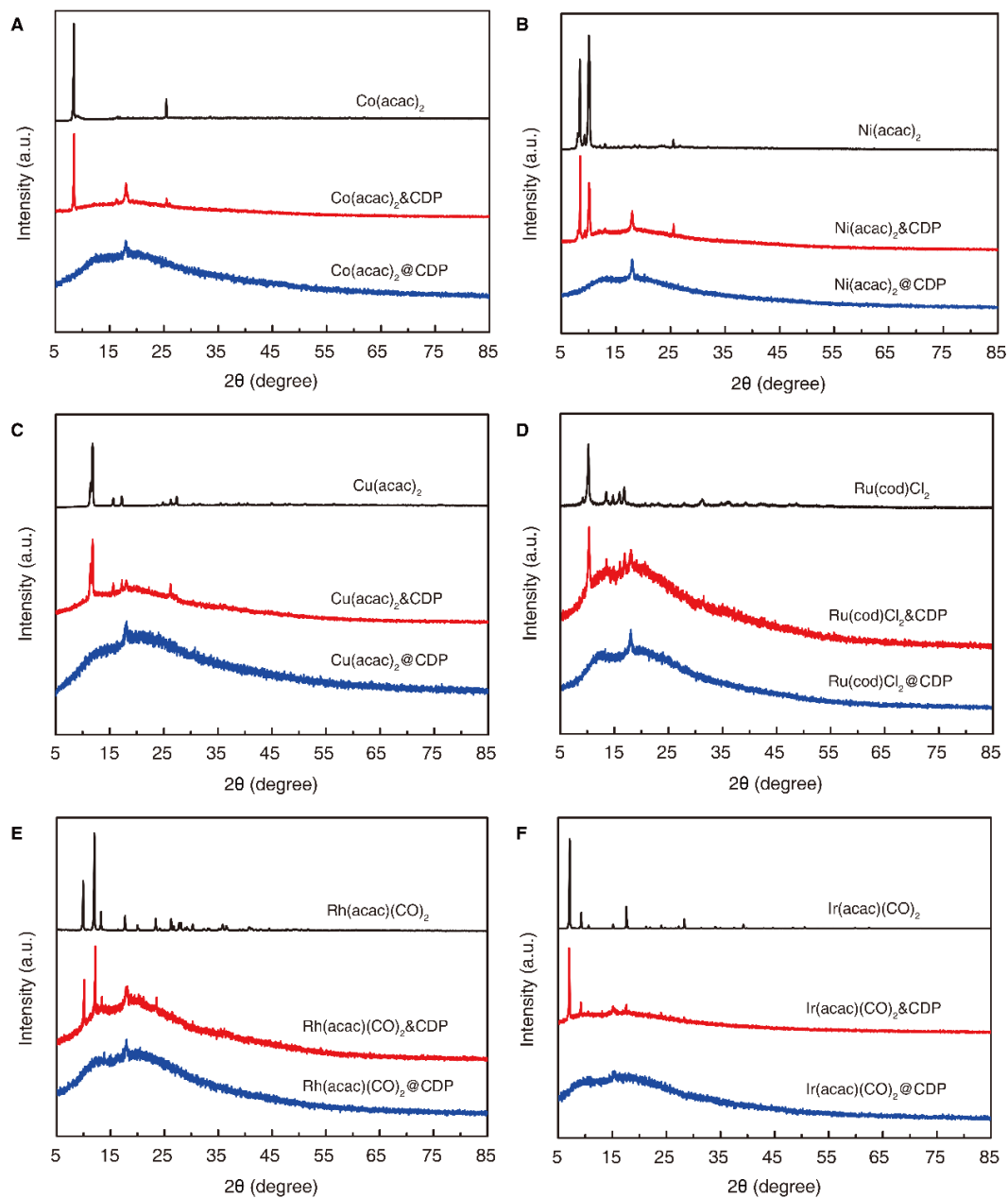


Figure S6. XRD patterns of other transition metal precursors, mechanical mixtures and inclusion complexes of CDP with a certain amount of the corresponding transition metal precursors (The amount of precursor was determined for loading 1 wt% metal).

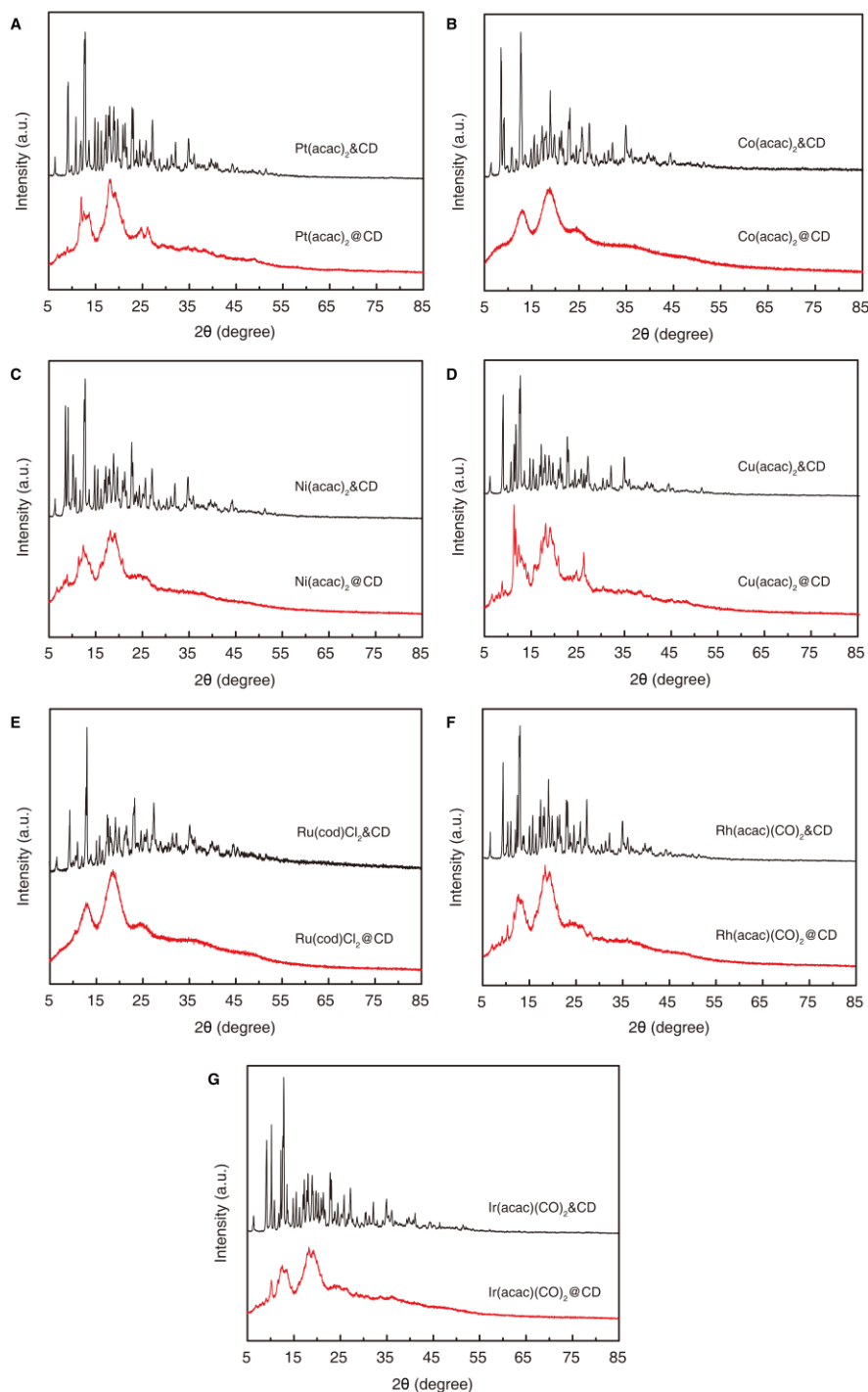


Figure S7. XRD patterns of mechanical mixtures and inclusion complexes of CD with a certain amount of the corresponding transition metal precursors (The amount of precursor was determined for loading 1 wt% metal).

For all transition metal precursors used in this work, different XRD signals compared with mechanical mixture of CD and the precursors were observed, which implied the formation of inclusion complexes and the host-guest chemistry principle involved in the general strategy.

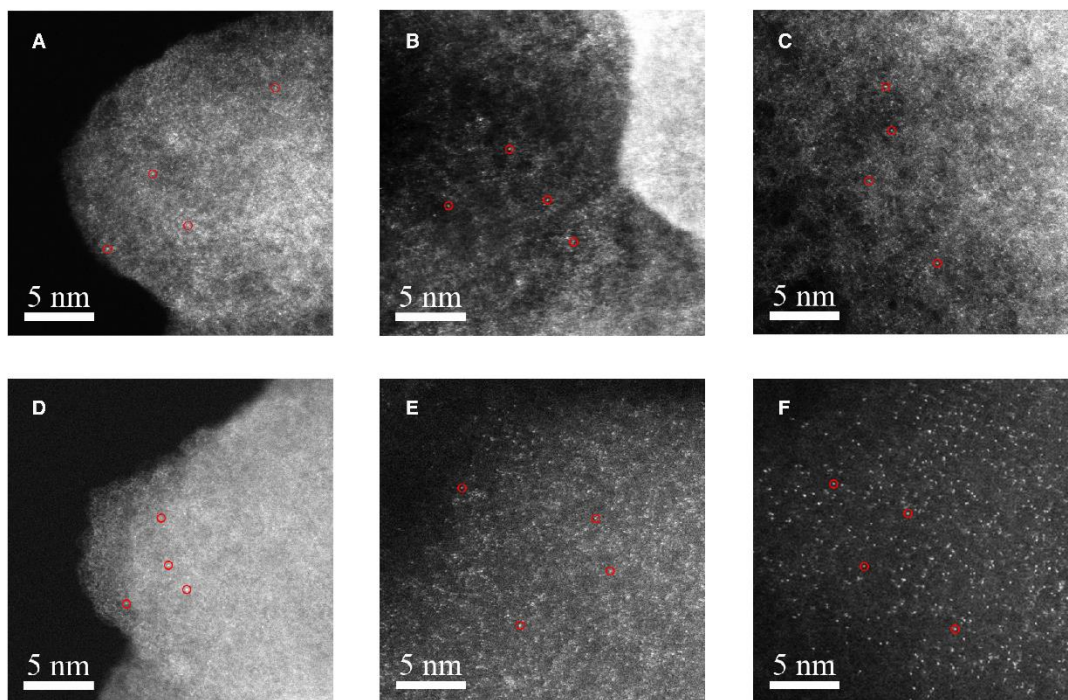


Figure S8. Aberration-corrected HAADF-STEM image of (A) Co₁/CDP, (B) Ni₁/CDP, (C) Cu₁/CDP, (D) Ru₁/CDP, (E) Rh₁/CDP and (F) Ir₁/CDP.

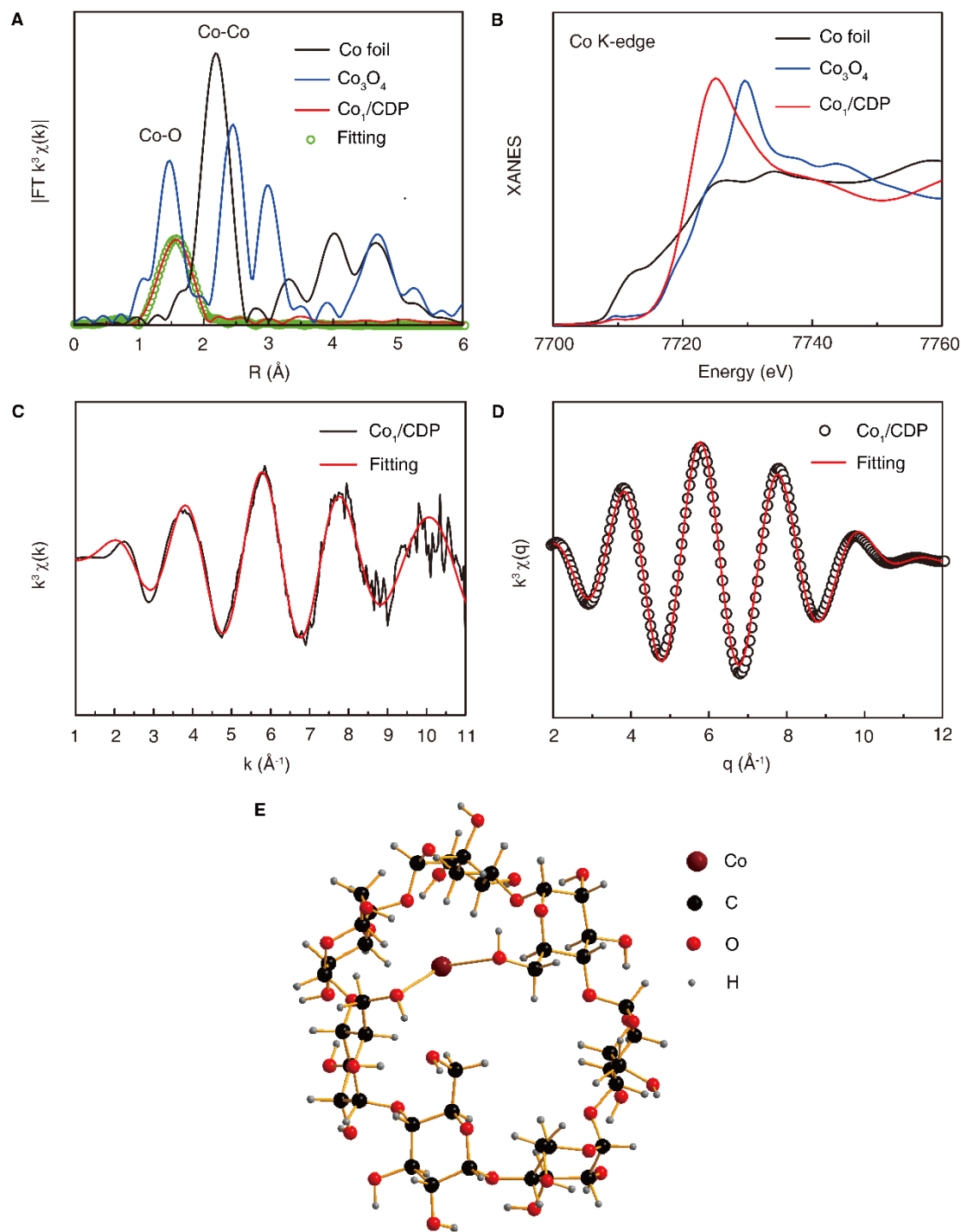


Figure S9. (A) Fourier-transformed EXAFS spectra at the Co K-edge for Co₁/CDP, Co foil, Co₃O₄ and EXAFS fitting curve for Co₁/CDP. (B) The normalized XANES spectra at the Co K-edge for Co₁/CDP, Co foil and Co₃O₄. The corresponding EXAFS fitting curves of Co₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Co₁/CDP.

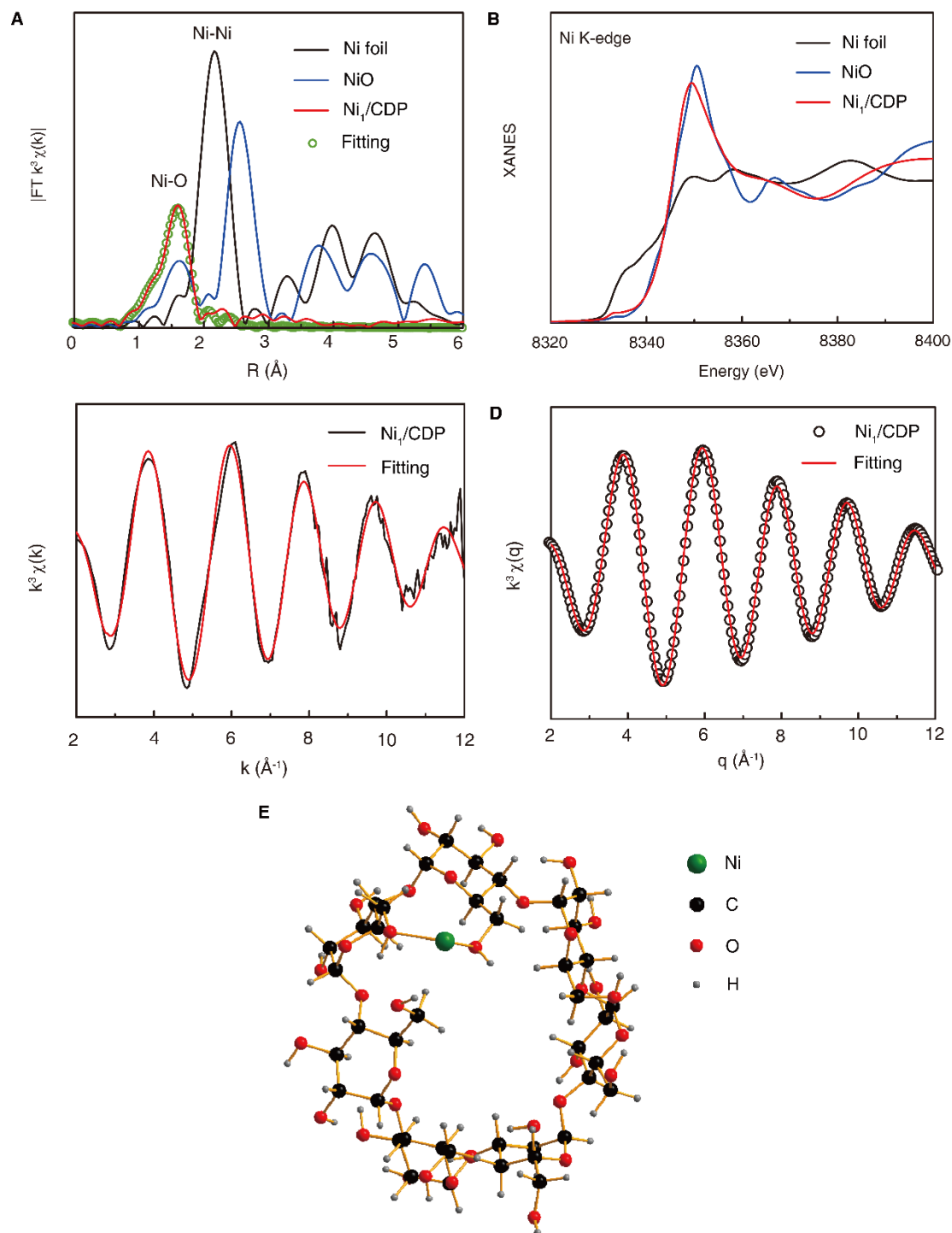


Figure S10. (A) Fourier-transformed EXAFS spectra at the Ni K-edge for Ni₁/CDP, Ni foil, NiO and EXAFS fitting curve for Ni₁/CDP. (B) The normalized XANES spectra at the Ni K-edge for Ni₁/CDP, Ni foil and NiO. The corresponding EXAFS fitting curves of Ni₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Ni₁/CDP.

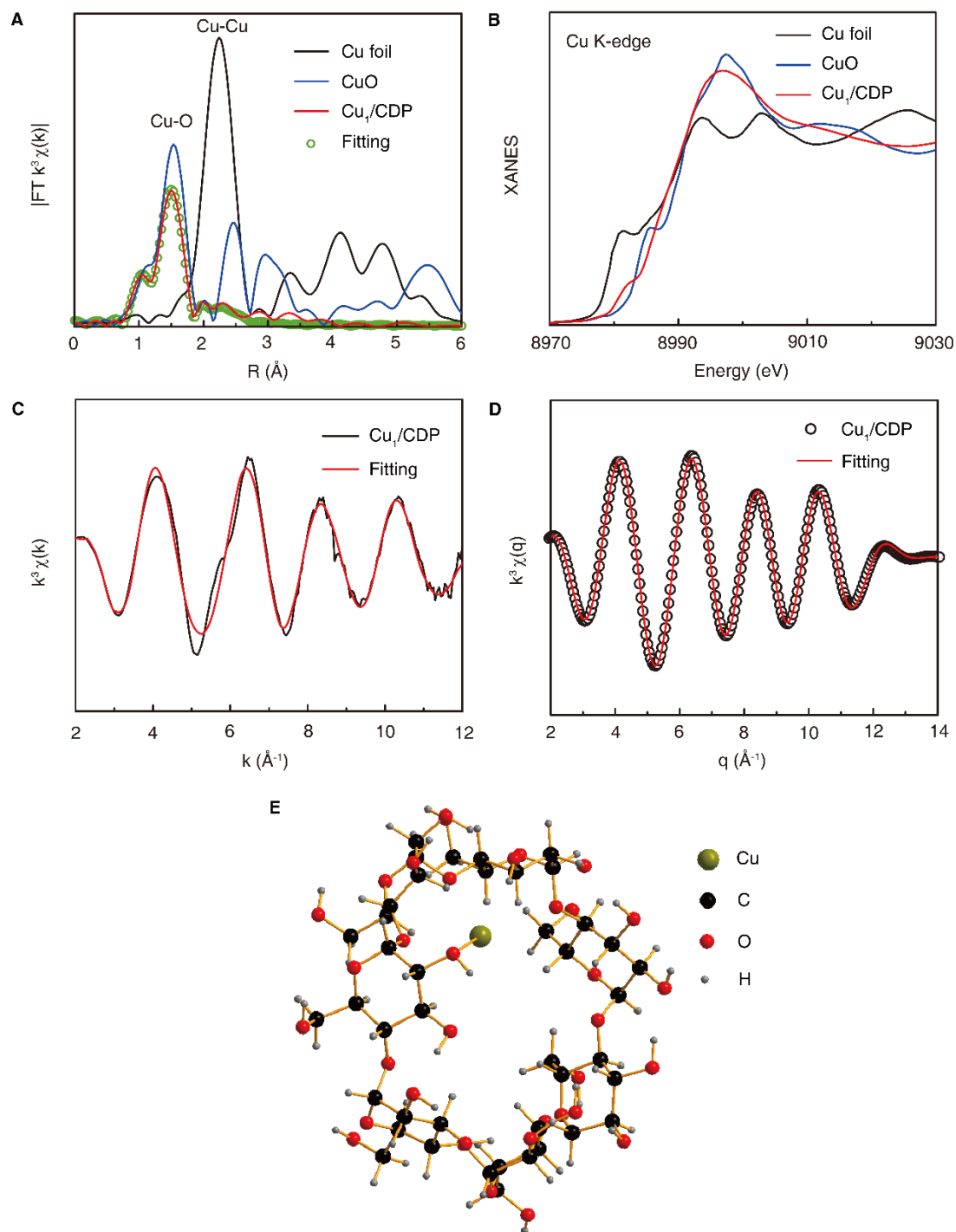


Figure S11. (A) Fourier-transformed EXAFS spectra at the Cu K-edge for Cu₁/CDP, Cu foil, CuO and EXAFS fitting curve for Cu₁/CDP. (B) The normalized XANES spectra at the Cu K-edge for Cu₁/CDP, Cu foil and CuO. The corresponding EXAFS fitting curves of Cu₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Cu₁/CDP.

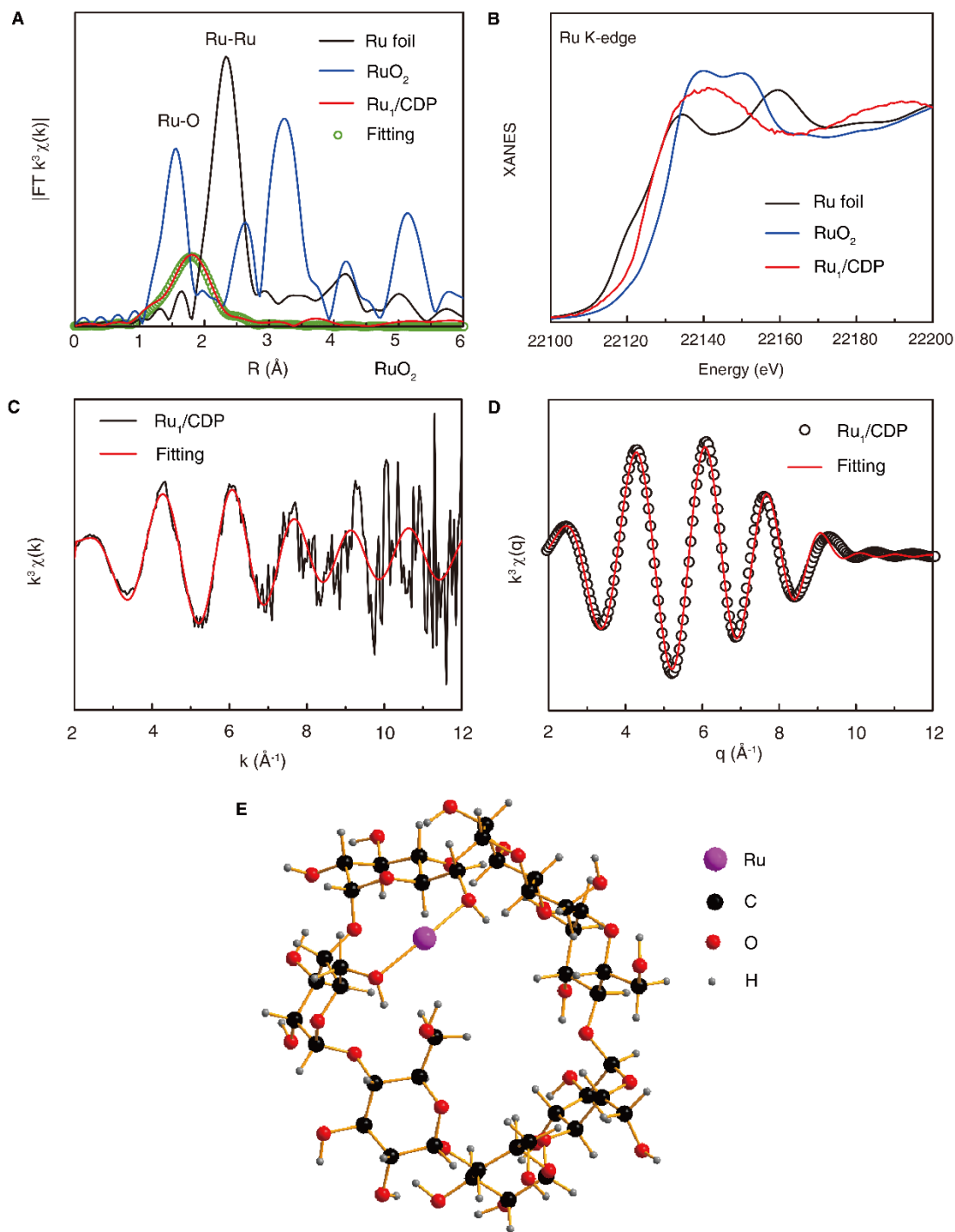


Figure S12. (A) Fourier-transformed EXAFS spectra at the Ru K-edge for Ru₁/CDP, Ru foil, RuO₂ and EXAFS fitting curve for Ru₁/CDP. (B) The normalized XANES spectra at the Ru K-edge for Ru₁/CDP, Ru foil and RuO₂. The corresponding EXAFS fitting curves of Ru₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Ru₁/CDP.

