

## Supporting Information

### ***N,N'*-Bis(imidazolyl)guanidinylphosphines: Powerful Initiators for Conjugate-Addition Polymerization of Michael-Type Monomers**

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## 1. General information

Unless noted otherwise, all manipulations were performed under an inert atmosphere of dry argon, using standard Schlenk or an argon-filled glovebox. Toluene and tetrahydrofuran (THF) were refluxed over sodium/benzophenone and distilled under argon atmosphere; hexane and dimethylformamide (DMF) were refluxed over CaH<sub>2</sub> and (vacuum) distilled under argon atmosphere. All of the solvents were stored over 4A molecular sieves before used.

$\alpha$ -Methylene- $\gamma$ -butyrolactone (MBL) was purchased from TCI. Methyl methacrylate (MMA), benzyl methacrylate (BnMA), furfuryl methacrylate (FMA), 4-vinylpyridine (4-VP), methyl acrylate (MA), *N,N*-dimethylacrylamide (DMAA) were purchased from Energy Chemical, Adamas or Macklin Inc. All monomers were dried over CaH<sub>2</sub> overnight, followed by vacuum distillation and stored in brown bottles inside a glovebox freezer at -30°C.

**NMR Experiments.** NMR spectra were recorded on 400 M or 600 M (<sup>1</sup>H NMR, 400 MHz or 600 MHz; <sup>13</sup>C{<sup>1</sup>H} NMR, 101 MHz, 126 MHz or 151 MHz; <sup>31</sup>P{<sup>1</sup>H} NMR, 162 MHz) spectrometer in CDCl<sub>3</sub>, DMSO-d<sub>6</sub>, C<sub>6</sub>D<sub>6</sub> at ambient temperature and chemical shifts are expressed in parts per million ( $\delta$ , ppm). Proton chemical shifts are referenced to 7.26 ppm (CDCl<sub>3</sub>), 2.50 ppm (DMSO-d<sub>6</sub>) or 7.16 ppm (C<sub>6</sub>D<sub>6</sub>) and carbon chemical shifts are referenced to 77.16 ppm (CDCl<sub>3</sub>), 39.52 ppm (DMSO-d<sub>6</sub>) or 128.06 ppm (C<sub>6</sub>D<sub>6</sub>).

**Electrospray ionization mass spectrometry (ESI-MS).** ESI-MS spectra of the resulting copolymers in positive ion mode were obtained using a ESI-Q-ToF (Waters, USA) mass spectrometer equipped with an orthogonal electrospray source (Z-spray).

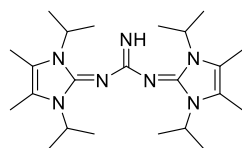
**Fourier transform infrared spectroscopy (FT-IR).** FT-IR spectra were performed on a Bruker EQUINOX55 spectrometer in the range from 4000 to 400 cm<sup>-1</sup> at a resolution of 2 cm<sup>-1</sup> and 32 times for each test.

**Gel Permeation Chromatography (GPC).** Molecular weights and molecular weight distributions of copolymers were measured by gel permeation chromatography (GPC) analysis at 30 °C and a flow rate of 1.0 mL/min, with THF as the eluent, on an Agilent 1260 instrument coupled with an Agilent RI detector and equipped with four PL gel columns. The sample concentration was about 0.1%, and the injection volume was 50  $\mu$ L. The curve was calibrated using monodisperse polystyrene standards covering the molecular weight range from 580 to 460000 Da.