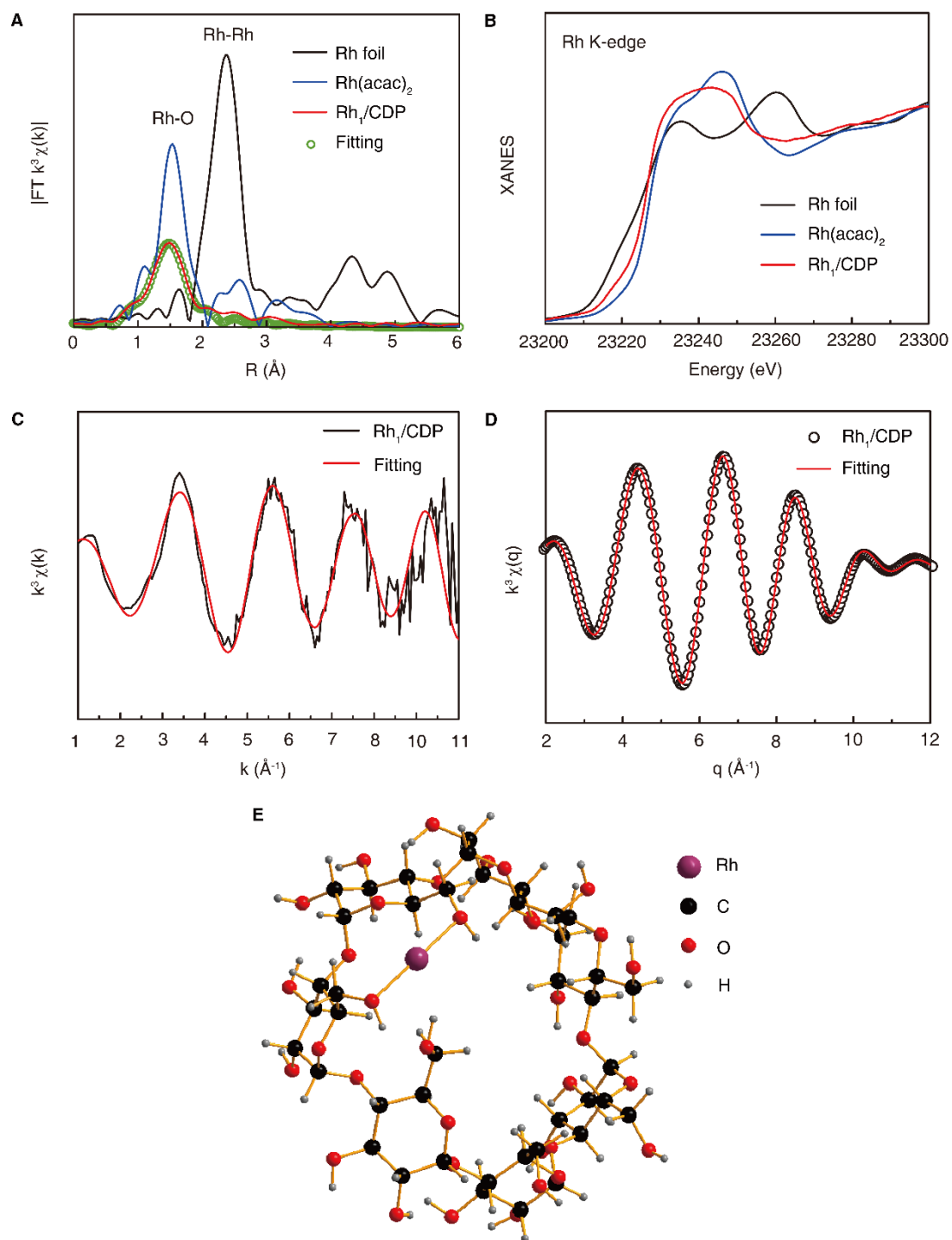


Figure S13. (A) Fourier-transformed EXAFS spectra at the Rh K-edge for Rh₁/CDP, Rh foil, Rh(acac)₃ and EXAFS fitting curve for Rh₁/CDP. (B) The normalized XANES spectra at the Rh K-edge for Rh₁/CDP, Rh foil and Rh(acac)₃. The corresponding EXAFS fitting curves of Rh₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Rh₁/CDP.

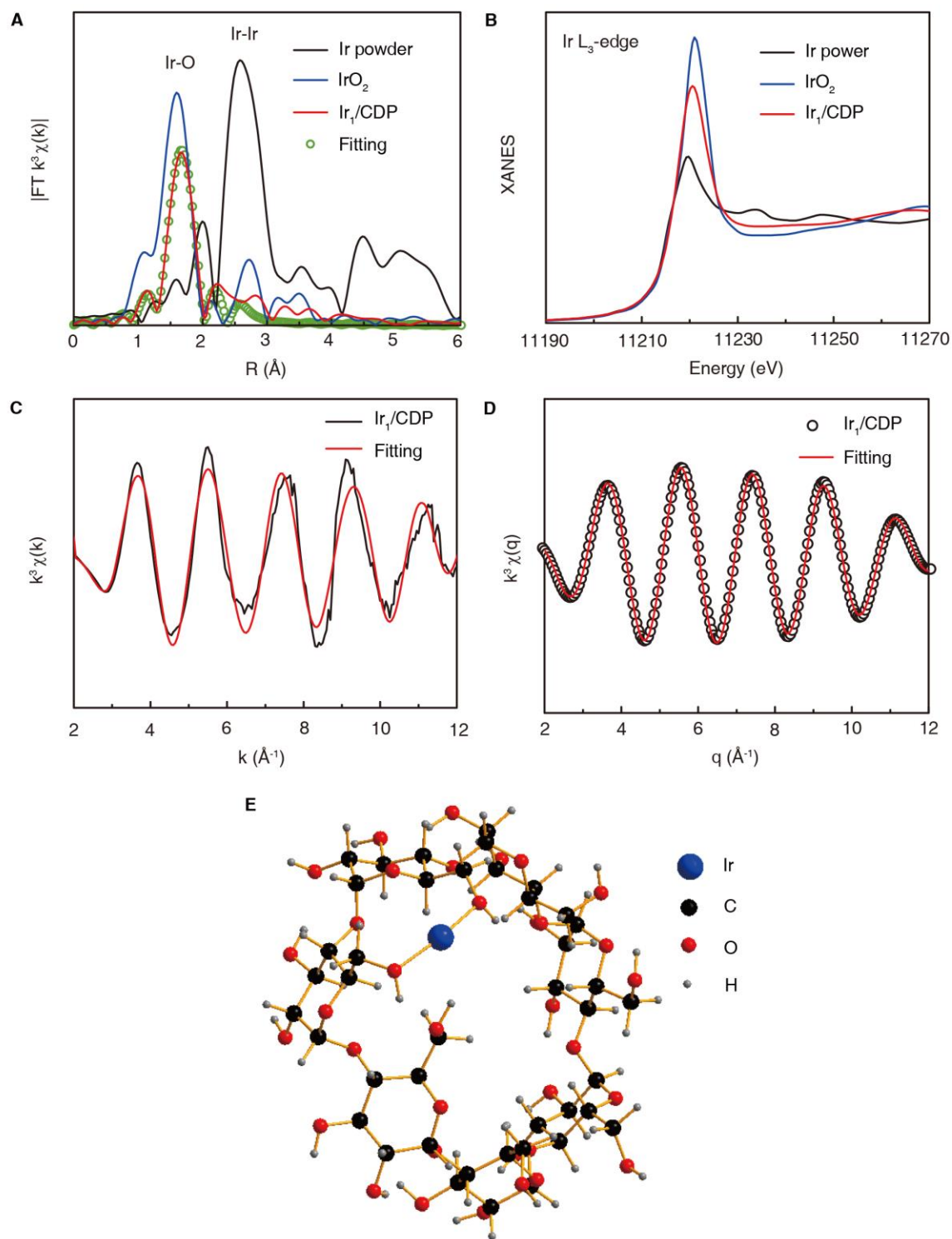


Figure S14. (A) Fourier-transformed EXAFS spectra at the Ir L₃-edge for Ir₁/CDP, Ir powder, IrO₂ and EXAFS fitting curve for Ir₁/CDP. (B) The normalized XANES spectra at the Ir L₃-edge for Ir₁/CDP, Ir powder, and IrO₂. The corresponding EXAFS fitting curves of Ir₁/CDP at (C) k space and (D) q space. (E) Schematic model of the mimicked enzyme catalytic pocket in Ir₁/CDP.

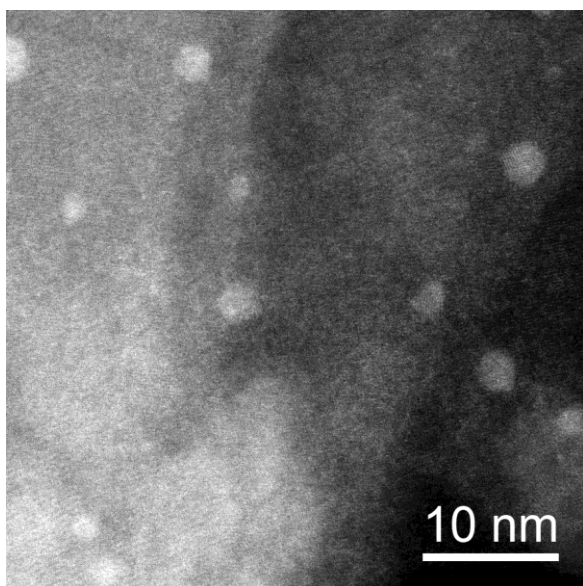


Figure S15. Aberration-corrected HAADF-STEM image of Ru/CDP prepared using $\text{Ru}(\text{acac})_3$ as metal precursor.

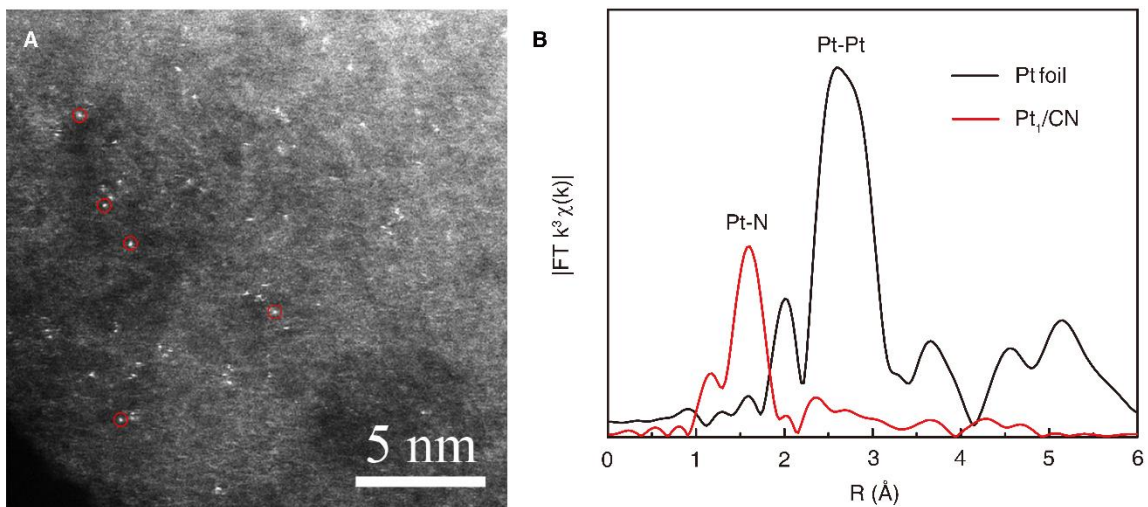


Figure S16. (A) Aberration-corrected HAADF-STEM image of Pt_1/CN . (B) Fourier-transformed EXAFS spectra at the Pt L_3 -edge for Pt_1/CN and Pt foil.

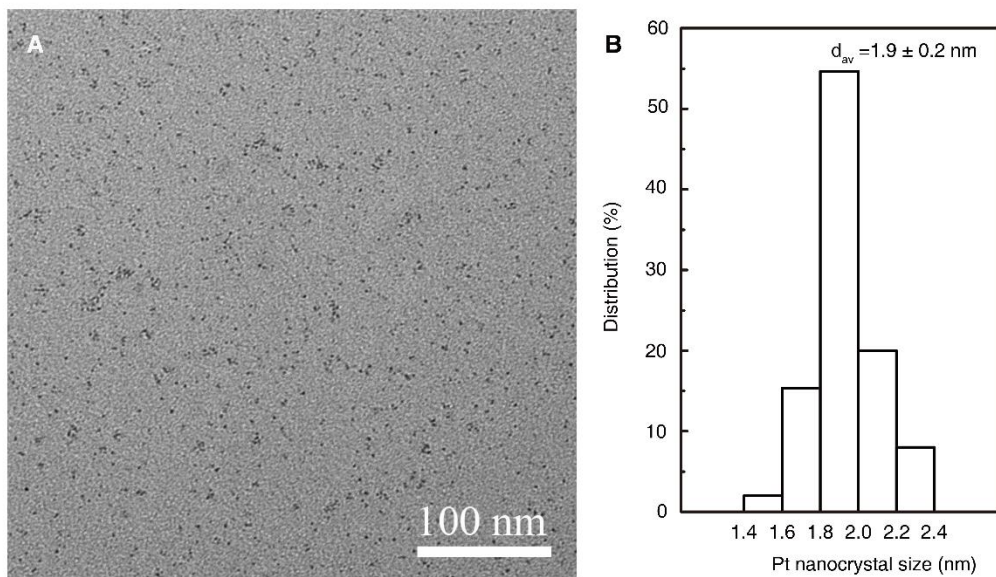


Figure S17. (A) TEM image and (B) nanocrystal size distribution histogram of the prepared Pt nanocrystals.

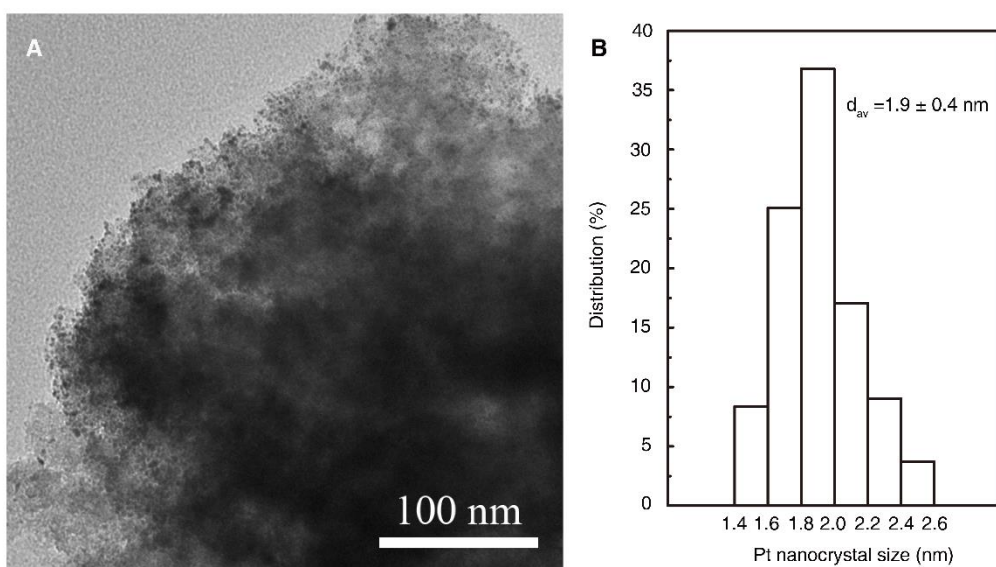


Figure S18. (A) TEM image and (B) nanocrystal size distribution histogram of Pt_{nano}/C.

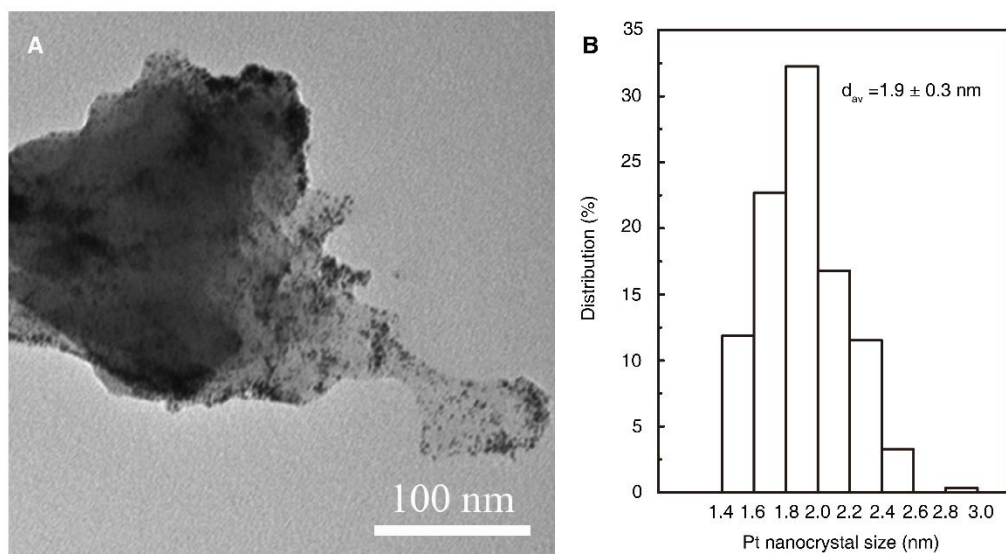


Figure S19. (A) TEM image and (B) nanocrystal size distribution histogram of Pt_{nano}/CDP.

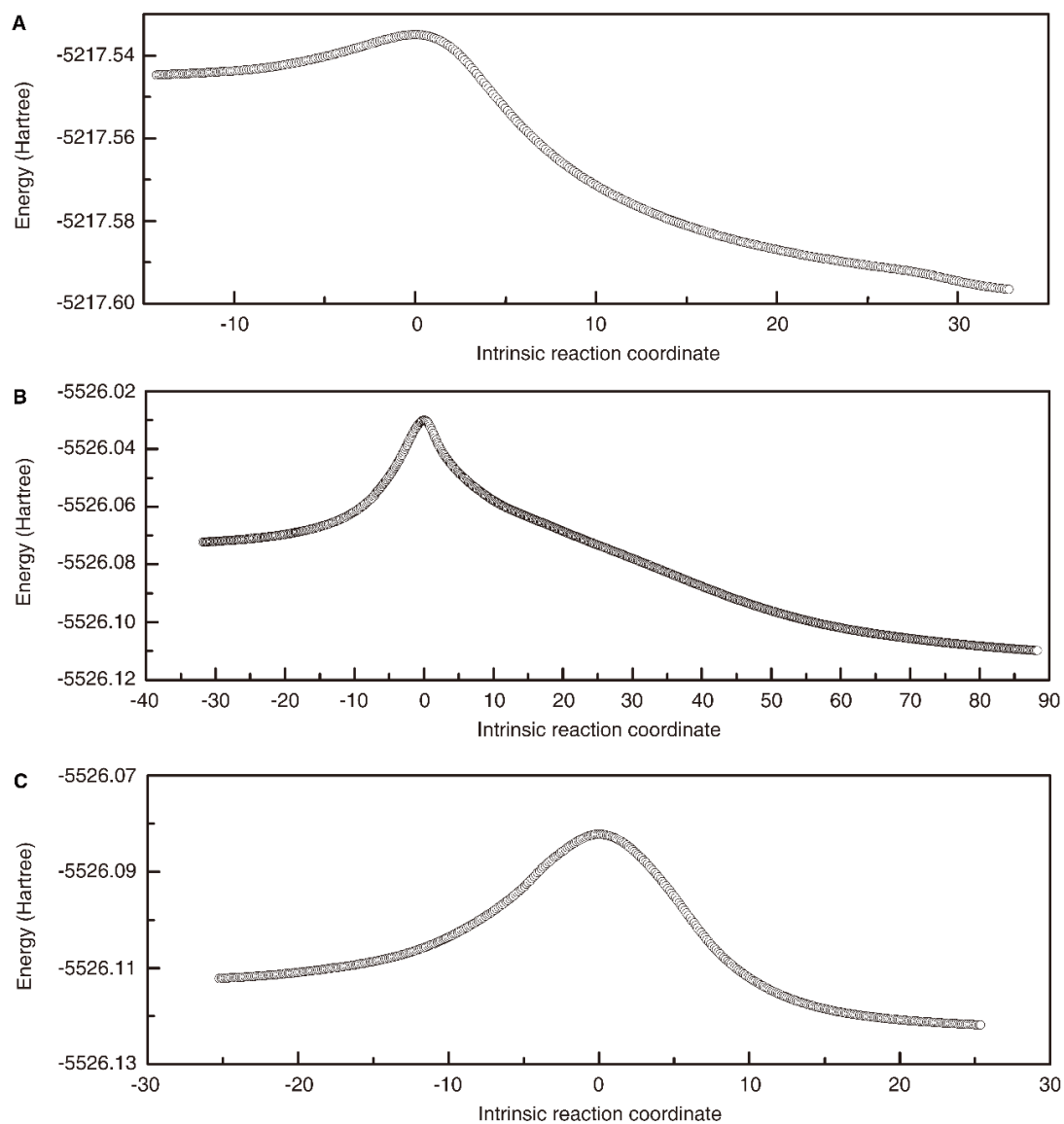


Figure S20. IRC reaction profiles of (A) the first step, (B) the second step and (C) the third step for the diboration of phenylacetylene over Pt₁/CD.

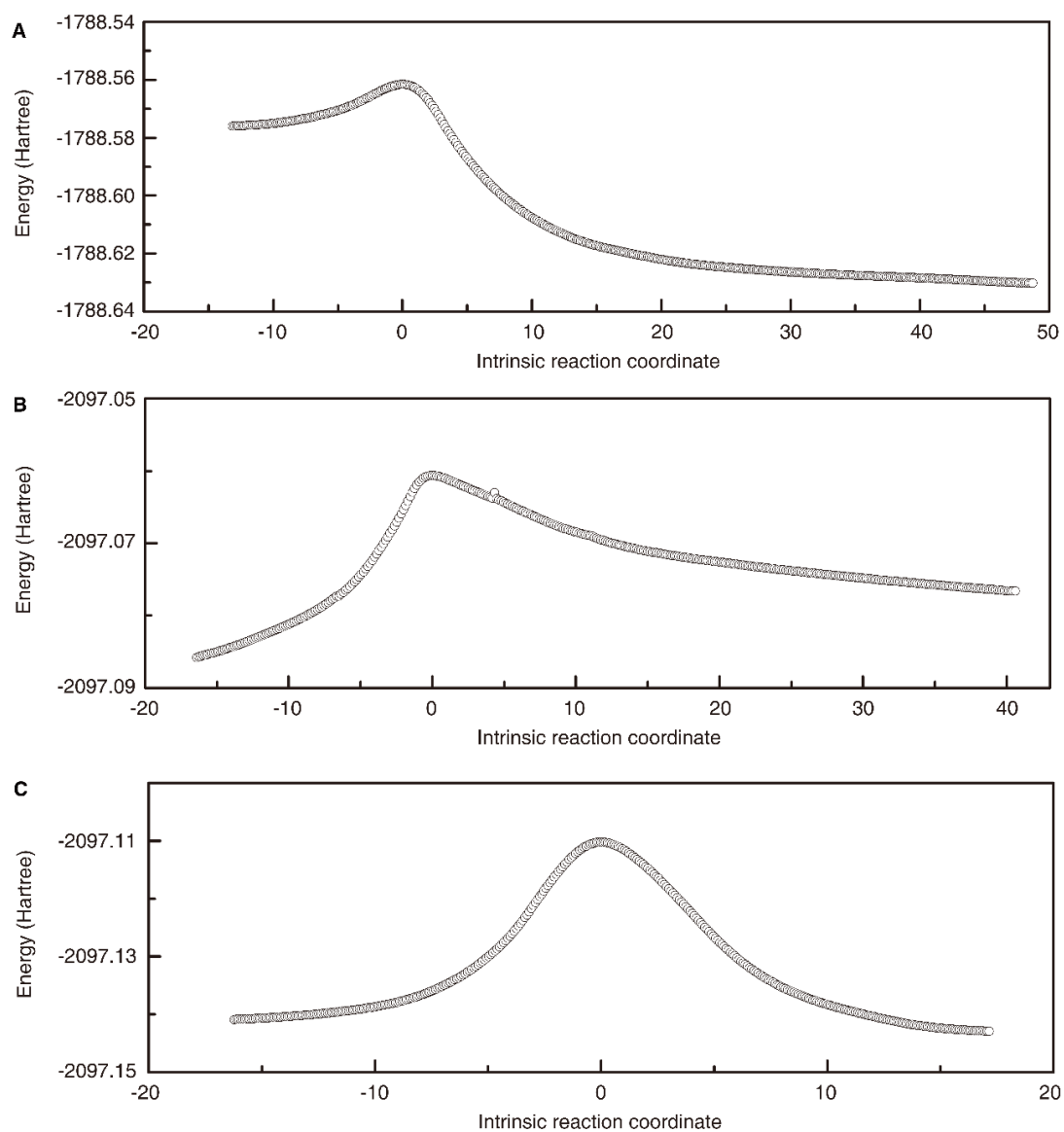


Figure S21. IRC reaction profiles of (A) the first step, (B) the second step and (C) the third step for the diboration of phenylacetylene over Pt₁/CD-b.

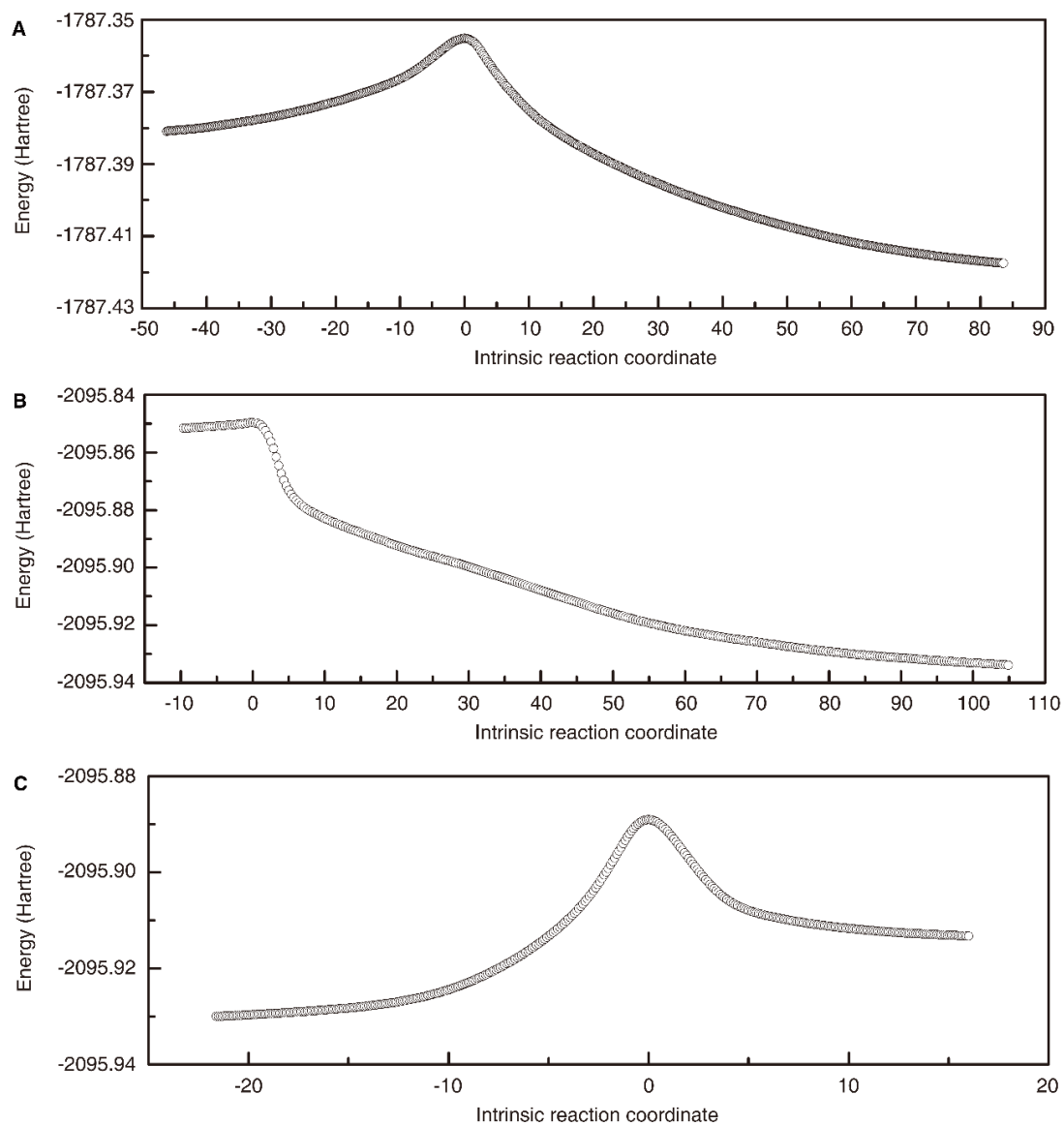


Figure S22. IRC reaction profiles of (A) the first step, (B) the second step and (C) the third step for the diboration of phenylacetylene over Pt₁/CD-b-nOH.

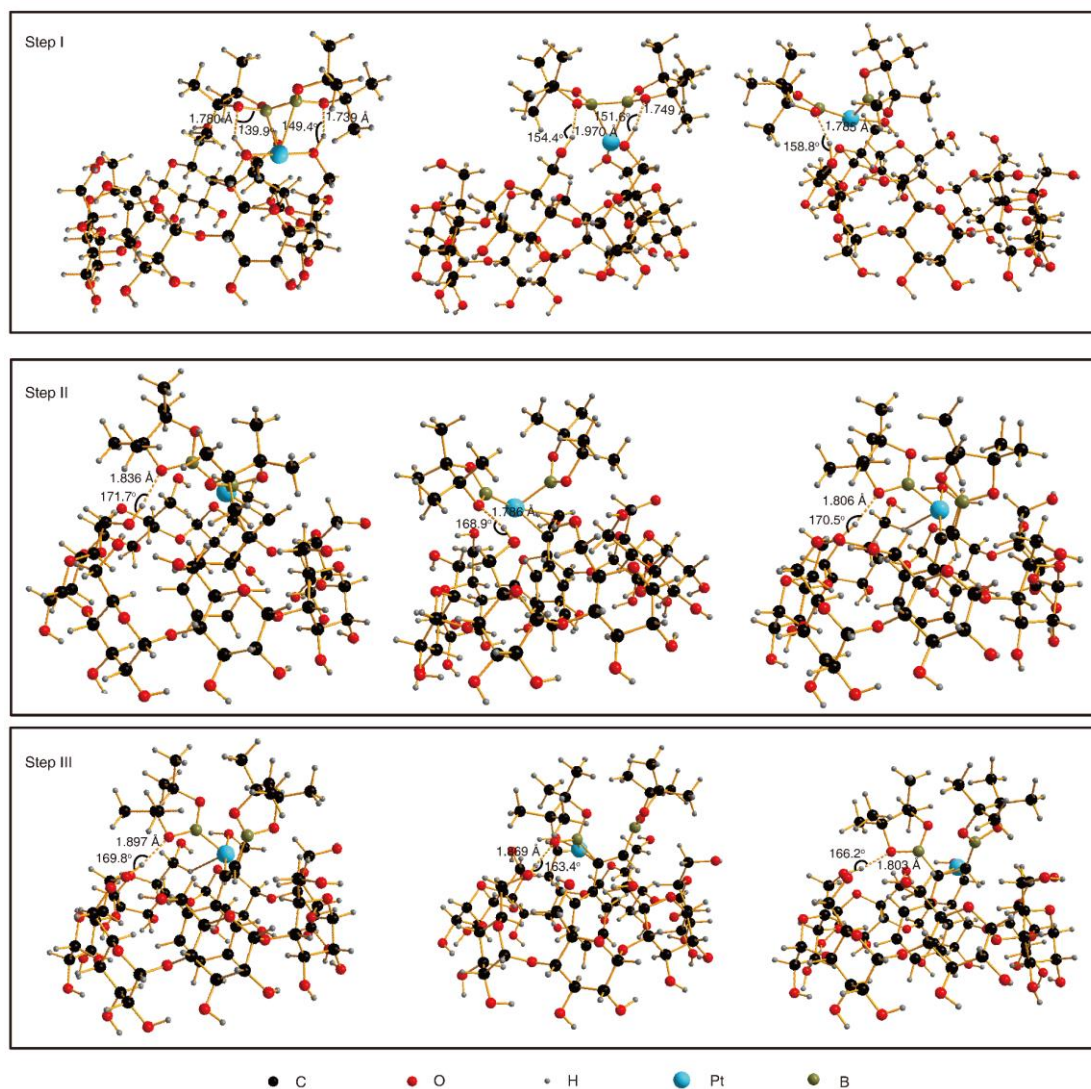


Figure S23. Schematic to show hydrogen bonds existing in diboration of phenylacetylene over Pt_1/CD .

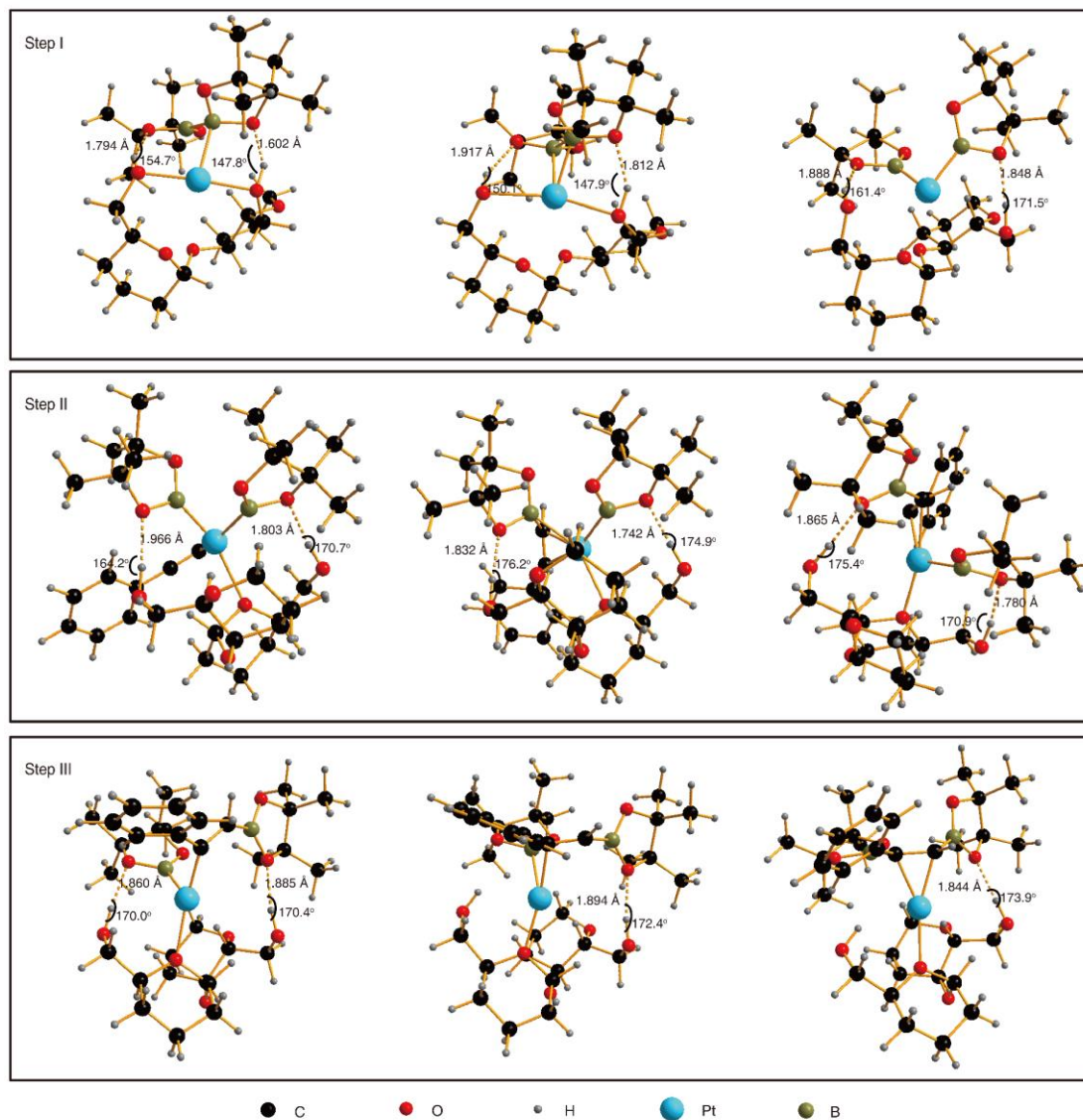


Figure S24. Schematic to show hydrogen bonds existing in diboration of phenylacetylene over Pt₁/CD-b.

Table S1. The precursor used to prepare atomically dispersed catalysts prepared in this work.

Catalyst	Transition metal precursor	Linear formula ^a	Purity and source
Pt ₁ /CDP	Bis(2,4-pentanedionate)platinum(II)	Pt(acac) ₂	Pt 48.0% min, Alfa Aesar
Co ₁ /CDP	Bis(2,4-pentanedionate)cobalt(II)	Co(acac) ₂	97%, Sigma Aldrich
Ni ₁ /CDP	Bis(2,4-pentanedionate)nickel(II)	Ni(acac) ₂	95%, Sigma Aldrich
Cu ₁ /CDP	Bis(2,4-pentanedionate)copper(II)	Cu(acac) ₂	98%, Alfa Aesar
Ru ₁ /CDP	Dichloro(1,5-cyclooctadiene)ruthenium(II)	Ru(COD)Cl ₂	97%, J&K Scientific Ltd. (China)
Rh ₁ /CDP	Dicarbonyl(2,4-pentanedionate)rhodium(I)	Rh(acac)(CO) ₂	99%, Shanghai Macklin Biochemical Co., Ltd. (China)
Ir ₁ /CDP	Dicarbonyl(2,4-pentanedionate)iridium(I)	Ir(acac)(CO) ₂	97%, Aladdin Industrial Corporation (China)

^a The linear formula of the corresponding precursor.

Table S2. The metal loading contents of the catalysts prepared in this work.^a

Catalyst	Content (wt%) ^b
Pt ₁ /CDP	0.8
Co ₁ /CDP	0.7
Ni ₁ /CDP	0.8
Cu ₁ /CDP	0.6
Ru ₁ /CDP	0.8
Rh ₁ /CDP	0.7
Ir ₁ /CDP	0.6
Pt ₁ /CN	0.7
Pt _{nano} /CDP	0.6
Pt _{nano} /C	0.9

^a The metal contents were determined by ICP-AES measurement.

^b The contents of the corresponding metals.

Table S3. Structural parameters extracted from the Co K-edge, Ni K-edge, Cu K-edge, Ru K-edge, Rh K-edge, Ir L₃-edge and Pt L₃-edge EXAFS fitting ($S_0^2 = 0.85$).^a

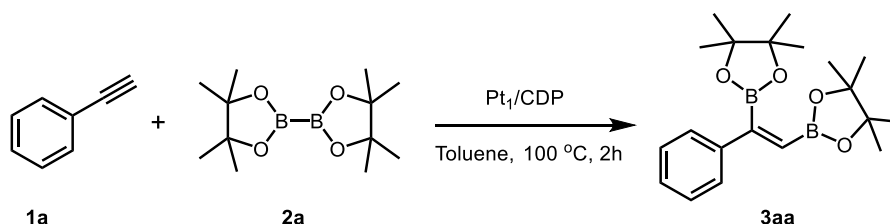
sample	Scattering pair	CN ^b	R (Å) ^c	σ^2 (10 ⁻³ Å ²) ^d	ΔE_0 (eV) ^e	R factor ^f
Pt foil	Pt-Pt	12 ^g	2.76	4.2	6.8	0.009
Pt ₁ /CDP	Pt-O	2.4	1.98	6.4	4.9	0.017
Co ₁ /CDP	Co-O	2.3	2.11	5.3	1.55	0.005
Ni ₁ /CDP	Ni-O	2.1	2.15	5.5	0.5	0.006
Cu ₁ /CDP	Cu-O	1.4	2.05	4.4	1.0	0.005
Ru ₁ /CDP	Ru-O	2.2	2.09	5.9	1.5	0.007
Rh ₁ /CDP	Rh-O	2.4	1.99	4.8	2.0	0.005
Ir ₁ /CDP	Ir-O	2.3	2.03	5.7	2.5	0.006

^a S_0^2 is the amplitude reduction factor; Error bounds that characterize the structural parameters obtained by EXAFS spectroscopy were estimated as $N \pm 20\%$, $R \pm 1\%$, $\sigma^2 \pm 20\%$, $\Delta E_0 \pm 20\%$. ^b The coordination number. ^c The interatomic distance (the bond length between central atoms and surrounding coordination atoms). ^d The Debye-Waller factor (a measure of thermal and static disorder in absorber-scatterer distances). ^e The edge-energy shift (the difference between the zero kinetic energy value of the sample and that of the theoretical model). ^f R factor is used to value the goodness of the fitting. ^g This value was fixed during EXAFS fitting, based on the known structure.

Table S4. The binding energy of the catalysts prepared in this work.

Catalyst	Binding energy (eV) ^a	Binding energy for the corresponding zero-valent metal (eV) ^b
Pt ₁ /CDP	73.1 (4f _{7/2})	71.2 (4f _{7/2})
Co ₁ /CDP	781.4 (2p _{3/2})	778.3 (2p _{3/2})
Ni ₁ /CDP	858.9 (2p _{3/2})	852.7 (2p _{3/2})
Cu ₁ /CDP	932.9 (2p _{3/2})	932.7 (2p _{3/2})
Ru ₁ /CDP	281.2 (3d _{5/2})	280.1 (3d _{5/2})
Rh ₁ /CDP	309.8 (3d _{5/2})	307.2 (3d _{5/2})
Ir ₁ /CDP	62.8 (4f _{7/2})	60.9 (4f _{7/2})

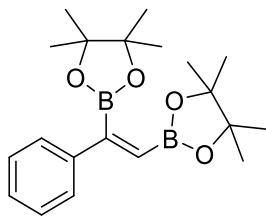
^a The binding energies of the corresponding metal in the atomically dispersed catalysts prepared in this work (The core-level for the binding energy is listed in parenthesis). ^b Data from the literature [8].

Table S5. Recoverability and reusability of the Pt₁/CDP catalyst. ^a

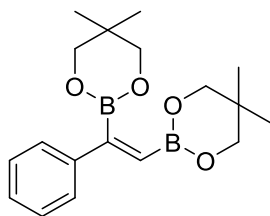
Entry	Catalyst	Conversion (%) ^b	Selectivity (%) ^b
1	Pt ₁ /CDP	88.2	100
2	Recovered from entry 1	86.7	100
3	Recovered from entry 2	86.9	100
4	Recovered from entry 3	86.8	100
5	Recovered from entry 4	87.0	100

^a Reaction conditions: phenylacetylene (0.5 mmol), B₂pin₂ (0.55 mmol), catalyst (0.1 mmol% based on metal), toluene (2 mL), temperature (100 °C), reaction time (1 h). ^b Conversion and selectivity is determined by GC and GC-MS.

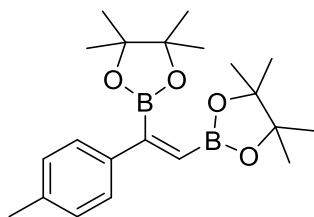
NMR Data of Diboration Products



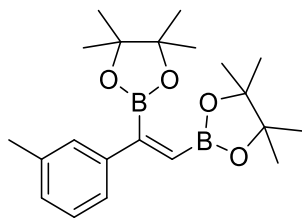
(E)-2,2'-(1-phenylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3aa).^[9] ¹H NMR (400 MHz, Chloroform-*d*) δ 7.47 (d, J = 7.4 Hz, 2H), 7.33 (dd, J = 8.2, 6.6 Hz, 2H), 7.29–7.23 (m, 1H), 6.32 (s, 1H), 1.41 (s, 12H), 1.33 (s, 12H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 129.17, 128.32, 127.64, 126.57, 84.14, 83.60, 25.11, 24.91.



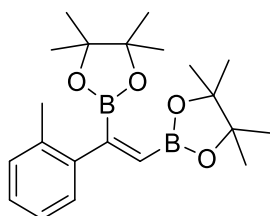
(E)-2,2'-(1-phenylethene-1,2-diyl)bis(5,5-dimethyl-1,3,2-dioxaborinane) (3ab).^[10] ¹H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, J = 7.6 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 7.26 (q, J = 7.2, 6.5 Hz, 1H), 6.21 (s, 1H), 3.76 (s, 4H), 3.73 (s, 4H), 1.09 (s, 6H), 1.05 (s, 6H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 143.08, 128.28, 127.29, 126.60, 72.50, 72.44, 31.89, 31.71, 22.29, 21.99.



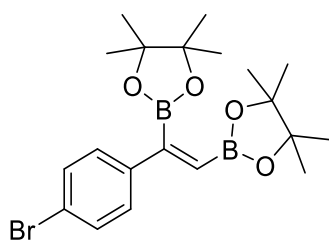
(E)-2,2'-(1-(p-tolyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ba).^[11] ¹H NMR (400 MHz, Chloroform-*d*) δ 7.34 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 7.9 Hz, 2H), 6.26 (s, 1H), 2.31 (s, 3H), 1.37 (s, 12H), 1.29 (s, 12H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 155.12, 140.18, 137.44, 129.08, 127.91, 126.48, 84.09, 83.53, 25.13, 24.91, 21.20.



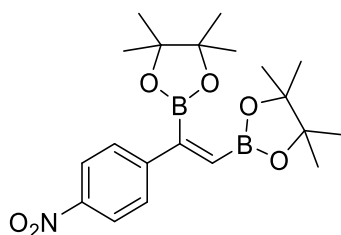
(E)-2,2'-(1-(m-tolyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ca).^[12] ¹H NMR (400 MHz, Chloroform-*d*) δ 7.24 (d, *J* = 10.9 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.3 Hz, 1H), 6.27 (s, 1H), 2.32 (s, 3H), 1.37 (s, 12H), 1.30 (s, 12H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 155.49 , 143.05 , 137.76 , 128.42 , 128.18 , 127.35 , 123.70 , 84.10 , 83.56 , 25.10 , 24.91 , 21.50 .



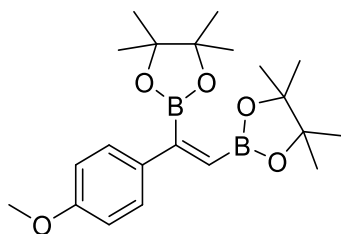
(E)-2,2'-(1-(o-tolyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3da).^[9] ¹H NMR (400 MHz, Chloroform-*d*) δ 7.15 (s, 4H), 6.06 (s, 1H), 2.34 (s, 3H), 1.36 (s, 12H), 1.33 (s, 12H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 144.63 , 134.54 , 129.89 , 128.01 , 126.69 , 125.60 , 83.93 , 83.60 , 24.96 , 24.89 , 20.48 .



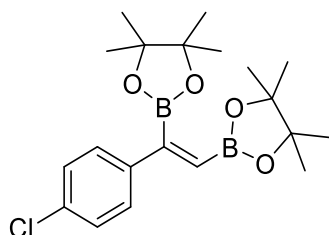
(E)-2,2'-(1-(4-bromophenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ea). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 6.28 (s, 1H), 1.36 (s, 12H), 1.30 (s, 12H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 131.42 , 128.25 , 84.28 , 83.73 , 25.05 , 24.89. HRMS (APCI) calcd for C₂₀H₂₉B₂BrO₄ (M+H⁺): 435.1508, found: 435.1505



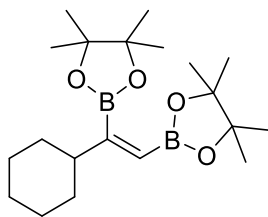
(E)-2,2'-(1-(4-nitrophenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3fa). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.18 (d, J = 8.7 Hz, 2H), 7.58 (d, J = 8.7 Hz, 2H), 6.43 (s, 1H), 1.38 (s, 12H), 1.34 (s, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.85 , 147.06 , 127.56, 123.87, 84.56 , 84.04 , 24.99 , 24.89 . HRMS (APCI) calcd for $\text{C}_{20}\text{H}_{29}\text{B}_2\text{NO}_6$ ($\text{M}+\text{H}^+$): 402.2254, found: 402.2256



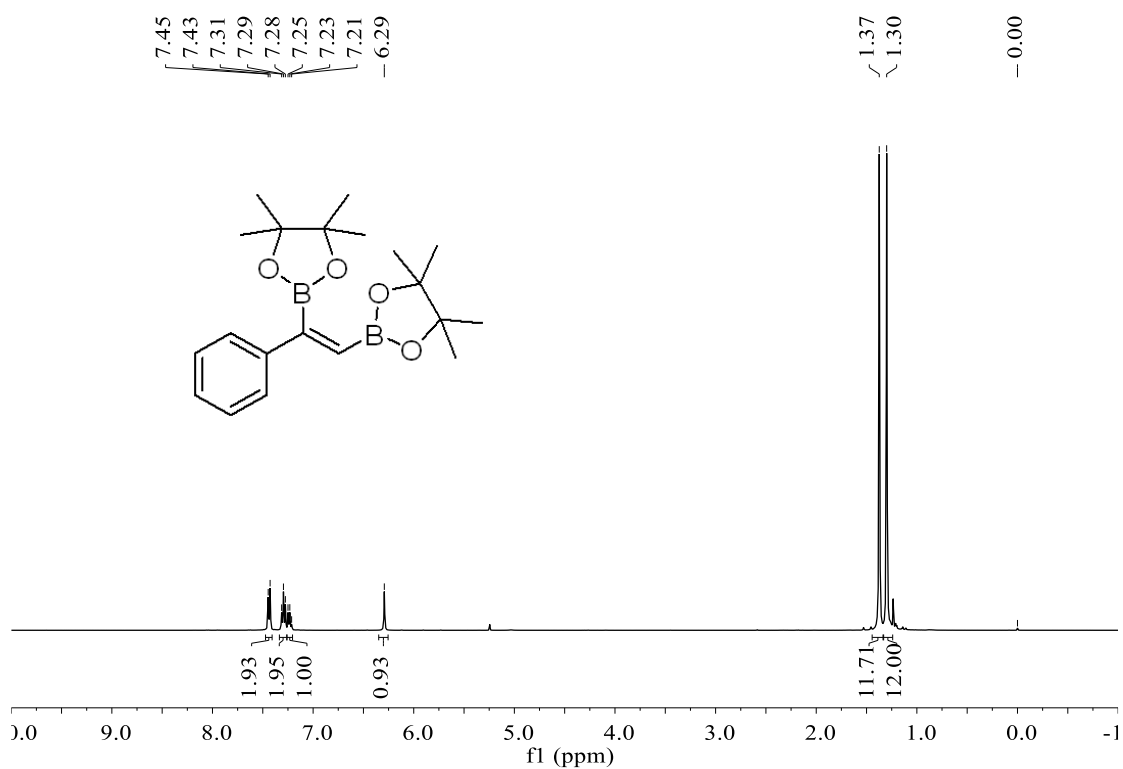
(E)-2,2'-(1-(4-methoxyphenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ga).^[9] ^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, J = 8.3 Hz, 2H), 6.84 (d, J = 8.3 Hz, 2H), 6.22 (s, 1H), 3.78 (s, 3H), 1.38 (s, 12H), 1.30 (s, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.42 , 135.43 , 127.77 , 113.74 , 84.10 , 83.50 , 25.12 , 24.86 .



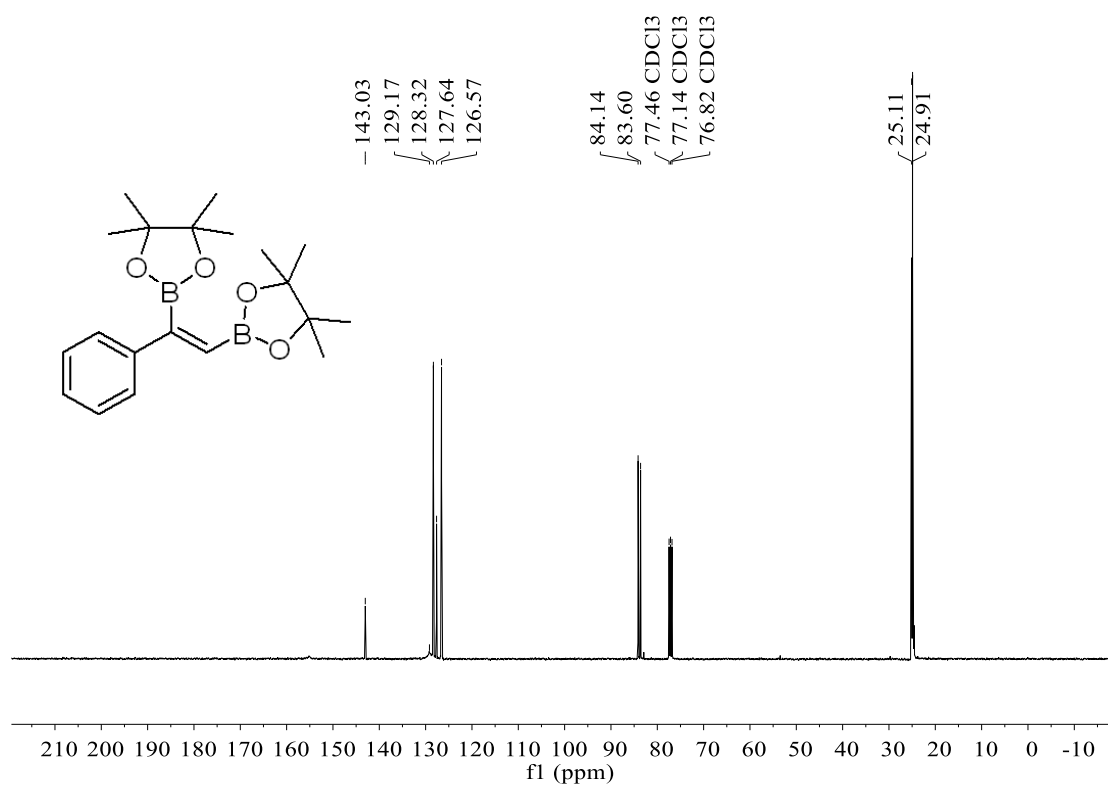
(E)-2,2'-(1-(4-chlorophenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ha).^[12] ^1H NMR (400 MHz, Chloroform-*d*) δ 7.37 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 8.5 Hz, 2H), 6.27 (s, 1H), 1.37 (s, 12H), 1.30 (s, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 128.48 , 127.91 , 84.27 , 83.72 , 25.06 , 24.89 .



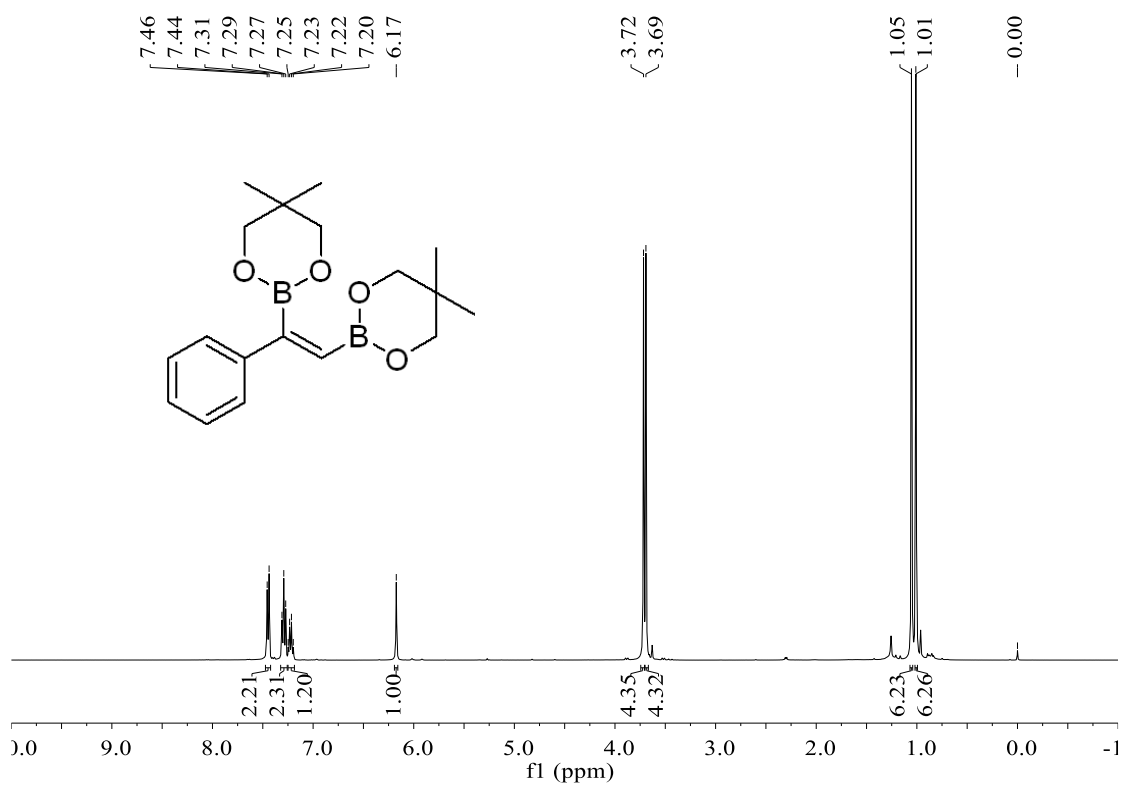
(*E*)-2,2'-(1-cyclohexylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3ia).^[11] ¹H NMR (400 MHz, Chloroform-*d*) δ 5.77 (s, 1H), 2.08 (t, *J* = 11.0 Hz, 1H), 1.72 (d, *J* = 10.9 Hz, 4H), 1.31 (s, 12H), 1.24 (s, 12H), 1.23 – 1.03 (m, 6H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 83.57 , 83.15 , 47.65 , 32.22 , 26.55 , 26.45, 25.04 , 24.84 .



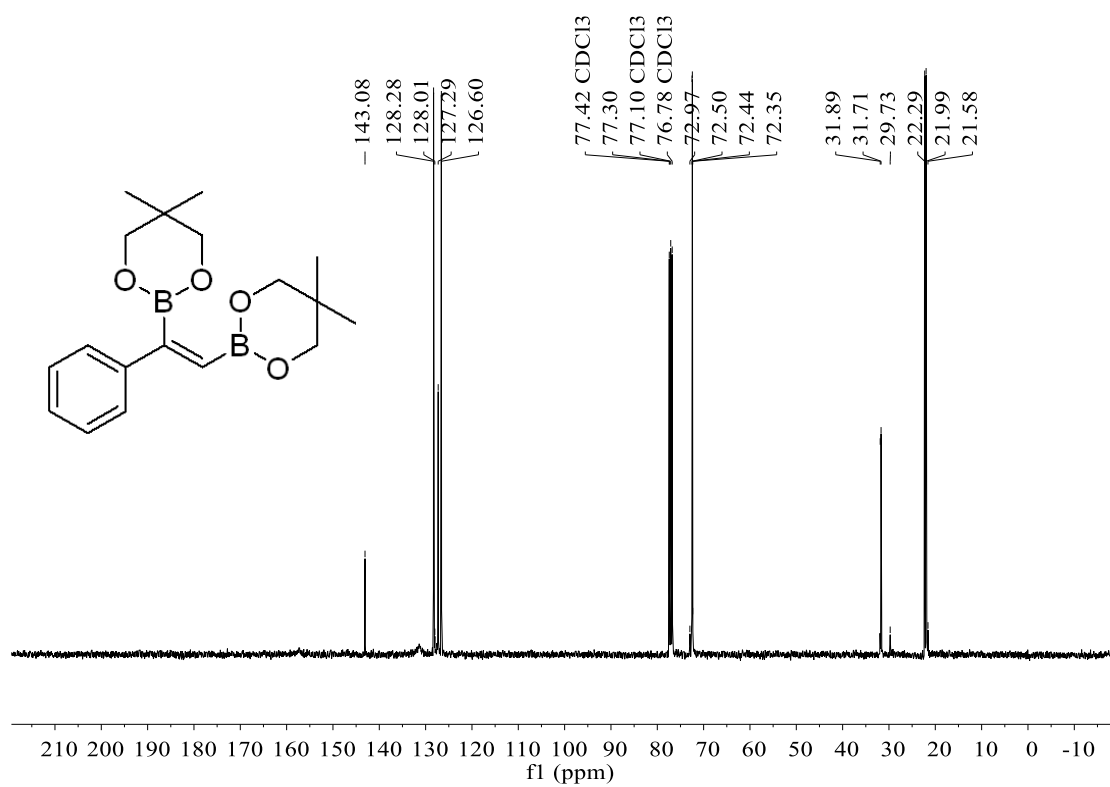
¹H NMR of 3aa.



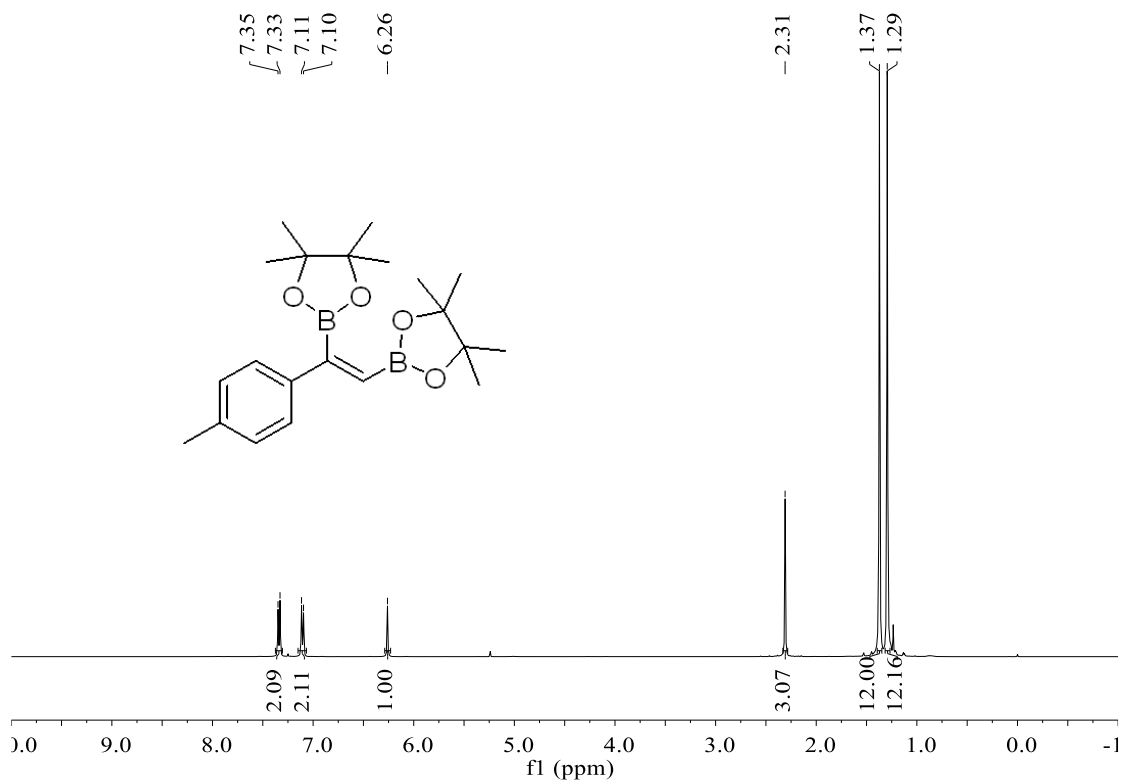
¹³C NMR spectrum of 3aa.



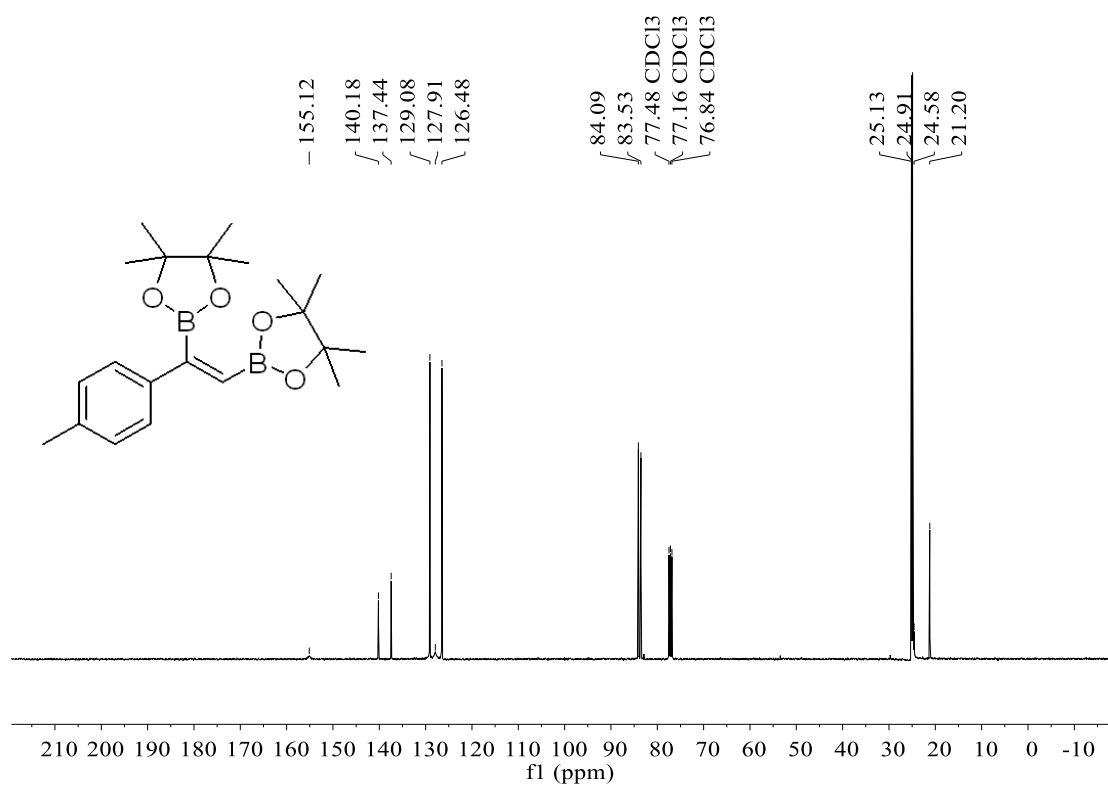
¹H NMR of 3ab.



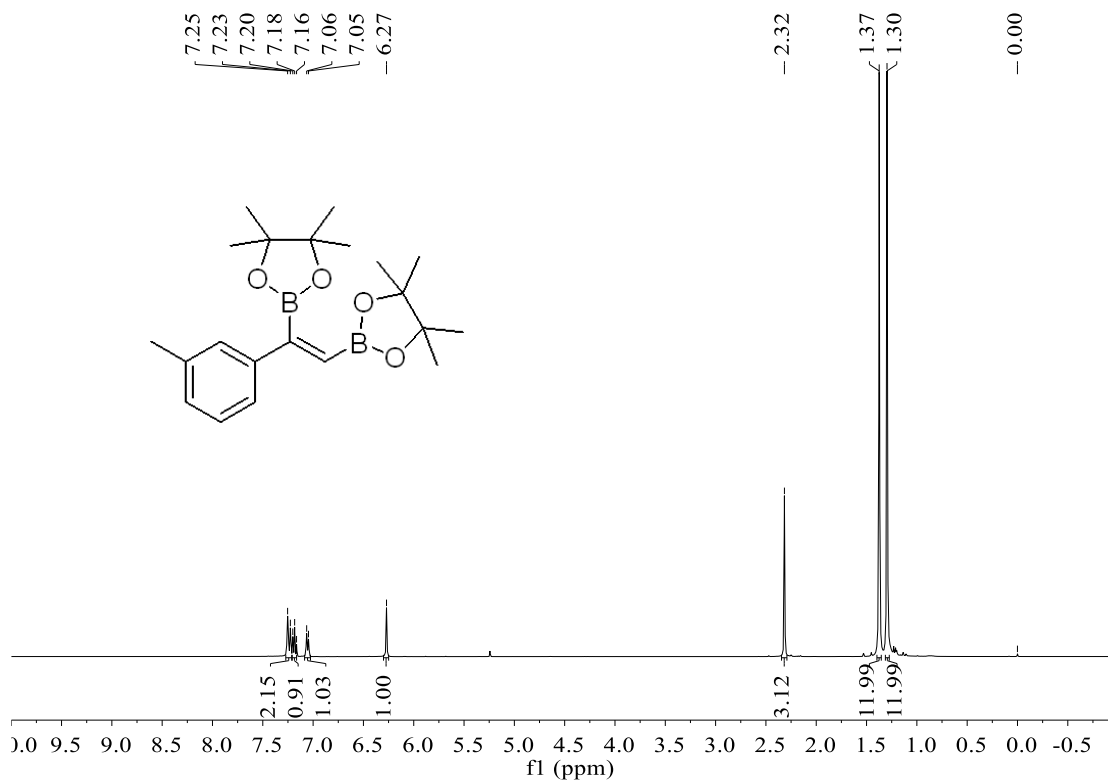
¹³C NMR spectrum of 3ab.



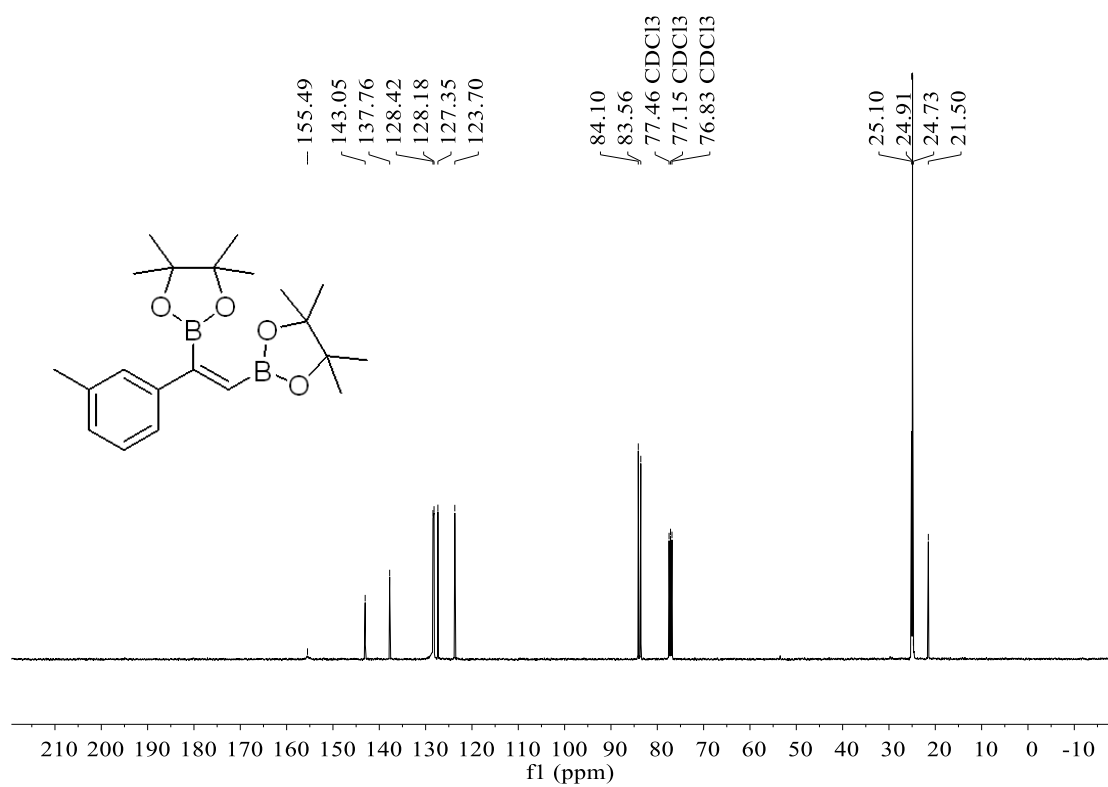
¹H NMR spectrum of 3ba.



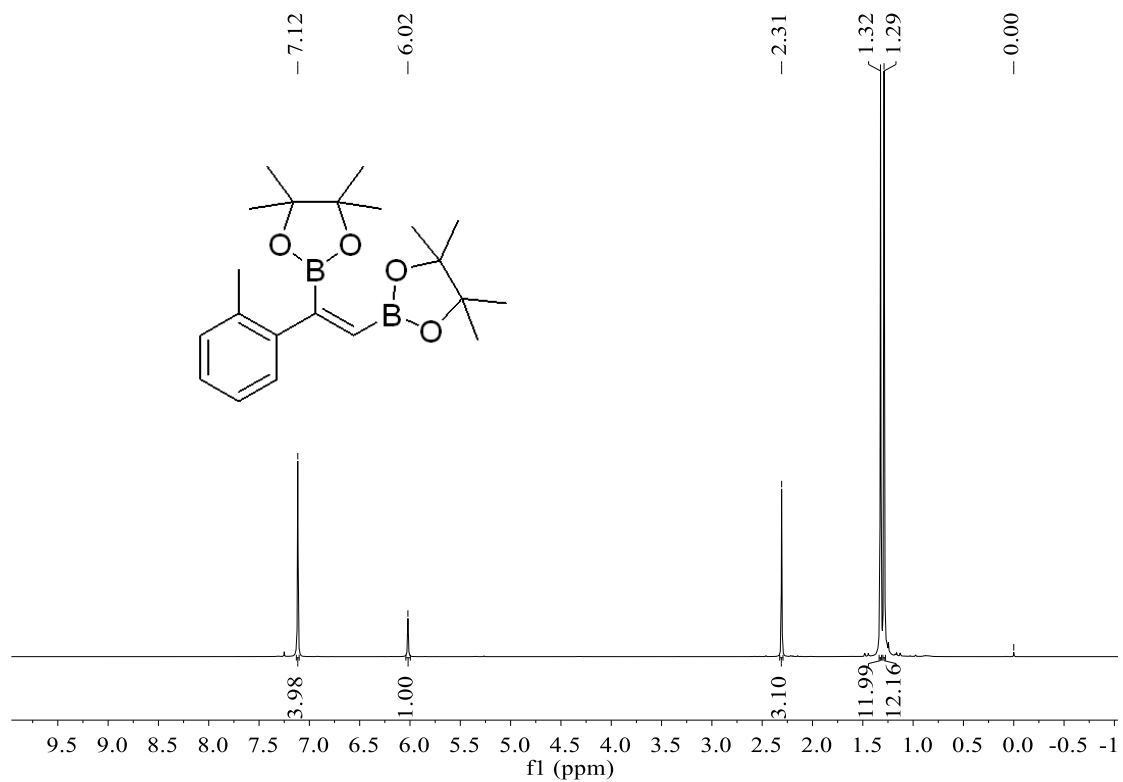
¹³C NMR spectrum of 3ba.



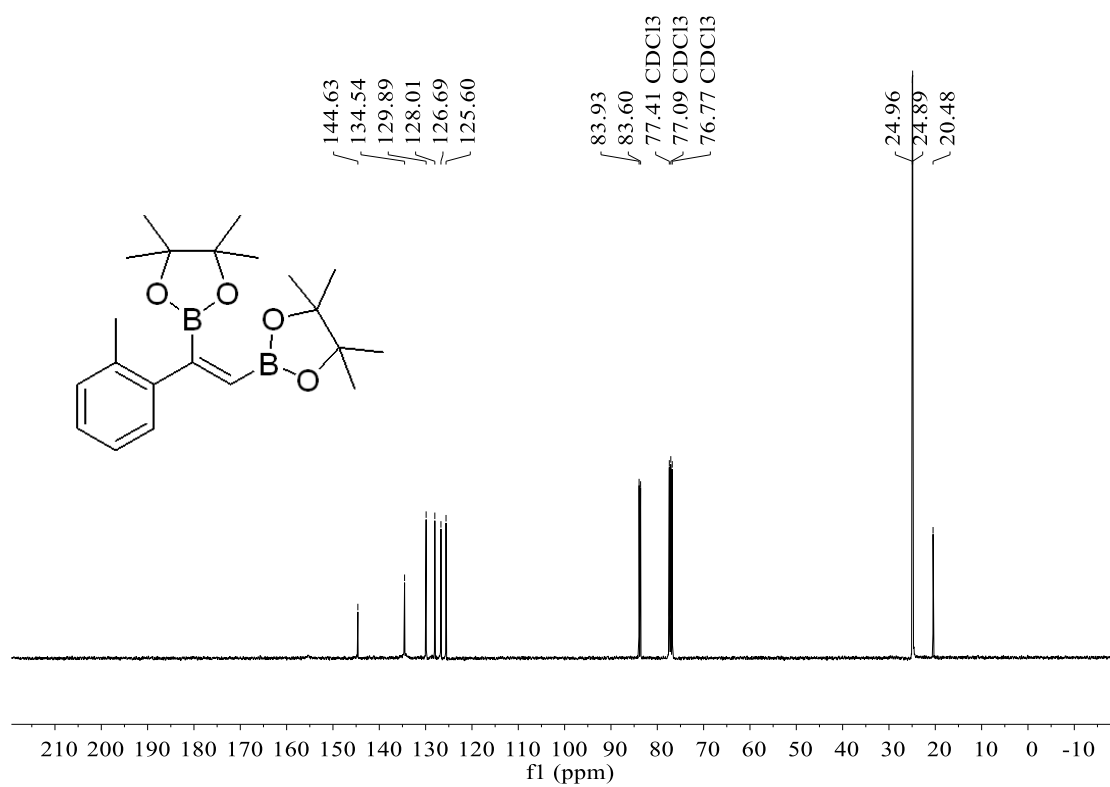
¹H NMR spectrum of 3ca.



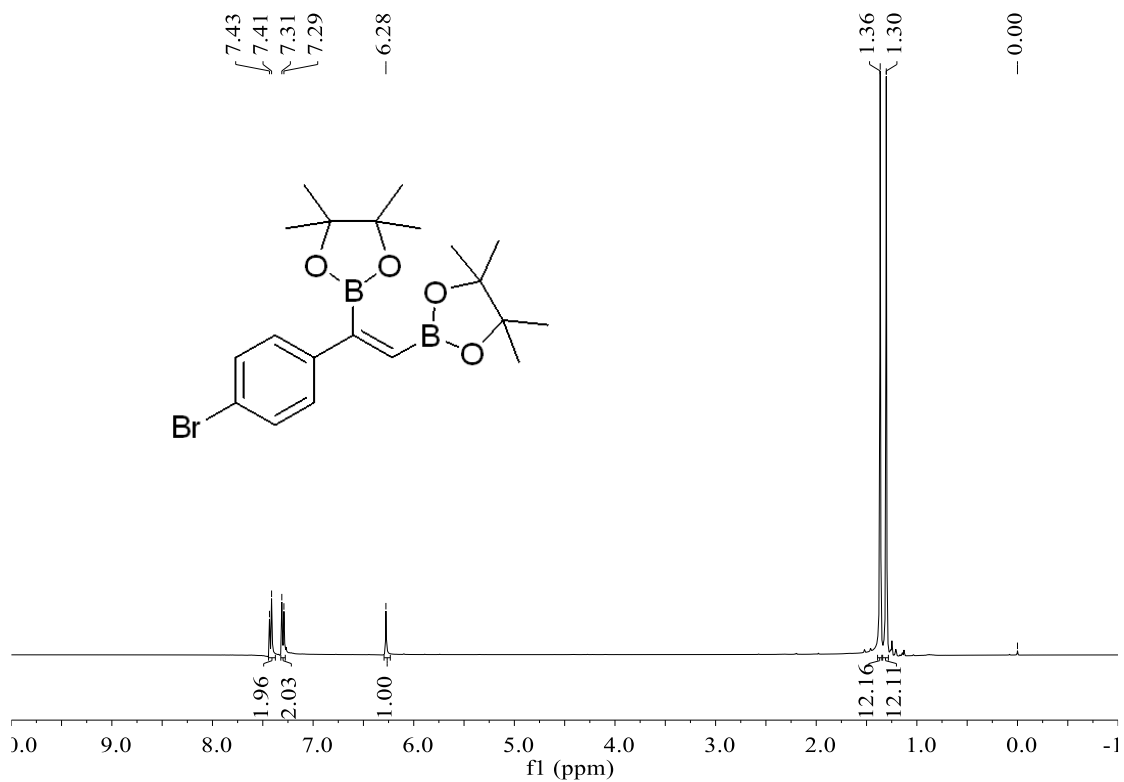
¹³C NMR spectrum of 3ca.



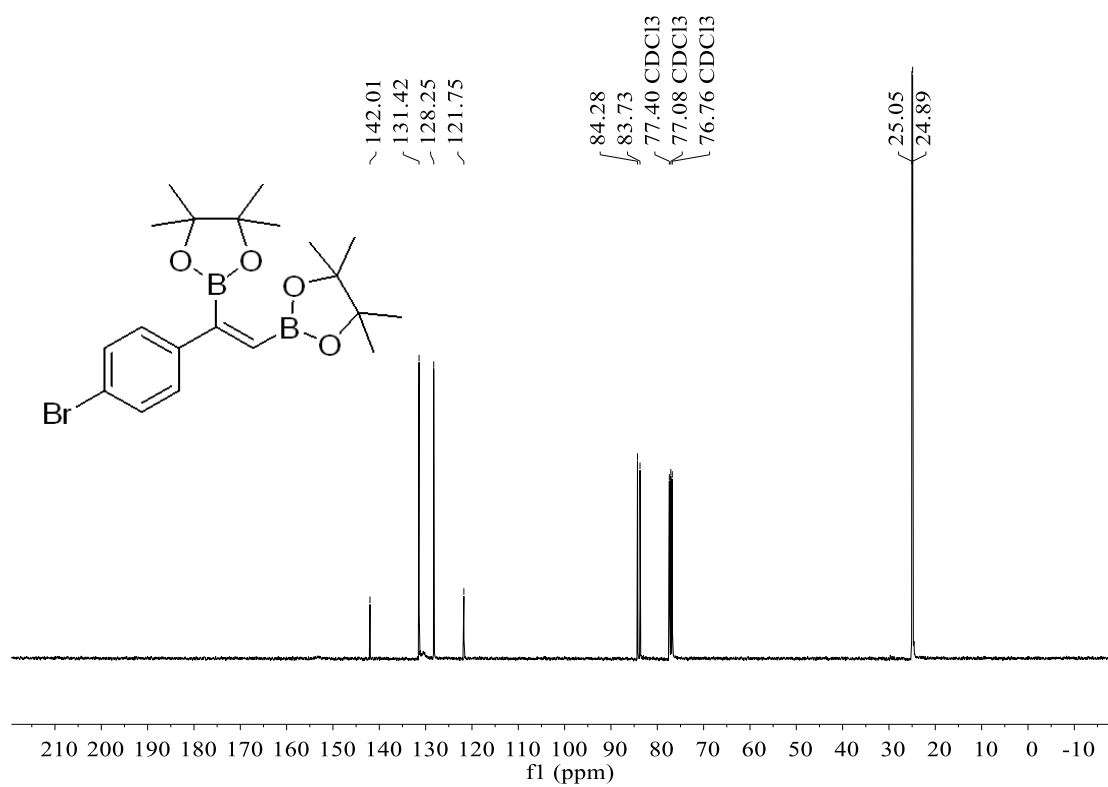
¹H NMR spectrum of 3da.



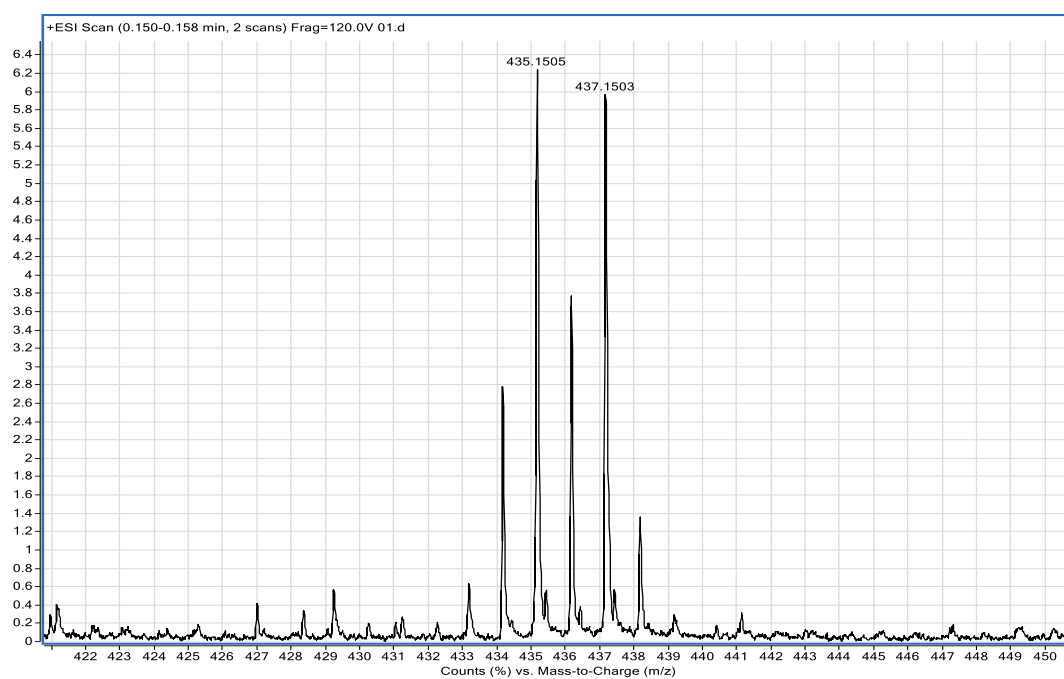
¹³C NMR spectrum of 3da.



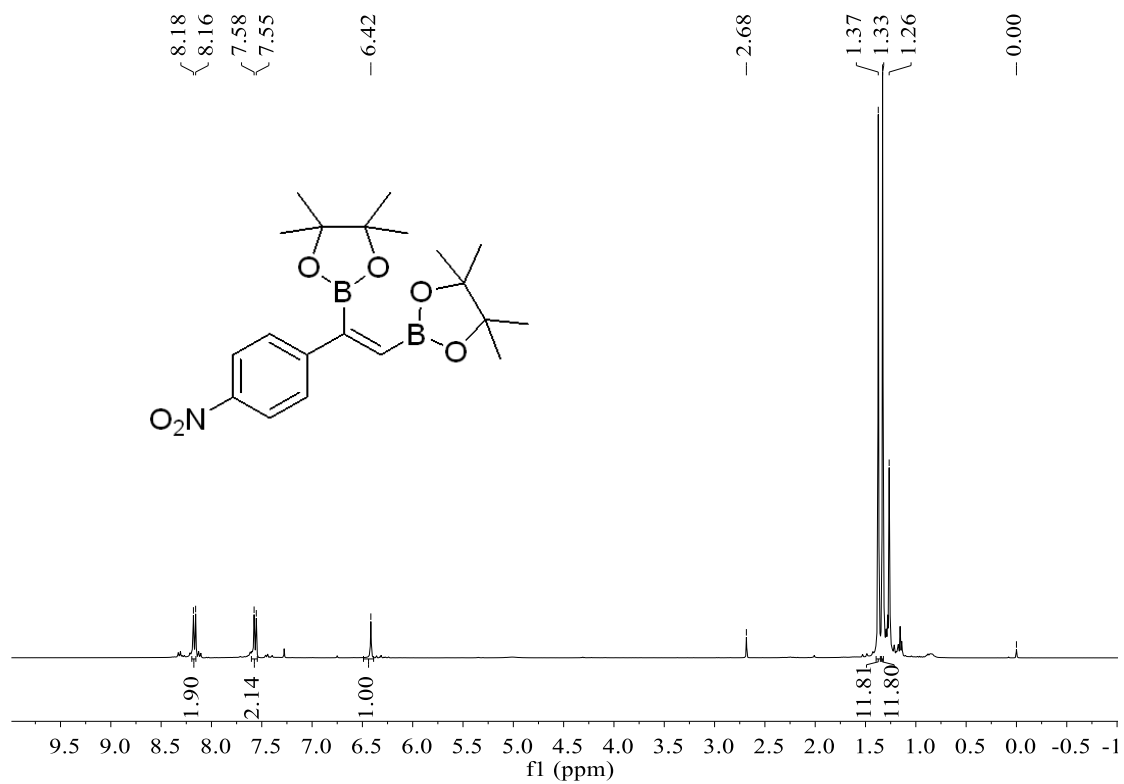
¹H NMR spectrum of 3ea.



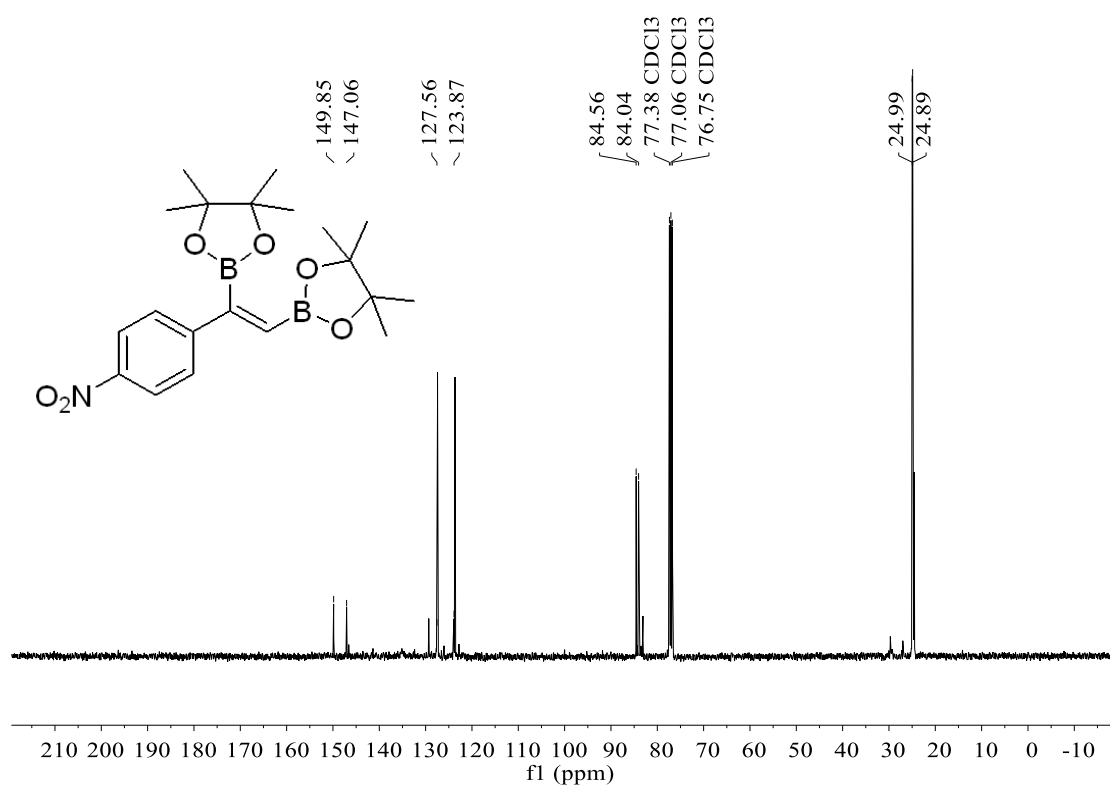
¹³C NMR spectrum of 3ea.



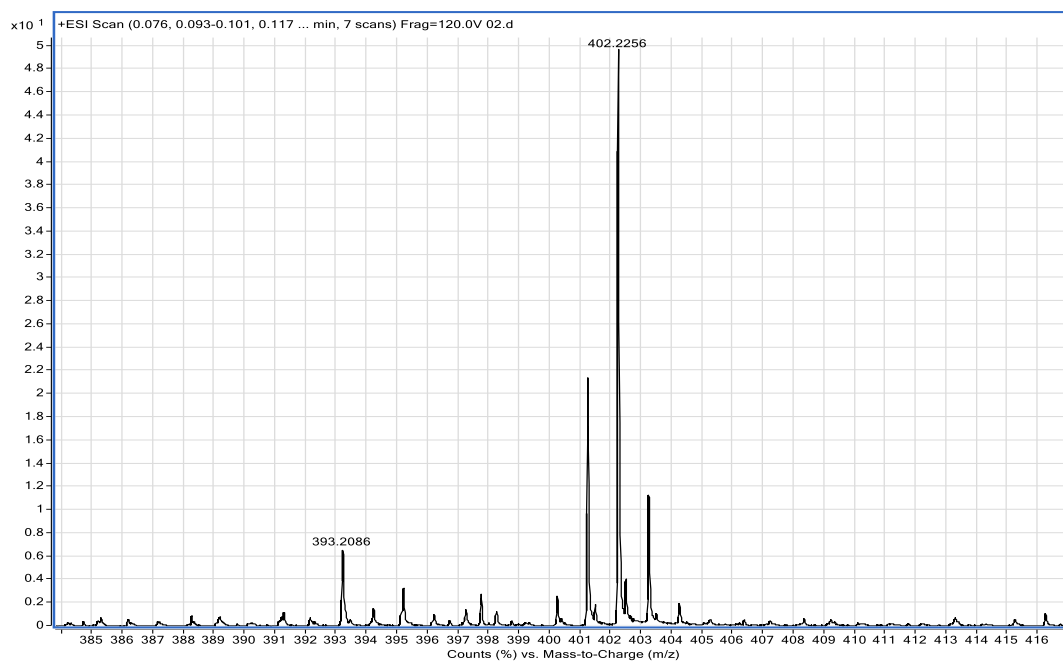
HRMS of 3ea.



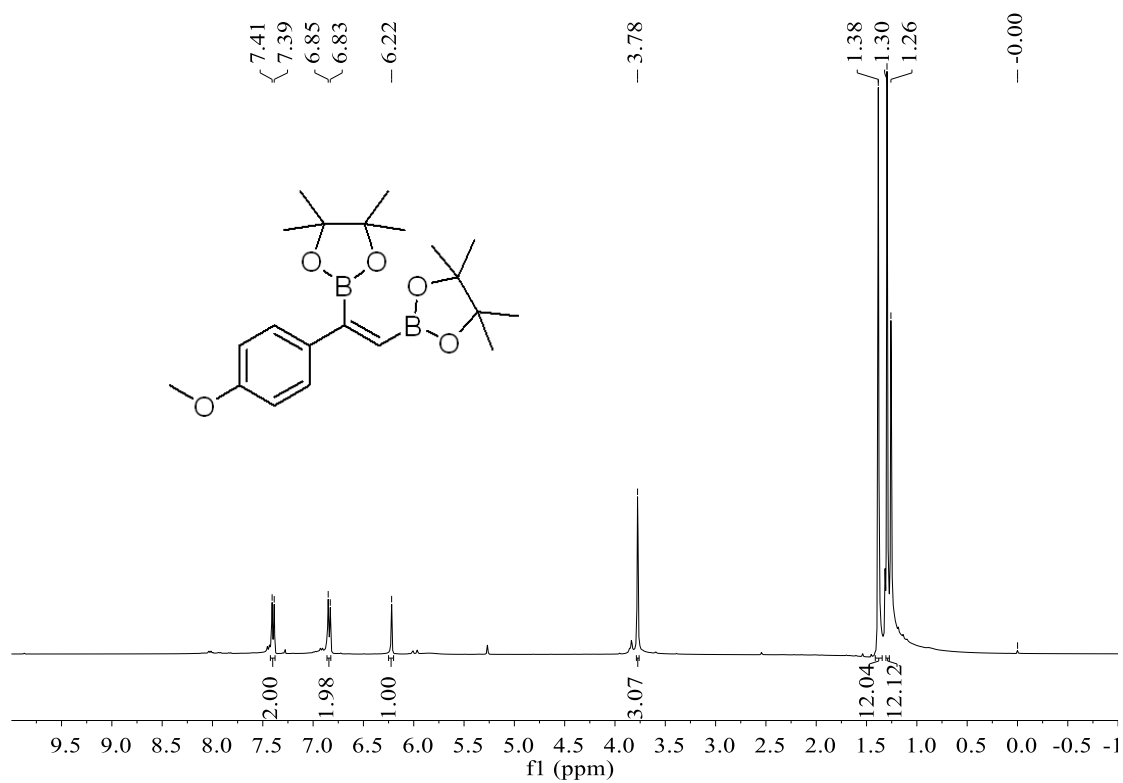
¹H NMR spectrum of 3fa.



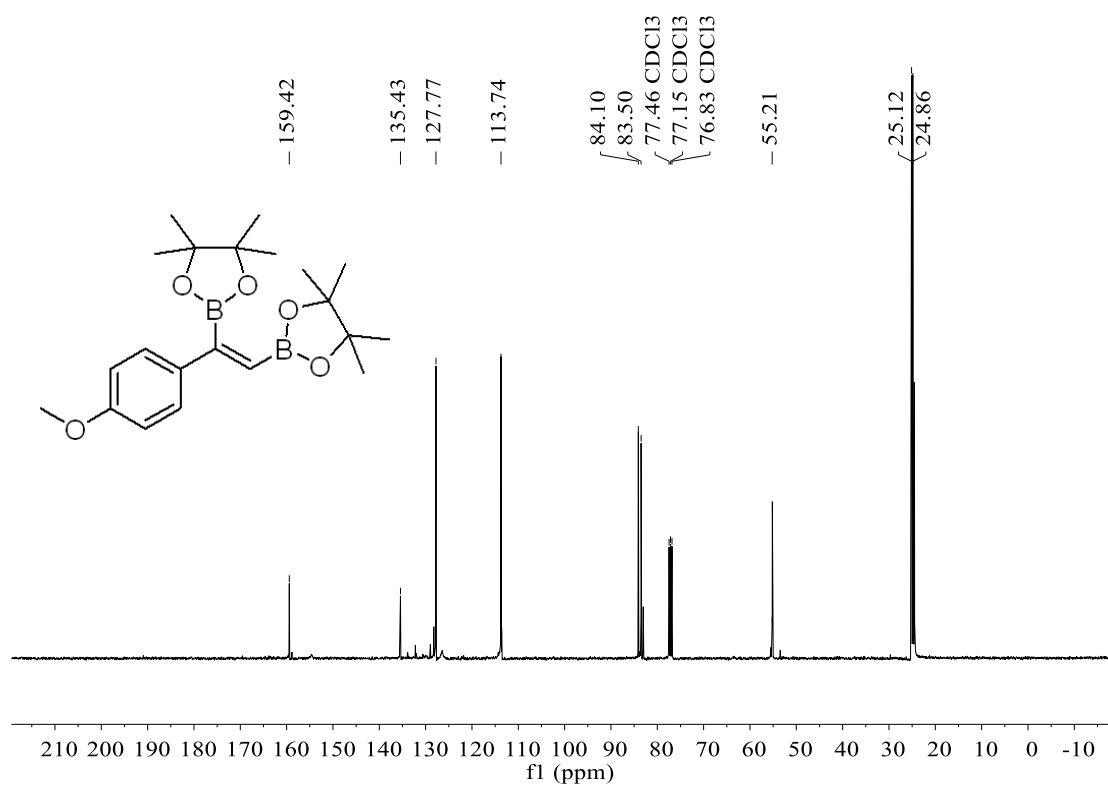
¹³C NMR spectrum of 3fa.



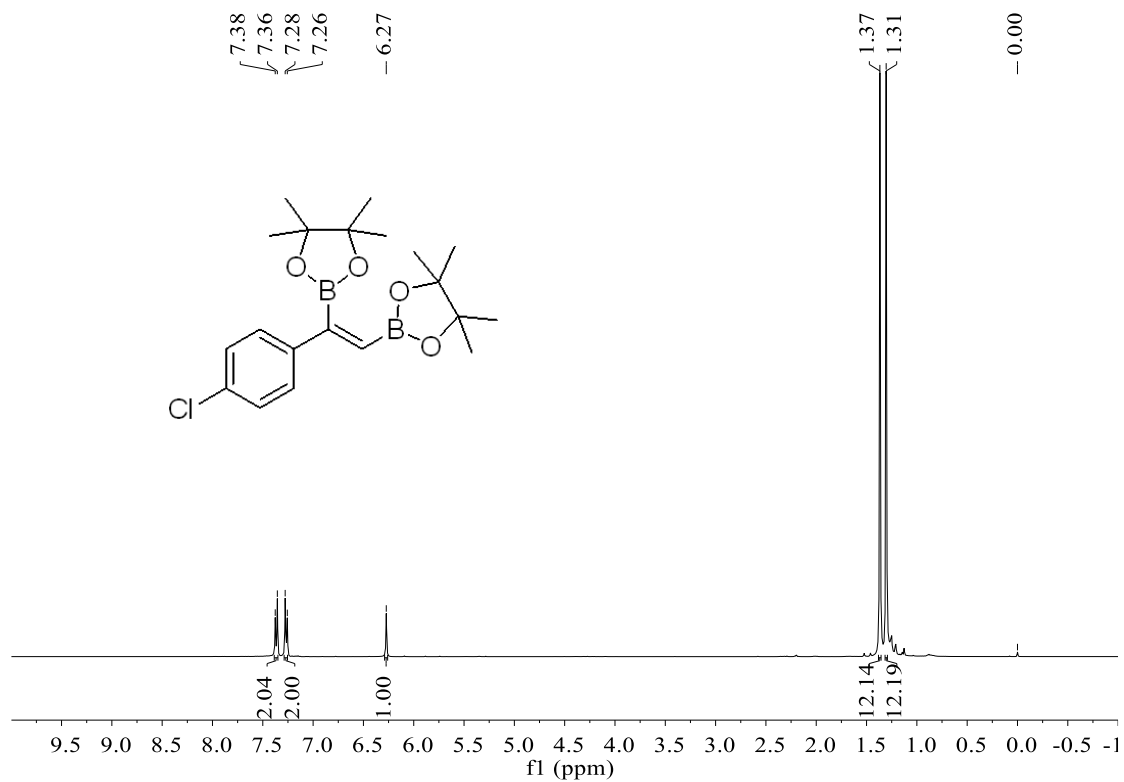
HRMS of 3fa.



¹H NMR spectrum of 3ga.



¹³C NMR spectrum of 3ga.



¹H NMR spectrum of 3ha.

O	-3.97132900	-5.24136700	2.19004800
H	-3.11844900	-5.09013200	2.61625900
C	-4.10468500	-4.25953500	1.16173900
C	-3.34057900	-4.63991900	-0.10101000
H	-3.73081100	-3.28950400	1.51350700
C	-5.58917400	-4.11222400	0.86979900
O	-1.97971400	-4.71807900	0.31628900
C	-3.61617200	-3.59660500	-1.19945800
H	-3.67626700	-5.62064300	-0.45974900
O	-6.28860700	-3.65590900	2.01906800
H	-5.98784900	-5.08234100	0.54030800
C	-5.77752000	-3.10243200	-0.26634200
C	-1.04045800	-5.32848900	-0.56309000
O	-5.04554500	-3.53311400	-1.39808500
C	-3.05385100	-3.93523600	-2.57359500
H	-3.24134900	-2.61734500	-0.87793200
H	-5.98347700	-4.21303300	2.75100200
O	-5.31916800	-1.85625400	0.18139500
H	-6.81886000	-3.04207600	-0.59160600
O	-0.22198000	-4.36962800	-1.17737100
C	-0.20296700	-6.28607000	0.27891400
H	-1.56334800	-5.85553100	-1.36532200
O	-3.43078600	-5.23825600	-2.99262900
H	-3.41033300	-3.16814900	-3.27653000
H	-1.96430300	-3.89956500	-2.55556900

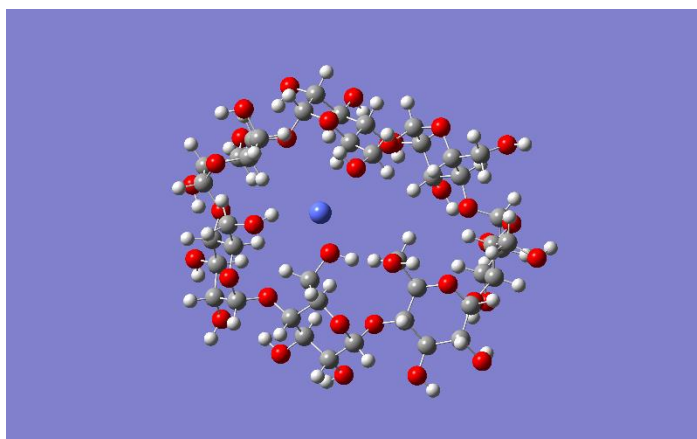
C	-6.20565000	-0.73528200	0.11530800
C	0.52208200	-3.55597900	-0.25573900
O	-1.01578300	-7.22243800	0.97415100
H	0.43860100	-6.86471300	-0.39296200
H	-4.39770000	-5.26370400	-2.96747800
C	-5.81371300	0.18030800	-1.04993700
H	-7.23571700	-1.07534600	-0.02531800
C	-6.09085400	-0.01682600	1.45046200
C	1.16127000	-2.44029200	-1.05459400
H	-0.17377300	-3.08373300	0.45070600
C	1.49108100	-4.43302400	0.55065200
H	-1.76262000	-6.71529800	1.32970700
O	-6.58255000	1.39026300	-0.99826800
C	-6.04271800	-0.47068200	-2.40252700
H	-4.74661300	0.42318700	-0.96171900
H	-5.03104600	0.22277200	1.62489500
C	-6.87278800	1.28718600	1.39037000
O	2.10536800	-2.94185600	-1.98888900
H	0.35513900	-1.91022800	-1.57980200
H	1.62495000	-1.73386700	-0.35335900
O	2.13443400	-3.58445000	1.50728500
H	2.23113000	-4.87528400	-0.12502800
C	0.69244400	-5.52526000	1.26038600
C	-6.40092000	2.12366700	0.19865500
O	-7.33409200	-1.06932300	-2.41712500

H	-5.94492800	0.30307300	-3.17625200
H	-5.26053500	-1.22544300	-2.55502700
O	-6.71252700	2.04168000	2.58272900
H	-7.93385500	1.04796300	1.23110000
H	2.44932000	-2.14196300	-2.47094200
C	3.40311900	-4.03638900	1.91774400
O	1.57353600	-6.43516500	1.89714100
H	0.05406700	-5.02242700	2.00493800
O	-5.05493500	2.45951900	0.40209800
H	-7.01500200	3.02316900	0.09019300
H	-7.46499500	-1.47270100	-3.28310700
H	-6.79554600	1.41254200	3.31419100
O	4.38054700	-3.82304400	0.90868200
C	3.83611900	-3.28228700	3.17376000
H	3.39061500	-5.11258900	2.09218300
H	1.02002700	-7.16727200	2.20665900
C	-4.63567000	3.80930000	0.18254400
C	4.51835100	-2.45900100	0.49272300
O	2.90433100	-3.48435700	4.21287700
C	3.99772400	-1.80012500	2.86681400
H	4.82600600	-3.68536400	3.44370900
C	-3.63661000	3.85752200	-0.96819100
H	-5.50391600	4.43989100	-0.05189400
C	-4.01868200	4.30242000	1.49878000
C	5.50812600	-2.49136900	-0.66330400

H	3.56781700	-2.06984400	0.11959400
H	3.14584900	-2.85055300	4.90368700
O	4.49739600	-1.18423500	4.04287000
C	4.91267600	-1.55568300	1.66808600
H	3.00691600	-1.40316300	2.60290000
O	-3.10633500	5.18690000	-1.08526400
C	-4.20385400	3.55045000	-2.34481600
H	-2.82243100	3.15415400	-0.75027700
O	-5.00829700	4.41126400	2.49267000
H	-3.22956300	3.58739100	1.78433000
C	-3.37322700	5.67740400	1.28866800
O	4.82442500	-2.56606600	-1.94065400
H	6.11945000	-1.59211100	-0.71597800
H	6.14707400	-3.37451400	-0.56274200
H	4.65070200	-0.24391200	3.84727600
O	4.69807700	-0.17970700	1.32055900
H	5.95755900	-1.71647600	1.96717300
C	-2.44535400	5.64399000	0.06614000
O	-3.18439100	3.58000000	-3.32909400
H	-4.64537700	2.55221300	-2.35329300
H	-5.00521100	4.27328100	-2.56609400
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O	-2.70436500	6.17134200	2.42319000
H	-4.18441800	6.38051200	1.05855400
H	4.00597100	-3.10234600	-1.82948900

C	5.76344400	0.67688000	1.03077300
O	-1.33421400	4.81518400	0.38225200
H	-2.09849800	6.65478400	-0.16738300
H	-2.74727800	4.44358900	-3.25909900
H	-1.76190500	5.94480900	2.35432200
O	5.64310000	1.24539200	-0.25473100
C	5.76787400	1.81944300	2.06326000
H	6.71834400	0.13694600	1.03074600
C	-0.05612700	5.25849800	-0.04558600
C	4.38548100	1.90538900	-0.47112800
O	5.77559500	1.35239600	3.41571500
C	4.49906000	2.64881300	1.92217200
H	6.63725400	2.46183300	1.87480100
C	0.61060200	4.23106900	-0.97218300
H	-0.14723900	6.20217900	-0.59516500
C	0.81526900	5.46507400	1.18498100
C	4.30454100	2.32181800	-1.93874400
H	3.56699800	1.21027400	-0.25439700
C	4.28859800	3.10692200	0.48477600
H	6.65701100	1.02755300	3.64137300
O	4.55219600	3.80571900	2.74752500
H	3.64534200	2.01560300	2.19883900
O	1.92746700	4.71999000	-1.33420200
C	-0.12611900	3.99016400	-2.27800000
H	0.71566400	3.27502900	-0.44330900

O	0.20740600	6.44379500	2.01056200
H	0.89322600	4.50574600	1.71959400
C	2.21432800	5.91063300	0.76366400
O	3.64166000	1.35674300	-2.79947000
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H	5.31039300	2.43092700	-2.34461900
O	2.99113700	3.68067600	0.43998100
H	5.05208000	3.85604700	0.23319700
H	4.69992400	3.50251000	3.65418100
C	2.79235900	4.90841200	-0.23863900
O	-0.45389100	5.18770200	-2.96192200
H	0.49357000	3.32823700	-2.90328200
H	-1.06871100	3.47881300	-2.08953200
H	0.87192300	6.69483800	2.66957200
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H	2.12453700	6.88024900	0.26032800
H	2.68540300	1.40993700	-2.65405700
H	3.73876900	5.27412500	-0.65135700
H	0.37574000	5.61919000	-3.20586600
H	3.36567600	5.24867100	2.20878200
O	-6.62369900	-0.77700500	2.51883600
H	-6.34466400	-1.70499200	2.40911100
Pt	4.16198500	-0.64451200	-2.46579500



O	6.49708500	1.15559300	2.71597800
H	5.99936600	1.98146100	2.65875800
C	6.01048900	0.30645100	1.68500200
C	6.31959000	0.85250900	0.28909300
H	4.92029100	0.19279000	1.76360100
C	6.63694400	-1.05933700	1.91655000
O	5.63432000	2.11754200	0.27659500
C	5.89843500	-0.19229200	-0.76965500
H	7.39469500	1.03469300	0.17803700
O	6.21485200	-1.60705900	3.15659800
H	7.73136200	-0.95962000	1.89062700
C	6.21182600	-1.99429900	0.78656700
C	5.34694200	2.74181500	-0.95385300
O	6.59782400	-1.41256200	-0.44760100
C	6.30881300	0.08201500	-2.21457500
H	4.81772500	-0.36205400	-0.72344900
H	6.31285800	-0.89874900	3.81010100
O	4.82534700	-2.15250400	0.86139600
H	6.72303700	-2.95874300	0.83295800

O	4.16562400	2.21383600	-1.52958000
C	5.18386500	4.23278700	-0.67287700
H	6.15264400	2.57201000	-1.67122900
O	7.64661400	0.53591700	-2.32793200
H	6.15336200	-0.85371200	-2.77065600
H	5.66691900	0.83822700	-2.66209900
C	4.27654900	-3.47072600	0.78750700
C	2.99431500	2.35372400	-0.69414500
O	6.32715400	4.77476300	-0.03036700
H	5.09431600	4.74771600	-1.63485600
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C	3.62141400	-3.70221800	-0.57786400
H	5.06432000	-4.21475600	0.93585300
C	3.26532500	-3.57599500	1.91992200
C	1.88567000	1.58974100	-1.39403800
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C	2.70490100	3.84502400	-0.50284500
H	6.56080200	4.14503400	0.66830600
O	2.93006300	-4.95314700	-0.57236600
C	4.62891300	-3.72775900	-1.71478500
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H	2.52931100	-2.76544400	1.81022800
C	2.53556500	-4.90566600	1.80780600
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H	2.20092500	0.54687200	-1.53214000

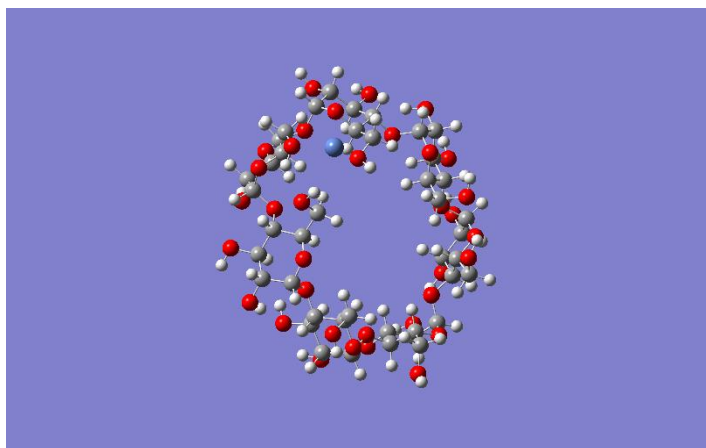
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C	1.92096900	-5.04347100	0.41396400
O	5.74630300	-4.51827200	-1.33112600
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H	4.93397500	-2.69592700	-1.92643400
O	1.50517300	-5.02324700	2.77817500
H	3.27028300	-5.71489000	1.92807400
H	2.31312700	2.20728800	-3.20047200
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O	3.69661000	5.92112300	0.17564300
H	4.02795400	4.11493600	1.14910800
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H	1.47250300	-6.02993100	0.28962100
H	6.41223600	-4.44986800	-2.02489500
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C	-1.12057500	3.86351700	-0.79022900
O	0.87565300	5.82724200	2.27713100

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C	-1.24281000	-5.01711500	0.64618500
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O	-1.89858700	5.37305400	2.55502100
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O	-5.07631700	-3.63718900	2.15524800
H	-4.38593400	-1.74282400	1.64832100
C	-6.52084900	-1.81435400	1.44567200
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O	-5.63685800	0.23162600	0.77279400
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H	-5.75574100	2.24356100	3.76829000
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O	-5.84441800	-3.18230300	-2.86906200
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O	-6.75136900	-1.33198500	2.75745000
H	-7.29061300	-2.56511800	1.23731000
H	-3.93937100	1.21704100	-2.80806900
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H	-6.72774800	-2.89126700	-2.60225600

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O	3.88879400	-3.53210900	3.19015400
H	4.51326800	-2.78398700	3.19878600
Co	-1.77121800	0.34136800	-1.86241100



O	2.60754300	-5.04797900	-2.16692400
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C	3.14585000	-4.17636200	-1.15816800
C	2.57743800	-4.49654300	0.21512100
H	2.91494300	-3.13521100	-1.40716600
C	4.65944100	-4.33479600	-1.14334800
O	1.18372800	-4.25058600	0.14304500
C	3.24706000	-3.61771900	1.28015800
H	2.77225800	-5.54909700	0.45132100
O	5.23054800	-3.95242300	-2.38669700
H	4.91251200	-5.37904100	-0.91134000
C	5.23434600	-3.43755600	-0.03803200
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C	-0.41966200	-6.01371000	-0.08186300
H	0.91063100	-5.69266400	1.61420200
O	3.07497100	-5.34906400	2.98589100
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C	5.93436500	-1.12217900	-0.40287400
C	-1.37220300	-3.44479800	0.84581500
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H	-1.04389200	-6.70221600	0.49688100
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C	5.80068600	-0.20364000	0.81722600
H	6.92114300	-1.59377900	-0.39845700
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C	-2.20496000	-4.23070300	-0.17604800
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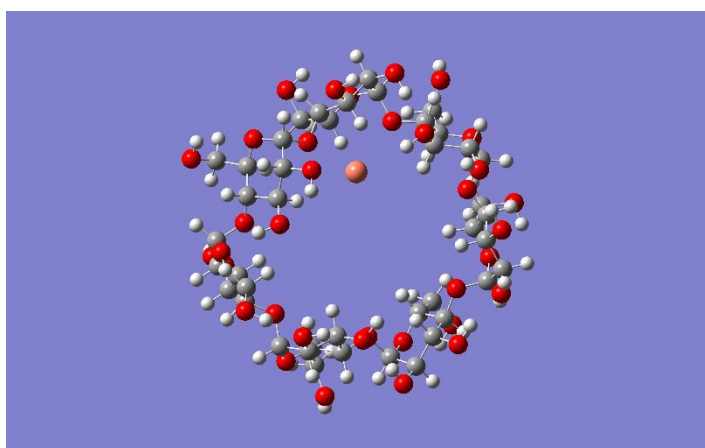
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H	-3.51953400	-2.97265000	3.20608400
C	-4.07199800	-3.65175100	-1.53882000
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H	7.61856000	-2.03681100	2.76146600
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H	-5.31996500	-3.35405700	-3.22884100
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H	-5.09404100	-3.00716900	1.75210400
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O	4.39206900	2.59358900	-0.15792900
C	3.21914000	3.95360800	1.44636500
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H	2.42863500	3.19553900	1.38775900
H	1.25848400	5.75541200	-2.07946800
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H	1.46439100	6.70314800	0.90772000
O	6.07650100	1.42506800	0.94675300
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O	5.07065900	4.73143800	2.80892800
H	3.45126600	3.64425300	3.55896300
H	4.63494300	2.76816500	2.55361800
C	-0.46600300	5.38140000	-0.02812000
C	5.35794800	0.17948000	1.02165200
O	5.75475700	2.31713000	-2.57047600
H	7.12496700	1.23510800	-1.45324800
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C	-1.49257600	5.45559200	1.11594600
H	-0.29893300	6.38504400	-0.42642900
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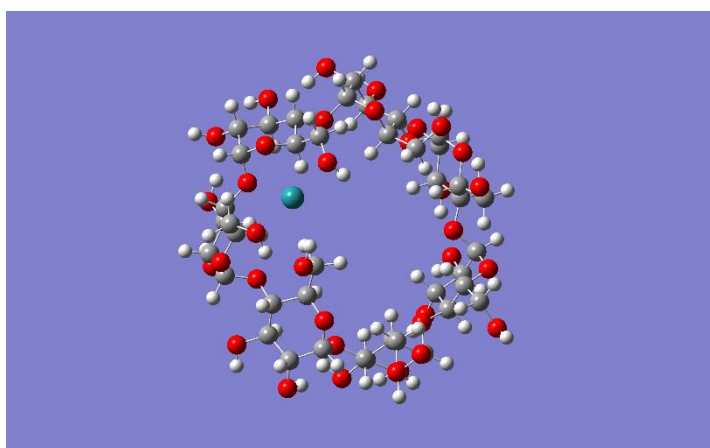
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H	-2.21882100	6.06806700	-1.94249100
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O	5.59729200	-0.45276400	-2.70664700
H	4.17976500	0.46205300	-1.48726700
O	-3.48920000	3.77394800	0.10317100

H	-4.26860200	5.53021400	-0.66222300
H	-0.46295400	8.24346400	2.38229000
H	-2.17106600	4.01608400	-3.21522800
O	4.99720700	-3.74621600	0.84926700
C	4.32329900	-3.74788400	-1.45957200
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O	4.47441800	-3.05199800	-2.68917500
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C	3.66077100	-4.54028200	2.66864300
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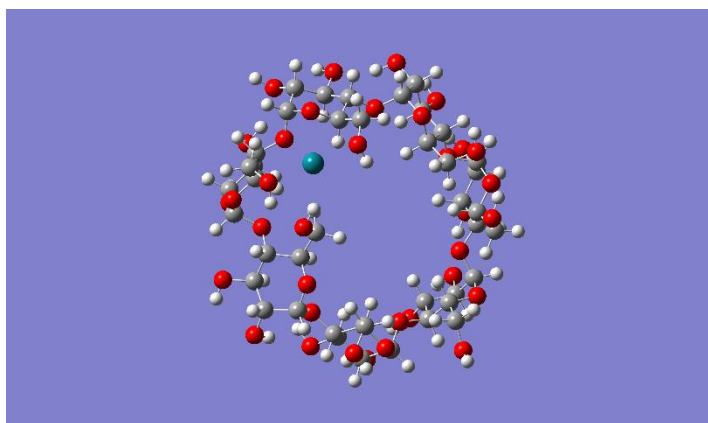
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H	1.19461300	-6.76151900	-1.13378300
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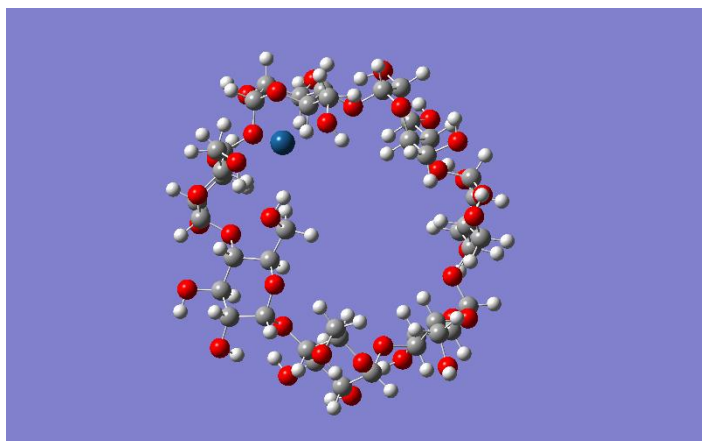
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O	5.02945900	2.18170300	-0.50342900
H	7.02640200	2.63536000	-0.25065500
H	7.27009400	-1.76413500	3.26372100
H	6.63648600	0.94391600	-3.41541200
O	-4.83271400	-3.69662700	-0.80162900
C	-4.26378500	-3.05056800	-3.02955900
H	-3.86638800	-4.94948500	-2.04290500
H	-1.59570300	-7.11992200	-2.01096400
C	4.69227500	3.56097100	-0.33040200
C	-4.92263000	-2.35776000	-0.30268000
O	-3.35865500	-3.25361000	-4.09211000

C	-4.33110000	-1.57909300	-2.64512100
H	-5.27837400	-3.38355800	-3.30235400
C	3.77050700	3.71960900	0.87386800
H	5.60375900	4.15684400	-0.18654500
C	4.01656200	4.01115400	-1.63313300
C	-5.98040700	-2.40331000	0.79822000
H	-3.97420600	-2.05466500	0.14468800
H	-3.57104000	-2.57430400	-4.74822400
O	-4.81298400	-0.87617900	-3.78020300
C	-5.21103200	-1.34604400	-1.41923300
H	-3.31413400	-1.25697600	-2.38184500
O	3.30350600	5.07555300	0.94558700
C	4.40663700	3.46099000	2.22996800
H	2.91698500	3.04185000	0.74346700
O	4.94687600	4.02056400	-2.68856300
H	3.18239100	3.31772900	-1.83020700
C	3.44111000	5.42216300	-1.46435400
O	-5.39521700	-2.52853500	2.10596600
H	-6.57715700	-1.49083800	0.83607500
H	-6.64349900	-3.25487600	0.60757100
H	-4.94854900	0.05202000	-3.52570800
O	-4.86373400	-0.02884600	-0.95453500
H	-6.26526400	-1.37589900	-1.72663200
C	2.59116100	5.49673200	-0.18842000
O	3.44585000	3.55630300	3.26737700

H	4.82875900	2.45464100	2.25891100
H	5.23329300	4.17537600	2.37227100
H	5.35912600	3.13891600	-2.73561100
O	2.72113800	5.87777000	-2.58439400
H	4.29242700	6.10137500	-1.32435000
H	-4.58574000	-3.06990600	2.02278700
C	-5.85205900	0.87618300	-0.56029000
O	1.42963000	4.70182000	-0.38910500
H	2.30071600	6.53325700	0.00627800
H	3.01651800	4.42276400	3.18372500
H	1.77410400	5.72774900	-2.42797200
O	-5.58149500	1.39057000	0.72592800
C	-5.89862400	2.04329000	-1.56298400
H	-6.83055300	0.38753600	-0.48140900
C	0.20613400	5.21550500	0.11422200
C	-4.31162300	2.05441000	0.85306800
O	-6.04902700	1.60377700	-2.91557300
C	-4.58676800	2.81202100	-1.52695000
H	-6.71803000	2.71848500	-1.28541400
C	-0.44447300	4.23412500	1.09980000
H	0.38069900	6.16002900	0.64165000
C	-0.73371800	5.45042800	-1.05929300
C	-4.17174000	2.49753700	2.30512900
H	-3.50648800	1.35390200	0.60055700
C	-4.24715200	3.25196000	-0.11034000

H	-6.95830900	1.31525900	-3.06768700
O	-4.65538600	3.97489500	-2.34145800
H	-3.78742600	2.14265300	-1.87253800
O	-1.71461300	4.78474700	1.53366100
C	0.36179400	3.98546500	2.36258500
H	-0.62243200	3.27440100	0.59829000
O	-0.13341300	6.38773800	-1.93715800
H	-0.89311500	4.49016800	-1.57364500
C	-2.07910600	5.96849900	-0.55393400
O	-3.87455700	1.42768300	3.21731800
H	-3.38231800	3.25128900	2.38177200
H	-5.12018600	2.92220000	2.64164400
O	-2.93133800	3.77887100	-0.16389100
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H	-4.89959200	3.68588900	-3.23180800
C	-2.63738500	5.00087300	0.49307400
O	0.78837600	5.18107400	2.99564300
H	-0.24598500	3.36733300	3.04030900
H	1.26636500	3.42736000	2.12720700
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O	-2.97849400	6.20603600	-1.61556000
H	-1.91030300	6.93546900	-0.06611300
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H	-3.53999100	5.40862300	0.96056900
H	-0.00208100	5.65212000	3.29066000

H	-3.35589600	5.35549700	-1.91189100
O	6.34672200	-1.21011100	-2.54290500
H	6.01485800	-2.11481700	-2.39355500
Rh	-4.66991500	-0.55543800	2.74200100



O	-3.82785900	-5.31382600	2.18381600
H	-2.98414500	-5.13243200	2.61647200
C	-3.98947300	-4.33521400	1.15613600
C	-3.20878400	-4.68909100	-0.10398000
H	-3.64886700	-3.35410600	1.51080400
C	-5.47673500	-4.23605900	0.85774700
O	-1.84757600	-4.72440600	0.31664900
C	-3.51260700	-3.65356000	-1.20193300
H	-3.51250100	-5.67931100	-0.46516900
O	-6.19603900	-3.80351200	2.00399100
H	-5.84203900	-5.21840400	0.52580600
C	-5.69291100	-3.23183000	-0.27856200
C	-0.89057000	-5.31685900	-0.55673900
O	-4.94232200	-3.63645700	-1.40774900

C	-2.93099100	-3.97142100	-2.57287100
H	-3.17157900	-2.66324200	-0.87675200
H	-5.87718000	-4.35164800	2.73682800
O	-5.27740200	-1.97219700	0.17312900
H	-6.73430100	-3.20509800	-0.60820000
O	-0.08688000	-4.34274000	-1.16520100
C	-0.04126200	-6.25925500	0.29021200
H	-1.39825200	-5.85330700	-1.36244700
O	-3.26495700	-5.28450900	-2.99703900
H	-3.30573100	-3.21415000	-3.27694200
H	-1.84304900	-3.90257500	-2.54714400
C	-6.19796300	-0.87946600	0.10227500
C	0.63786100	-3.51476700	-0.24050300
O	-0.84076100	-7.21098100	0.98016700
H	0.61539300	-6.82570200	-0.37747700
H	-4.23073500	-5.33998800	-2.97723500
C	-5.82919400	0.04706700	-1.06187500
H	-7.21641200	-1.25129000	-0.04251200
C	-6.11081900	-0.15816700	1.43809700
C	1.26001400	-2.38911900	-1.04074600
H	-0.07023700	-3.05436900	0.46176100
C	1.61646700	-4.37539100	0.57315400
H	-1.59927100	-6.71853800	1.33179700
O	-6.63253700	1.23460000	-1.01250800
C	-6.03520400	-0.60999100	-2.41522200

H	-4.76984100	0.32050300	-0.97037600
H	-5.05918900	0.11153400	1.61776600
C	-6.92898000	1.12323600	1.37492300
O	2.21079500	-2.87157500	-1.97540800
H	0.44444000	-1.87360100	-1.56585100
H	1.70817500	-1.67145300	-0.33965900
O	2.23853100	-3.51763400	1.53678900
H	2.36907600	-4.80448000	-0.09718100
C	0.83272300	-5.48183400	1.27737000
C	-6.47506600	1.97225600	0.18514000
O	-7.30851600	-1.24610500	-2.43374100
H	-5.95779300	0.16649800	-3.18851600
H	-5.23088200	-1.34150500	-2.56561400
O	-6.79422300	1.88232500	2.56764500
H	-7.98234000	0.85469800	1.21146300
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C	3.51065100	-3.94887900	1.95787200
O	1.72551200	-6.37524200	1.92148700
H	0.17986500	-4.99038200	2.01695300
O	-5.13904300	2.34239300	0.39447200
H	-7.11177700	2.85563000	0.07445100
H	-7.42483400	-1.65318900	-3.30007300
H	-6.86266500	1.25133200	3.29901700
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C	3.92411600	-3.18545500	3.21506100

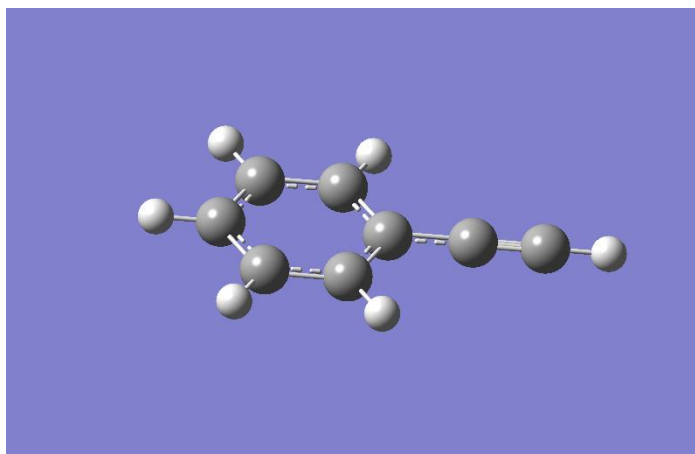
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C	-4.75168600	3.70180300	0.17684600
C	4.59609100	-2.35353800	0.53626400
O	2.99215900	-3.40403000	4.25062000
C	4.05685600	-1.70070100	2.90648500
H	4.92045800	-3.56922000	3.48919100
C	-3.75444400	3.77468600	-0.97419200
H	-5.63446600	4.31274100	-0.05537400
C	-4.14520000	4.20502700	1.49415500
C	5.57605100	-2.36253200	-0.62845400
H	3.63356700	-1.98937800	0.16896700
H	3.21882800	-2.76536800	4.94197600
O	4.54121000	-1.07164500	4.08185500
C	4.96695700	-1.43555400	1.70766700
H	3.05816900	-1.32571000	2.64039400
O	-3.25146600	5.11501900	-1.08764300
C	-4.31497800	3.45942500	-2.35165600
H	-2.92611600	3.08751000	-0.75805500
O	-5.13687900	4.28987400	2.48836200
H	-3.34109000	3.50612700	1.77777600
C	-3.52870900	5.59361800	1.28757800
O	4.85890000	-2.45165900	-1.89016700
H	6.15786000	-1.44514700	-0.69856000
H	6.23495300	-3.23181000	-0.54396200

H	4.66328500	-0.12660500	3.88688700
O	4.70875700	-0.06883600	1.35315600
H	6.01603600	-1.56304000	2.00741400
C	-2.60031300	5.58231800	0.06507400
O	-3.29522400	3.50687800	-3.33488600
H	-4.73976800	2.45397200	-2.36150900
H	-5.12811500	4.16901800	-2.57287900
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H	-4.35425000	6.28035200	1.05892800
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C	5.74454300	0.82246900	1.06134700
O	-1.47243100	4.77532600	0.37915300
H	-2.27392500	6.60060400	-0.16544400
H	-2.87208300	4.37732400	-3.26407300
H	-1.92222100	5.89708800	2.35059600
O	5.60615200	1.38063800	-0.22671800
C	5.70598800	1.96957100	2.08790800
H	6.71765900	0.31625700	1.06497500
C	-0.20473400	5.24357700	-0.05279600
C	4.32570000	1.99011500	-0.44864800
O	5.72528600	1.51045900	3.44307200
C	4.41011300	2.75494000	1.93786000
H	6.55321600	2.64069000	1.89883900
C	0.48289000	4.22401800	-0.97283700

H	-0.31688700	6.18097400	-0.60919100
C	0.66268400	5.47828100	1.17546700
C	4.22906800	2.39261200	-1.91730800
H	3.53136000	1.26916600	-0.22609100
C	4.18894200	3.19706300	0.49656000
H	6.61822800	1.22378600	3.67502800
O	4.42343000	3.91795200	2.75598800
H	3.57691700	2.09582400	2.21664600
O	1.79018200	4.73707200	-1.33819700
C	-0.24842900	3.96147100	-2.27757700
H	0.60720100	3.27347300	-0.43849700
O	0.03358800	6.44924300	1.99421400
H	0.76235600	4.52488000	1.71704700
C	2.05097800	5.95161100	0.74937100
O	3.65310800	1.36408000	-2.77629900
H	3.59266800	3.27202800	-2.03563200
H	5.22479400	2.58417000	-2.31645600
O	2.87724800	3.73561100	0.44378800
H	4.93296900	3.96403000	0.24047900
H	4.57925700	3.62546000	3.66480900
C	2.65065100	4.95370100	-0.24448600
O	-0.59827400	5.14873500	-2.96851600
H	0.38373700	3.30735500	-2.89844700
H	-1.18139700	3.43370000	-2.08671400
H	0.69311100	6.72112200	2.64997600

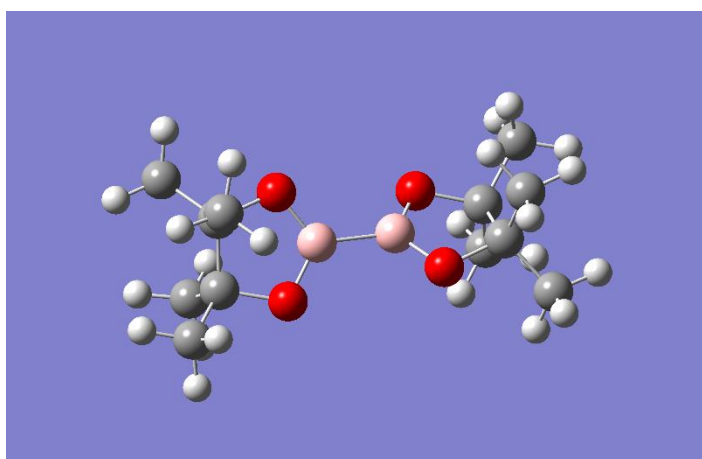
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H	3.58868300	5.33670300	-0.66075900
H	0.22303200	5.59553300	-3.21299800
H	3.21416000	5.32881800	2.20237200
O	-6.62663100	-0.93436900	2.50336600
H	-6.31791400	-1.85311100	2.39540600
Ir	4.26341100	-0.58645200	-2.54508200

XYZ-coordinates of optimized structures of molecules in Pt-catalyzed diboration of phenylacetylene ( represents C atom,  represents H atom,  represents O atom,  represents B atom,  represents Pt atom).



C	-1.51117300	-1.20856700	0.00000200
C	-0.11937000	-1.21376300	-0.00003000
C	0.59234900	-0.00000100	0.00000300
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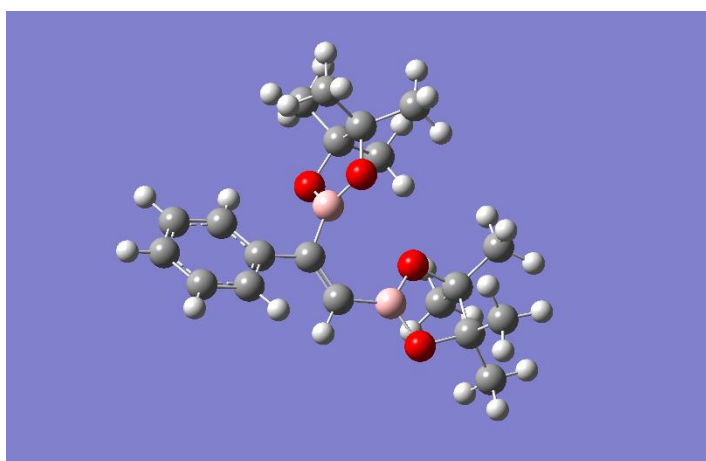
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H	0.42912200	-2.14979400	0.00002800
H	0.42913200	2.14978800	0.00001900
H	-2.05185100	2.15011100	-0.00002900
H	-3.29633700	0.00000600	0.00003900
C	2.02134000	-0.00000100	0.00000500
C	3.23177400	0.00000000	0.00000800
H	4.29880200	0.00000000	0.00000700



C	2.99604700	-0.59811700	0.50775800
C	2.99604700	0.59811700	-0.50775800
O	1.60887400	-1.05090000	0.45400600
O	1.60887400	1.05090000	-0.45400600
B	0.84926700	0.00000000	0.00000000
C	-2.99605900	-0.59771600	-0.50819400
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B	-0.84931000	0.00000000	0.00000000

O	-1.60893700	-1.05066600	-0.45453900
O	-1.60893700	1.05066600	0.45453900
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H	-4.94829300	-1.44430100	-0.09772400
H	-3.81581700	-2.55267100	-0.88643300
H	-3.63291600	-2.18965100	0.83368600
C	-3.25647800	-0.16482900	-1.95286300
H	-3.03504200	-1.00247200	-2.61975400
H	-4.29930500	0.12819500	-2.10423500
H	-2.61434900	0.67292800	-2.23823000
C	-3.90170100	1.76339500	0.13413100
H	-4.94829300	1.44430100	0.09772400
H	-3.81581700	2.55267100	0.88643300
H	-3.63291600	2.18965100	-0.83368600
C	-3.25647800	0.16482900	1.95286300
H	-3.03504300	1.00247200	2.61975400
H	-4.29930500	-0.12819500	2.10423500
H	-2.61434900	-0.67292800	2.23823000
C	3.90142800	1.76365400	-0.13261400
H	4.94808800	1.44477000	-0.09631700
H	3.81547800	2.55353900	-0.88426900
H	3.63238900	2.18904500	0.83551400
C	3.25682200	-0.16639600	1.95270500
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H	4.29966400	0.12660800	2.10400100

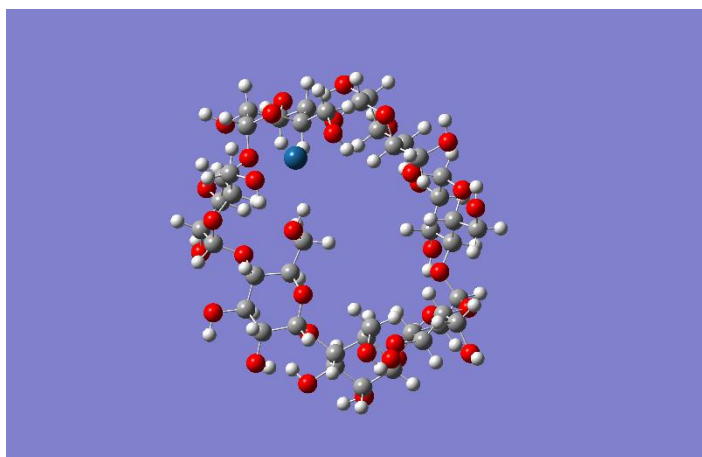
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H	3.81547700	-2.55353900	0.88426900
H	3.63238900	-2.18904500	-0.83551400
C	3.25682200	0.16639600	-1.95270500
H	3.03566400	1.00459500	-2.61898800
H	4.29966400	-0.12660800	-2.10400100
H	2.61470500	-0.67106300	-2.23895100



C	-4.10464900	-3.38514400	0.48925900
C	-2.80416500	-2.88923700	0.50859600
C	-2.49343700	-1.65246700	-0.08459100
C	-3.53813400	-0.92074300	-0.67813700
C	-4.83836000	-1.42166400	-0.70349200
C	-5.12794300	-2.65559200	-0.12058700
H	-4.32344400	-4.33901300	0.96045600
H	-2.02168500	-3.44941600	1.01004700

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H	-5.62685700	-0.84584600	-1.17933800
H	-6.14249500	-3.04241100	-0.13279600
C	-1.10933800	-1.11503800	-0.07848900
C	-0.02640600	-1.92707400	-0.09581000
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O	-0.72237500	1.11002700	1.17113500
O	-1.21938600	1.28337300	-1.06126500
C	-0.97478700	2.52624200	0.93783900
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B	1.43759400	-1.43993900	-0.07619700
O	1.81890000	-0.11688200	-0.14411600
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C	3.26041000	-0.09298900	-0.35399800
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C	0.51999500	2.92494000	-1.14513700
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C	-1.89281300	3.59832900	-1.26058700
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C	0.07457400	3.32998500	1.69424300

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H	-2.63011900	3.87052900	1.41401700
H	-3.13374200	2.22411400	0.97674700
C	4.87121700	-2.13931500	-0.50258700
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O	-3.82142300	-5.33006200	2.11419700
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C	-3.99693600	-4.33457700	1.10042000
C	-3.20795100	-4.66504600	-0.16076700
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O	-1.84430900	-4.65358800	0.24953500
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H	-5.84084800	-5.22778300	0.45116000
C	-5.70689800	-3.23432800	-0.33585300
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O	-4.95502700	-3.62284300	-1.46908800
C	-2.93331200	-3.95705900	-2.62418700
H	-3.18624700	-2.64472700	-0.93920200
H	-5.90830700	-4.38719100	2.66789600
O	-5.29955500	-1.97387000	0.12541600

H	-6.74988900	-3.21478600	-0.66167900
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H	-1.38485300	-5.87927000	-1.35906200
O	-3.27294200	-5.26571900	-3.06094500
H	-3.28589500	-3.19395000	-3.33343200
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C	-6.22655800	-0.88615500	0.07344000
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O	-0.94150500	-7.13245300	1.06032800
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C	-6.13293000	-0.18464100	1.42033200
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C	1.60430900	-4.37879000	0.60237900
H	-1.68548900	-6.59697500	1.38217700
O	-6.66428900	1.25116700	-1.00308900
C	-6.09218700	-0.57441100	-2.44142900
H	-4.80554600	0.32408600	-0.99930400
H	-5.07967700	0.07953400	1.59841400
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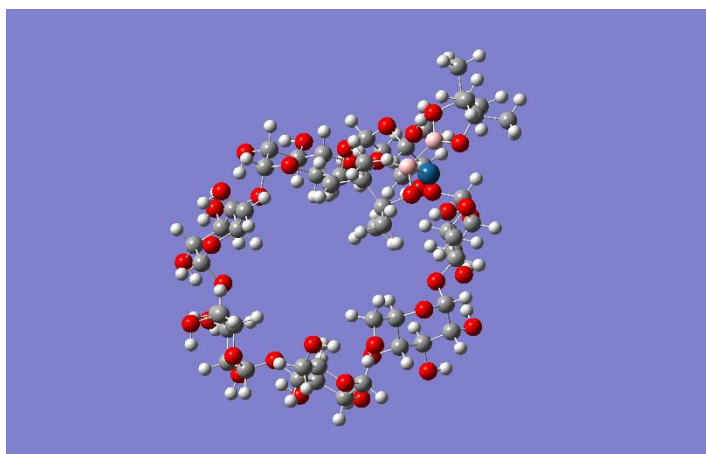
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C	0.77442700	-5.43703300	1.32879100
C	-6.49896600	1.96721900	0.20529500
O	-7.38558300	-1.16937800	-2.47524900
H	-5.98602100	0.20558800	-3.20833100
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H	-8.00408200	0.83900200	1.22324600
H	2.67222700	-2.20239200	-2.48432600
C	3.46392600	-3.89896200	2.02279100
O	1.63010500	-6.31732700	2.04192000
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O	4.47841800	-3.70430500	1.04703500
C	3.83602100	-3.09486800	3.26752300
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H	3.07449000	-2.62102800	4.95752800
O	4.41692500	-0.95507900	4.09307700
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O	-3.29449600	5.14633300	-1.02097500
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H	-5.19848000	4.28641100	-2.50013300
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H	3.54898700	2.15841700	2.15470500
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O	0.05675900	6.47000100	1.94123400
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H	3.59714100	3.23495400	-2.12723100
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H	-6.33225600	-1.89757900	2.34586100
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O	-4.36963500	-5.50685400	2.17575900
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C	2.50776800	-2.13488100	4.86295800
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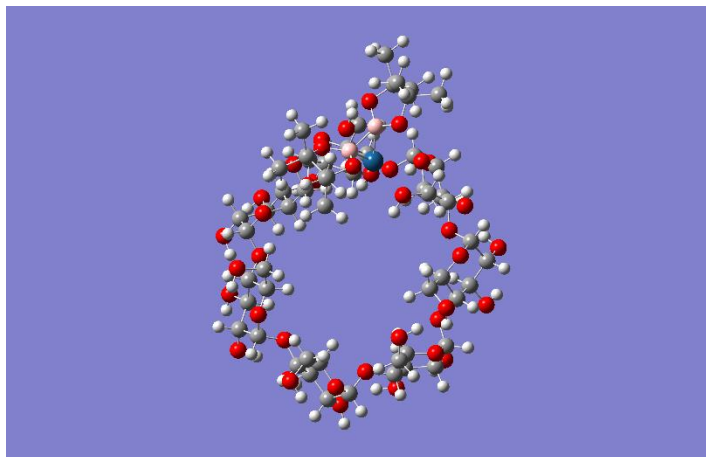
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H	1.97226600	1.81297600	-5.07555200
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H	1.34505900	1.58887800	-2.71098000
H	0.35329300	0.19691800	-3.14844500
H	1.55793700	0.05901200	-1.84213700
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H	0.82600200	-2.19992300	-4.66101600

H	1.73626700	-3.35943700	-3.67800000
H	0.84005000	-2.05515200	-2.89901400



O	-4.19158600	-5.46871500	2.60587000
H	-5.06263500	-5.43953900	3.03043700
C	-4.29432000	-4.66821000	1.43331800
C	-3.06715900	-4.91529100	0.57550500
H	-4.32417200	-3.60237500	1.70246400
C	-5.56269300	-5.01122100	0.65497100
O	-1.94166100	-4.45759200	1.31643600
C	-3.17095700	-4.16107000	-0.75822300
H	-2.97837700	-5.98809300	0.36948700
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O	-5.65867700	-2.84512800	-0.32213100
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C	1.17499400	-3.59278100	2.62700200
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H	-5.39829300	-0.64652500	-1.69104600

H	-6.43152100	-0.69396300	0.78202400
C	-8.31528200	-0.25772900	-0.13736600
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O	3.87473800	-1.98364000	3.30777500
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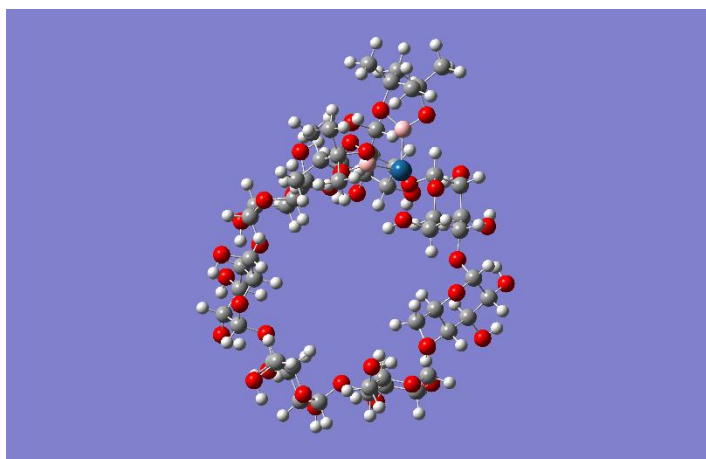
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O	1.33933600	-1.72427800	5.94862300
C	2.27729400	0.00891900	4.56481900
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O	2.19300000	1.01171100	5.57791100
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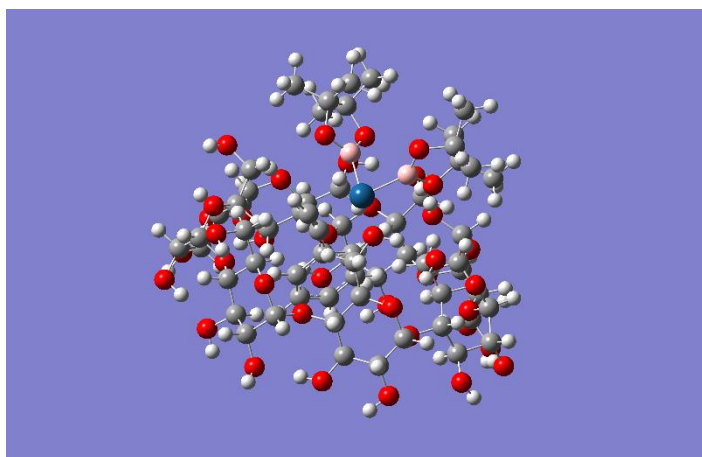
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H	1.19668400	3.39757100	2.80973700
O	-0.71918600	5.19428200	-1.21015100
C	-2.37788500	3.82432600	-2.25683000
H	-1.61080600	3.57006000	-0.28046800
O	-3.24950900	6.78927700	1.62207300
H	-2.10833200	5.05472800	1.76479000
C	-1.01393500	6.60120700	0.73304500
O	2.10922200	1.82627000	-1.86020700
H	0.92994700	3.52440200	-1.54472700
H	2.68436400	3.76448500	-1.70614100
O	0.30915900	4.63821300	0.80651500
H	2.30992100	5.17294000	0.60197500
H	2.00532300	5.29235800	4.01504700
C	-0.07825600	5.69092200	-0.05865500
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H	-1.49665500	3.57758700	-2.85543000
H	-2.90947100	2.88788400	-2.05989200
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O	-0.40658600	7.11504300	1.90285300
H	-1.25929000	7.46276700	0.10170100
H	1.41346900	1.22684300	-1.54975300

H	0.80073200	6.23958700	-0.41200800
H	-4.02473500	4.81753600	-2.58104900
H	0.09620200	6.39919700	2.33655000
O	-7.80958400	-2.57140900	1.10564000
H	-8.14794300	-2.10687900	1.88452600
Pt	4.22305400	1.00549100	-1.20032300
C	8.40604900	0.65994100	-1.16291300
C	8.05606700	-0.69763300	-0.46511700
C	4.06115700	-2.68624600	-3.15679700
C	4.83794900	-1.86754400	-4.24668100
B	6.12500200	0.51365500	-0.93414600
B	4.37344600	-0.53252800	-2.44323200
O	7.17021200	1.41490400	-1.01338500
O	6.61762300	-0.77901900	-0.69612300
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C	9.53832300	1.44141800	-0.51128300
H	10.47269200	0.87138500	-0.54351300
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C	4.97211100	-3.54962300	-2.28040200
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H	5.34702200	-4.42034900	-2.82732100
H	5.82371800	-2.96902800	-1.91793700
C	6.09119200	-2.54454800	-4.78523200
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H	6.80249200	-2.76439600	-3.98731700
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H	4.49636600	-0.67313800	-6.00288400
H	3.65137800	-2.23184900	-6.04752900
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C	2.89578900	-3.51096700	-3.68660200
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O	5.14393400	-3.55488000	-3.37981400
H	5.63608400	-3.20959000	-4.13890600
C	5.02238200	-2.47739700	-2.45896900
C	4.48032700	-3.02867800	-1.15224300
H	4.30146200	-1.73827300	-2.83653300
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O	3.15250500	-3.45090100	-1.43097100
C	4.47865100	-1.95964800	-0.05241100
H	5.09725700	-3.87683300	-0.83349500
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C	6.23808800	-0.75574600	-1.12328200
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O	5.79290500	-1.36335600	0.06358200
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H	7.20019600	-0.28773400	-0.89421300

O	1.62537200	-4.31259100	0.09706900
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O	4.93612900	-3.59854100	1.70797200
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C	5.67288000	1.58950100	-1.59892600
C	0.45750900	-3.72750900	-0.52377700
O	3.23617400	-5.81779600	-2.85933900
H	1.97214100	-6.54130500	-1.45757700
H	5.84133300	-3.26195400	1.75505700
C	5.14591100	2.30041700	-0.34580200
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C	5.05816400	2.15081800	-2.87164200
C	-0.52204800	-3.33735800	0.56547600
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C	-0.09049900	-4.76823200	-1.50255600
H	3.66862300	-4.97020200	-3.07648100
O	5.23144900	3.73404200	-0.48858800
C	5.95928900	1.96425000	0.89523600
H	4.10284500	2.00889900	-0.20149900
H	3.99384500	1.88354100	-2.89718700
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O	-1.09950600	-4.47732400	1.16176700
H	0.00476400	-2.71637500	1.30177100

H	-1.28398900	-2.70008000	0.10446700
O	-1.29406200	-4.33401700	-2.13328700
H	-0.28656200	-5.67536500	-0.92352900
C	0.95685200	-5.02406700	-2.57063900
C	4.51603600	4.22876100	-1.60040100
O	7.32474800	2.31314500	0.73992500
H	5.50903600	2.47738900	1.75870700
H	5.92222800	0.88697400	1.07632600
O	4.53291600	4.13580500	-4.07968600
H	6.21953100	3.95426800	-2.87330300
H	-2.02926100	-4.24806800	1.36351000
C	-2.33019600	-5.29054200	-2.14514900
O	0.43973900	-5.94452300	-3.52940600
H	1.19734900	-4.07030100	-3.06381300
O	3.16630600	3.84137100	-1.55571800
H	4.61162000	5.31901400	-1.56073300
H	7.34130000	3.26127600	0.54796900
H	5.00456500	4.92030600	-4.38822200
O	-3.20092100	-5.14466600	-1.05171600
C	-3.10403400	-5.13053900	-3.45162500
H	-1.91879100	-6.30072200	-2.06409400
H	1.20787100	-6.25768500	-4.03116500
C	2.19513300	4.83846000	-1.22325900
C	-3.80295100	-3.84932600	-0.94503400
O	-2.29070800	-5.25168400	-4.60431500

C	-3.81349400	-3.77839800	-3.45365900
H	-3.86766800	-5.91987300	-3.48019200
C	1.20282100	4.32248700	-0.17307400
H	2.69830200	5.73250000	-0.83260500
C	1.43145100	5.18981800	-2.49643800
C	-4.52497100	-3.84982600	0.40565900
H	-3.02533900	-3.07794800	-0.92350500
H	-1.35758300	-5.25935500	-4.32232700
O	-4.65999000	-3.64046200	-4.58707200
C	-4.65757500	-3.58280600	-2.19860100
H	-3.04045600	-2.99598300	-3.45532000
O	0.23851600	5.37814900	0.06433700
C	1.83981800	3.98033900	1.16740800
H	0.69457100	3.43695600	-0.57080100
O	2.28011600	5.74601600	-3.48521700
H	0.94114600	4.27800200	-2.86744400
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O	-3.66064100	-3.46400400	1.47063500
H	-5.39624200	-3.19634700	0.39020400
H	-4.85319900	-4.87325900	0.60911600
H	-4.12129000	-3.90770500	-5.34644200
O	-5.08963900	-2.22114500	-2.28229500
H	-5.52861100	-4.25217300	-2.22987200
C	-0.56133900	5.74989100	-1.07686500
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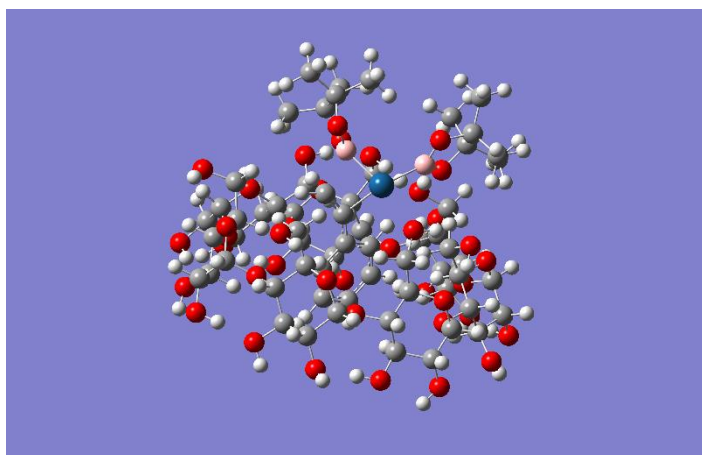
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C	-6.94345700	-0.80023500	-2.52011100
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C	-4.58135900	0.15438000	0.99508700
H	-4.17738200	-0.41561800	-1.00957700
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C	-5.12769300	4.49054700	-1.41022900
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O	5.74786500	1.57304500	-3.97315200
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B	-0.82599600	0.87725200	3.77625000
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O	-0.74881900	1.14153900	5.12696100
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C	3.29529300	-3.09250900	5.07741500
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H	-3.02247300	6.63054400	-0.90229300
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O	-6.41163600	-2.81964300	1.29059400
H	-4.42031000	-2.60562100	1.90420800
H	-5.23846600	-1.17246600	1.24243100
O	-4.53817900	-4.48049000	-3.98285400
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H	1.14120600	4.29109300	1.86240900
C	1.49682000	5.93797200	-1.35960400
O	-1.28197200	6.50672700	-2.85685100
H	-1.81108700	4.50600400	-2.71556300

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C	2.32006900	6.11179200	-2.63600200
H	0.98995200	6.87215400	-1.10045800
H	-2.03753500	6.77057300	-3.40327100
C	-1.66365600	-4.99219000	-1.79627100
C	3.06518400	4.41774400	-0.40508500
O	1.53663200	6.40366700	-3.77727900
C	3.14655700	4.85025700	-2.87112300
H	3.01044000	6.95001400	-2.47065300
C	-0.66165700	-4.61181200	-0.70284000
H	-2.05043700	-6.00343200	-1.61137200
C	-0.98701500	-4.95118800	-3.16048000
C	3.75849600	4.20518500	0.93873200
H	2.36850700	3.58839400	-0.57330800
H	0.60148500	6.22294200	-3.56647500
O	4.02995300	5.00599100	-3.97509300
C	3.97527800	4.49598000	-1.64319700
H	2.45122400	4.01758800	-3.05246500
O	0.46477100	-5.51899200	-0.78298200
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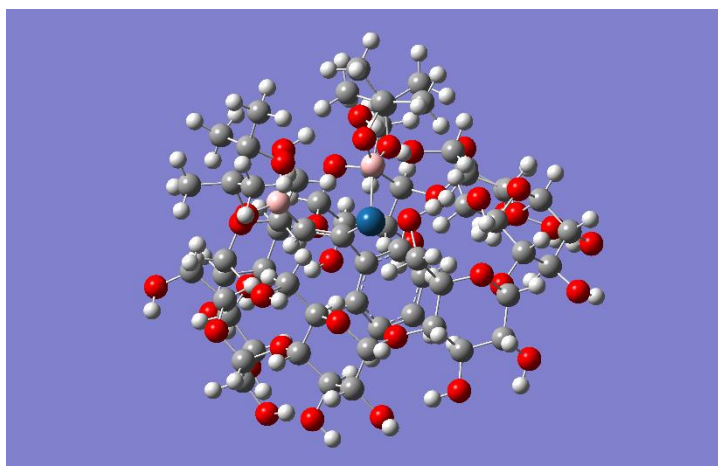
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H	4.06991700	5.18370300	1.31864400
H	3.48812700	5.36926900	-4.69129100
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H	4.76796800	5.24366200	-1.50113100
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H	-0.12885800	-6.88632900	-2.93556200
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C	5.81105900	2.88506000	-1.45684900
O	1.77200600	-4.25555300	-2.25128400
H	1.94632800	-6.27421500	-1.92176800
H	0.38578500	-4.23512400	1.74005100
H	0.21350500	-5.88323800	-5.06894800
O	5.71325600	2.08418500	-0.29606400
C	6.52021400	2.12196700	-2.58028500
H	6.37692100	3.77616600	-1.16357400

C	3.10213400	-4.09444200	-1.73953100
C	4.91164400	0.90584400	-0.49558300
O	6.54836900	2.86150300	-3.78528500
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C	3.14001500	-2.96497200	-0.70514900
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C	4.04406000	-3.76547200	-2.89075300
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C	5.67405400	0.00683300	-1.48119900
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O	6.61101600	-0.04462300	-3.68040800
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C	2.21945200	-3.11335200	0.49030100
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O	4.95585400	-1.17737000	-1.79638800
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O	2.18153200	-4.40526500	1.09854300
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H	2.64050000	-1.17841800	6.96542000
C	4.92323500	-1.71648600	3.74311800
H	5.42711100	-0.89836000	3.22469600
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H	4.84269800	-2.55986000	3.05542700
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C	-2.12229900	3.29211600	4.06740500
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C	-0.71938900	-0.18731700	-0.29573300
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C	-1.26819300	-0.33134700	1.03515800
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O	-3.26031100	3.53633600	-4.15882300
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C	-4.66296000	2.49883900	-0.82850700
H	-4.49499700	4.25456900	-2.08138700
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O	-4.50487900	0.06927200	-2.19602500

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O	3.16850200	6.08967900	-3.28661200
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H	5.01032800	4.77430600	-3.93252800
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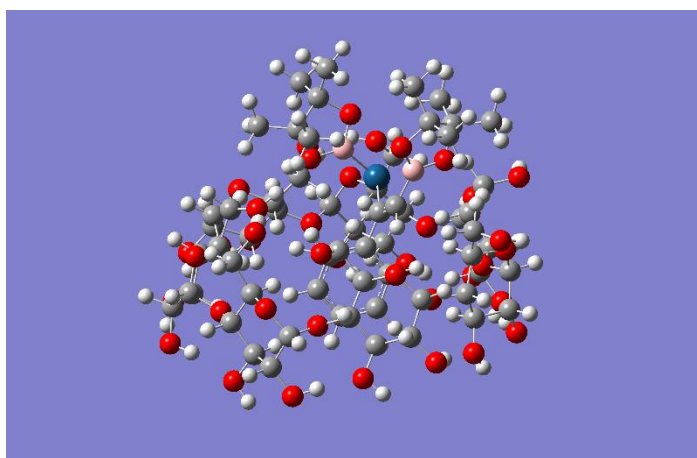
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C	1.74991800	-0.48085800	-1.92023300
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H	-0.90031000	-0.21902400	-4.03505000
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H	1.63833400	-0.29269700	0.22189900
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H	1.55505600	-0.62168000	-4.06542200
C	-1.03113700	0.04750800	0.61803000
C	-1.76479200	1.13652400	0.92028800
H	-1.82080500	1.93307900	0.17793400



O	-3.60806500	4.00965100	-3.97582400
H	-3.79904900	3.66134600	-4.85914000
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C	-3.86925000	3.51280000	-1.65666300
H	-3.07582900	2.19140700	-3.13240400
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O	-2.52703900	3.88254000	-1.37100000

C	-4.34866900	2.48317700	-0.62284700
H	-4.52881000	4.38796200	-1.62672900
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H	-5.99354600	3.04474900	-3.34072000
C	-5.50813500	1.23868700	-2.30709900
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O	-5.57659100	1.84484600	-1.04473200
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O	-4.46839100	0.27124600	-2.35922200
H	-6.47845400	0.76112900	-2.47461200
O	-1.51485900	4.81241200	0.49040900
C	-1.58460000	6.06054900	-1.59531500
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O	-5.68257200	4.11447000	0.60532000
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H	-3.79030500	3.59381000	1.13518600
C	-4.79960000	-1.10619800	-2.40861200
C	-0.21040200	4.24716500	0.20423100
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C	-4.30693200	-1.81305300	-1.13809900
H	-5.88563700	-1.23890300	-2.47913700

C	-4.13000900	-1.68560900	-3.64628400
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H	-0.34812800	3.33066400	-0.37916500
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H	-2.58166800	5.46787400	-3.18129300
O	-4.47195100	-3.24643300	-1.27848900
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H	-3.24739500	-1.57472700	-0.97993800
H	-3.05250400	-1.47853900	-3.59401400
C	-4.33835400	-3.19045500	-3.68167200
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H	0.64431000	6.18830300	-0.02413900
C	-0.18689600	5.53916800	-1.91241300
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O	-6.48009700	-1.77906300	-0.05270300
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H	-5.06007200	-0.35768500	0.25387200
O	-3.66486800	-3.68079100	-4.84586300
H	-5.41348200	-3.39564600	-3.75444500
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O	0.53924600	6.48843300	-2.69285800

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O	-2.42534000	-3.62167700	-2.31232900
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H	-6.50327600	-2.73530600	-0.19515500
H	-4.06026800	-4.52166900	-5.11085800
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C	3.92995000	5.61451800	-1.83889300
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C	-1.57493400	-4.74958000	-2.09835800
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C	-0.84893400	-4.60441500	-0.75796900
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C	-0.56681600	-4.77856300	-3.24001200
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H	3.26493100	3.28214700	0.32111300
H	2.39530600	5.93179600	-3.02007500
O	5.56565100	4.14991700	-2.88922500
C	5.13797500	3.80752700	-0.56359500
H	3.73499900	3.50785100	-2.14121400
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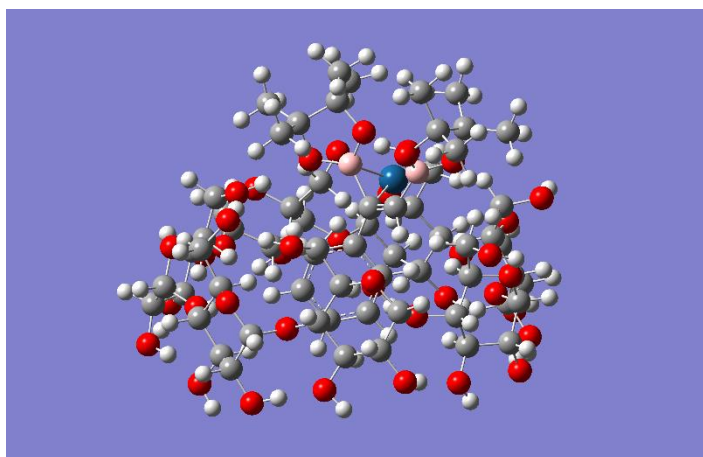
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O	3.42529100	3.44240600	2.82232100
H	5.27434700	2.95216500	2.04135200
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O	5.52754400	2.44133000	-0.74509800
H	6.02624700	4.41937100	-0.35299500
C	1.13615200	-5.70222600	-1.64830900
O	-1.32213000	-3.95334800	1.59012100
H	-2.75193000	-4.23482100	0.18606000
H	-1.94376600	-5.72966100	0.71112100
H	-1.84205100	-4.35171900	-4.64926700
O	1.42454000	-5.91159100	-4.02119000
H	-0.09227800	-6.83654200	-2.94775400
H	3.27965600	2.48342300	2.72177400
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O	1.91018500	-4.54910600	-1.61849900
H	1.73546600	-6.58572300	-1.41273800
H	-0.40771700	-4.25286500	1.82229000
H	0.93286800	-5.82008000	-4.85042900
O	6.06575900	1.18750600	1.14549700
C	7.39575200	1.01192000	-0.87180700

H	7.17694700	2.71937600	0.46271600
C	3.06400300	-4.59640400	-0.76586400
C	5.18472600	0.11835400	0.76449800
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H	8.31363200	0.73845600	-0.33919800
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C	4.32455100	-4.52511100	-1.61747700
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O	5.55835700	-1.61195200	-1.43240400
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O	1.54720200	-4.70791600	-0.04741600
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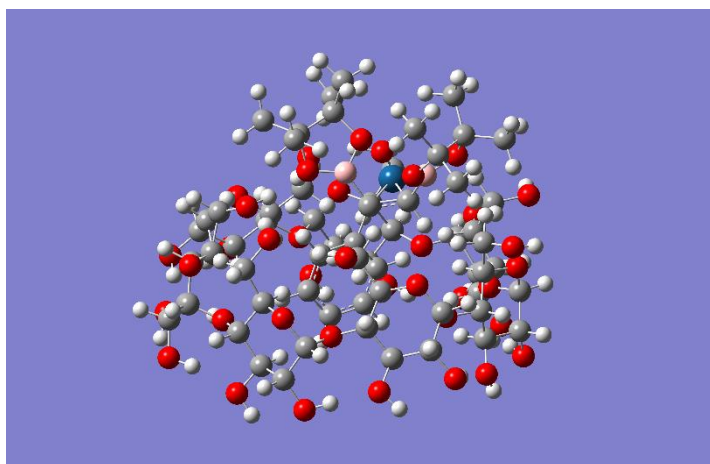
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C	-4.34184700	4.63582100	-1.13887200
C	-4.74610400	0.19846500	2.23880800
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O	-3.70704600	-0.73121800	2.56387200
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H	-6.79821000	3.39380700	-1.35697800
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H	4.88840500	-2.15417700	6.35650100
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H	-0.00805400	-4.06279500	-3.15968500
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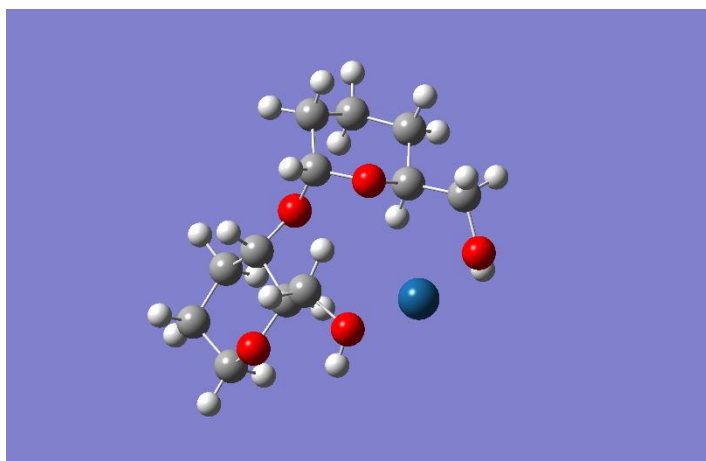
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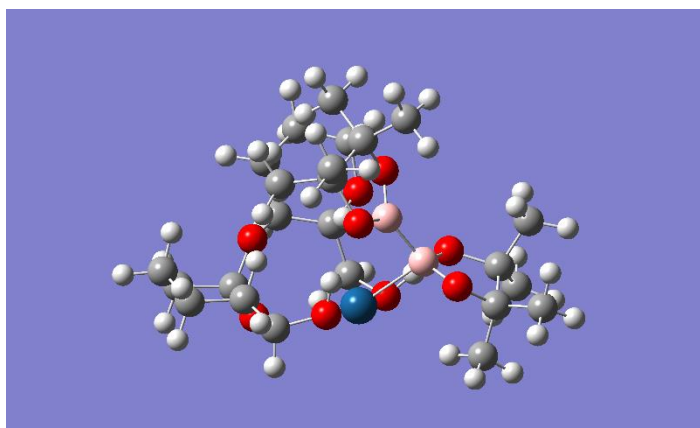
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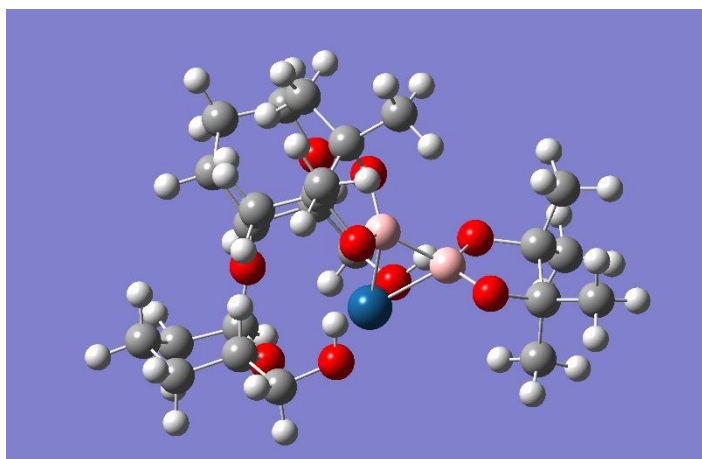


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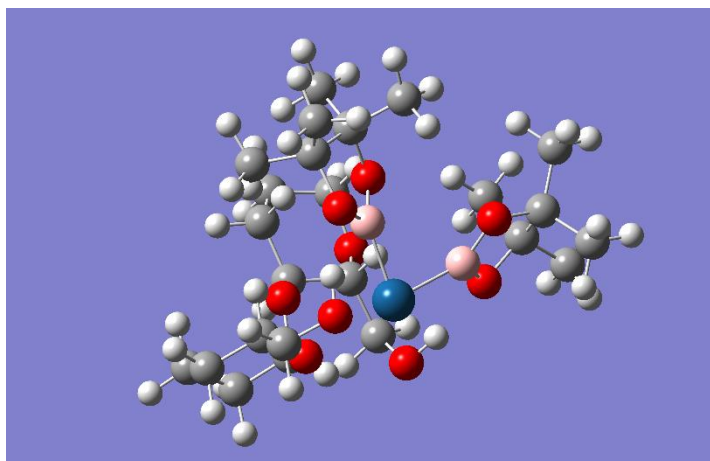
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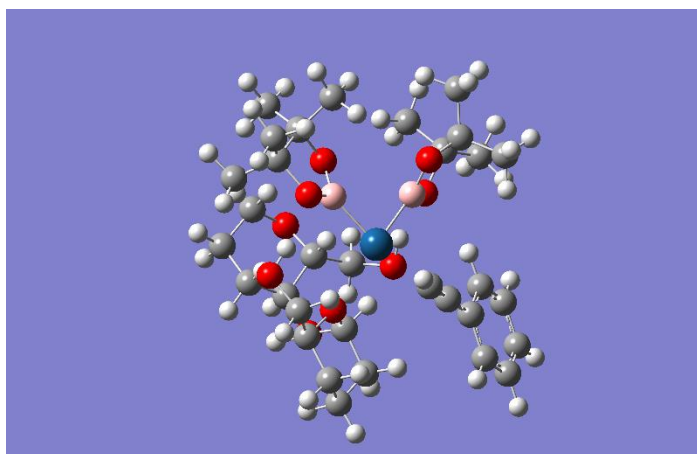


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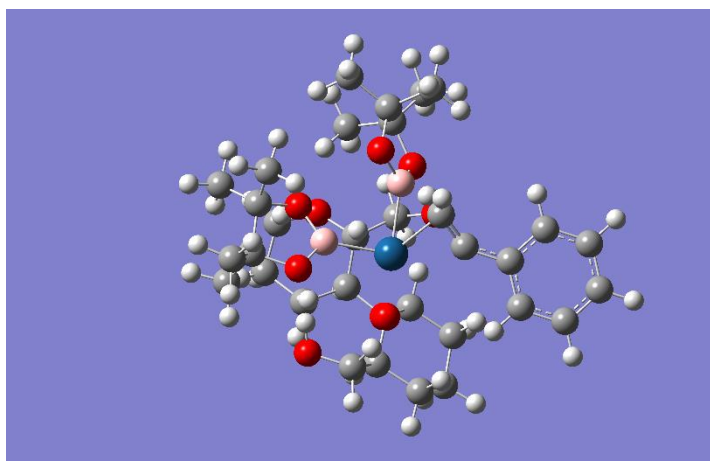


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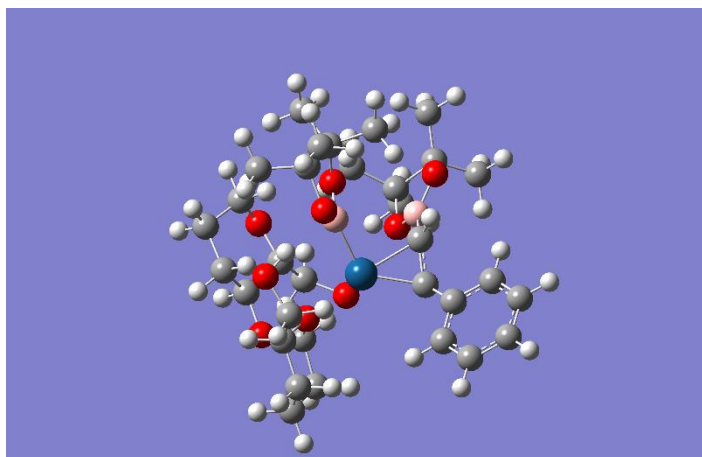
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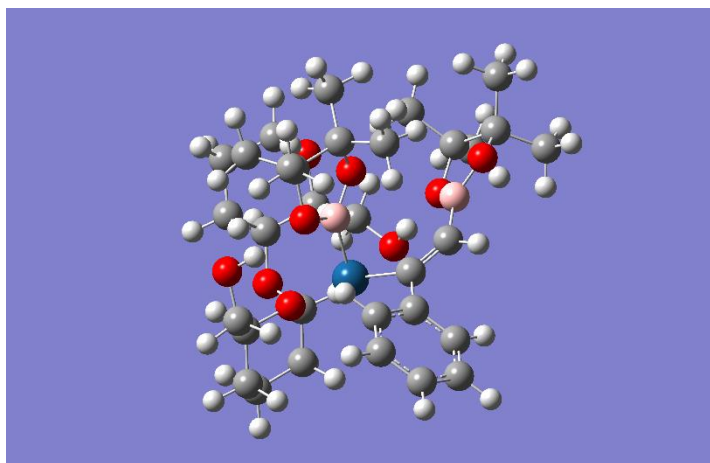
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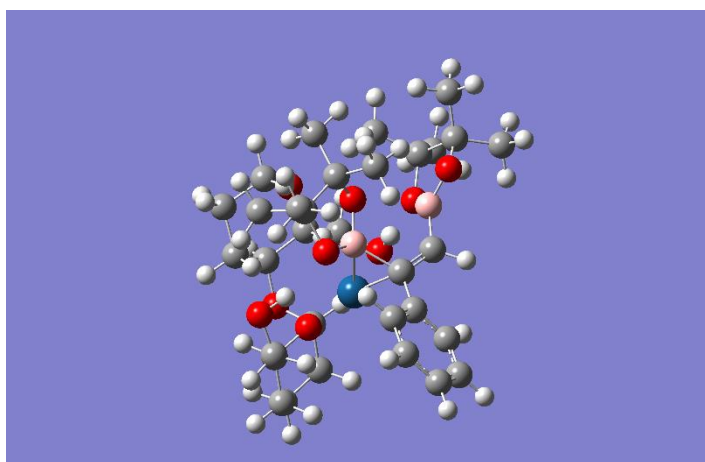
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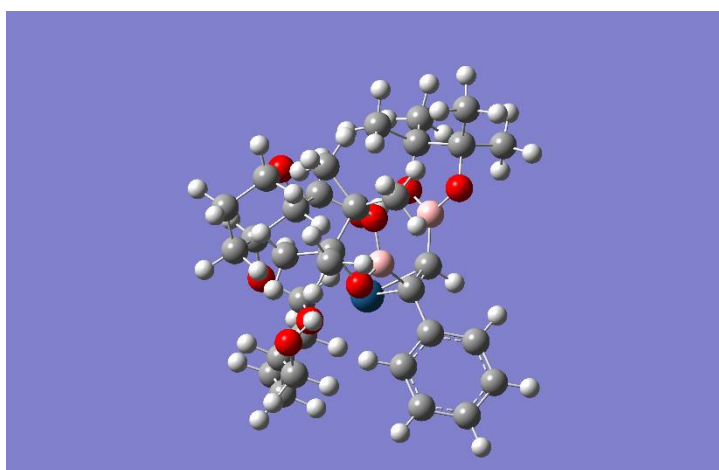
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O	-3.77672400	0.88652000	-1.12778100
O	-2.35055100	-0.86678600	-1.49937200
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O	-1.61516200	0.69515000	1.19934900
C	-0.76506600	3.04812100	3.90669200
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H	-1.42861000	2.90427700	4.76580400
C	-0.01233200	0.65768000	3.83784100
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C	0.76169900	3.45869900	-2.48449200
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H	2.54763500	6.33944900	-2.17523200
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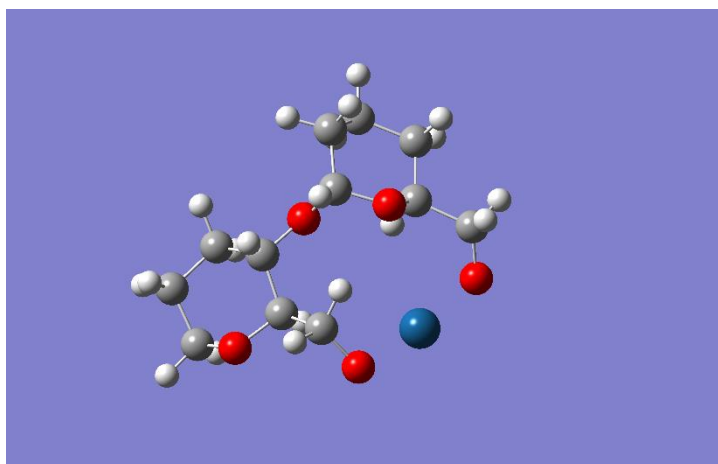
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H	0.50697400	-2.03150700	0.27899000
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H	1.98403600	-0.97960500	2.08921500
O	0.56157000	-3.26129800	-1.86865500
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O	2.81141500	-0.37923200	-0.24858100
C	4.31531400	-1.72362200	-1.62317900
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H	4.03484700	-1.19326100	-2.54018400
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C	5.11673600	0.37603400	-0.51269900

H	5.84228700	-1.61915100	-0.09909700
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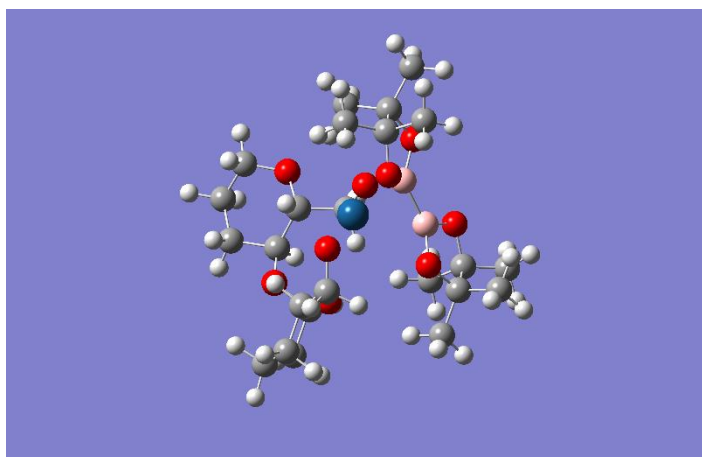
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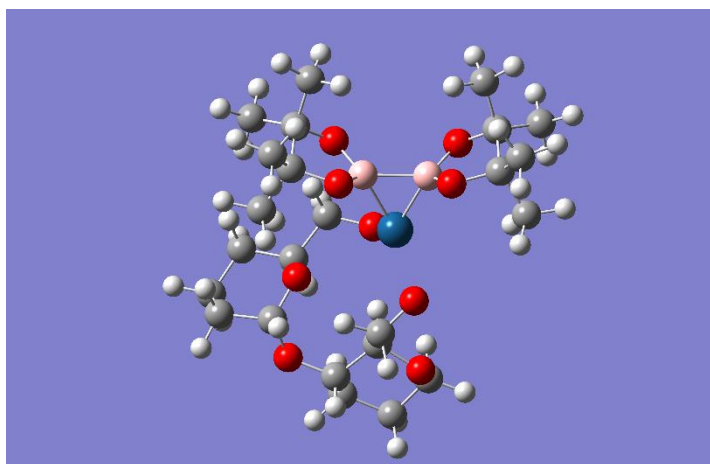


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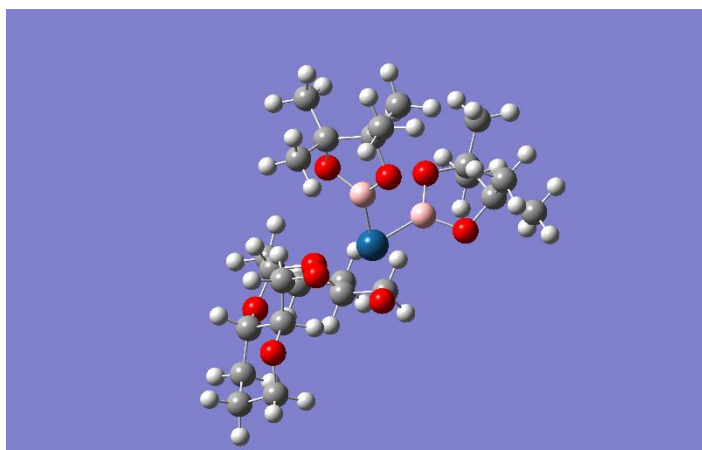


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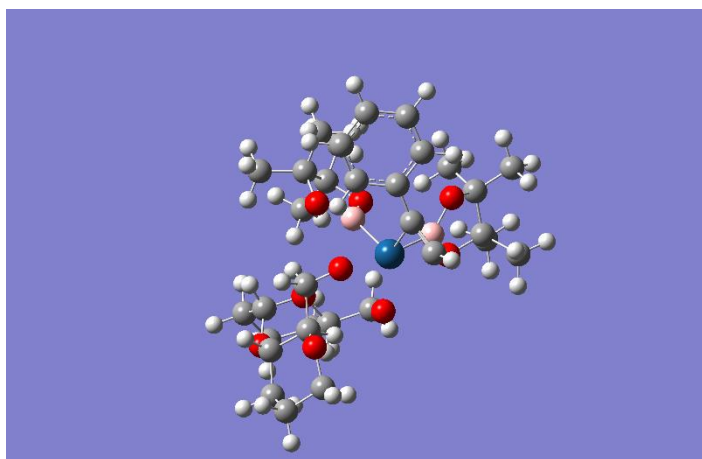


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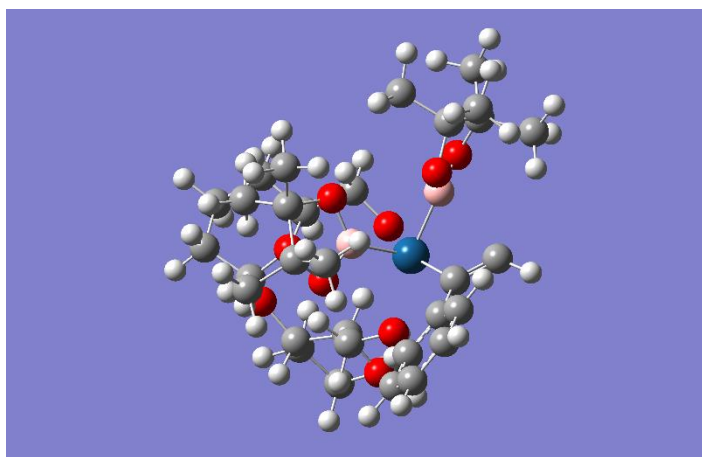
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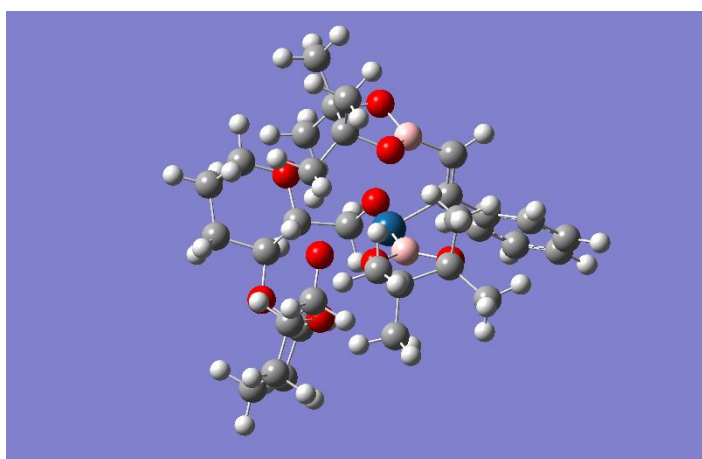
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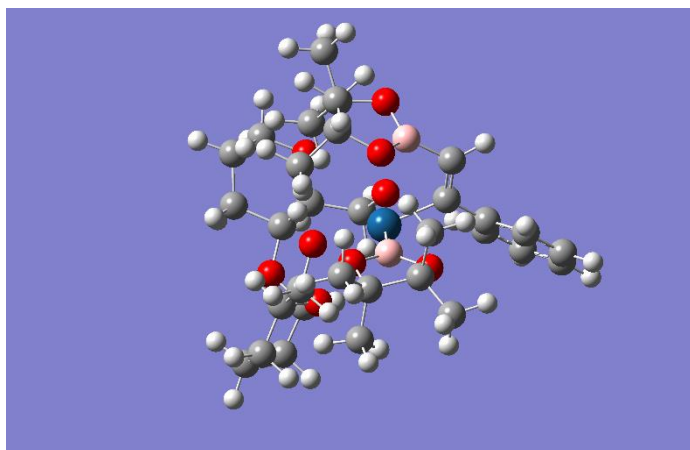
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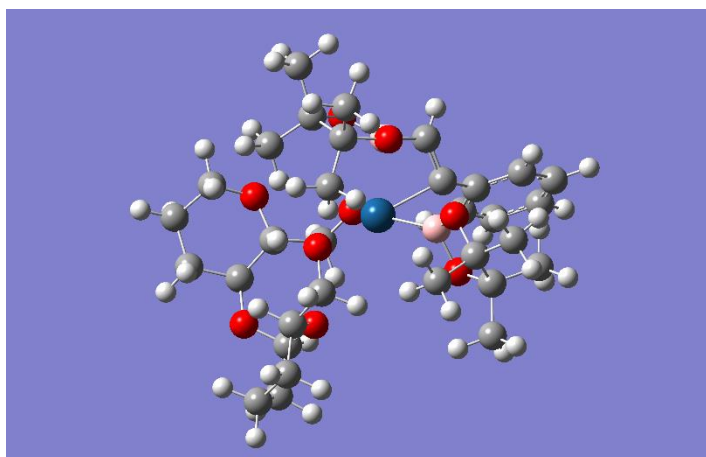
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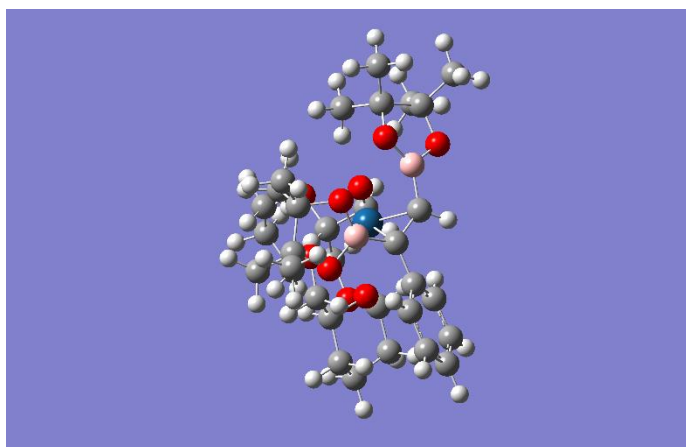
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C	-0.14118300	4.96661000	-2.15851100
C	0.92818300	4.61724000	-2.98332200
H	2.06382200	2.96612300	-3.78551600
H	0.72515600	1.23371600	-2.63062000
H	-1.72893400	4.26568100	-0.88772400
H	-0.37853100	6.01627800	-1.99069500
H	1.53299800	5.38375600	-3.46425500
C	-1.47703500	1.56389500	-1.05218400

C	-1.75227200	0.34141200	-1.82316300
H	-1.33146400	0.34398100	-2.83259900

Video S1: This video is referred to as Video S1 in the text, which shows IRC reaction pathway for the diboration of phenylacetylene over Pt₁/CD.

Video S2: This video is referred to as Video S2 in the text, which shows IRC reaction pathway for the diboration of phenylacetylene over Pt₁/CD-b.

Video S3: This video is referred to as Video S3 in the text, which shows IRC reaction pathway for the diboration of phenylacetylene over Pt₁/CD-b-noH.

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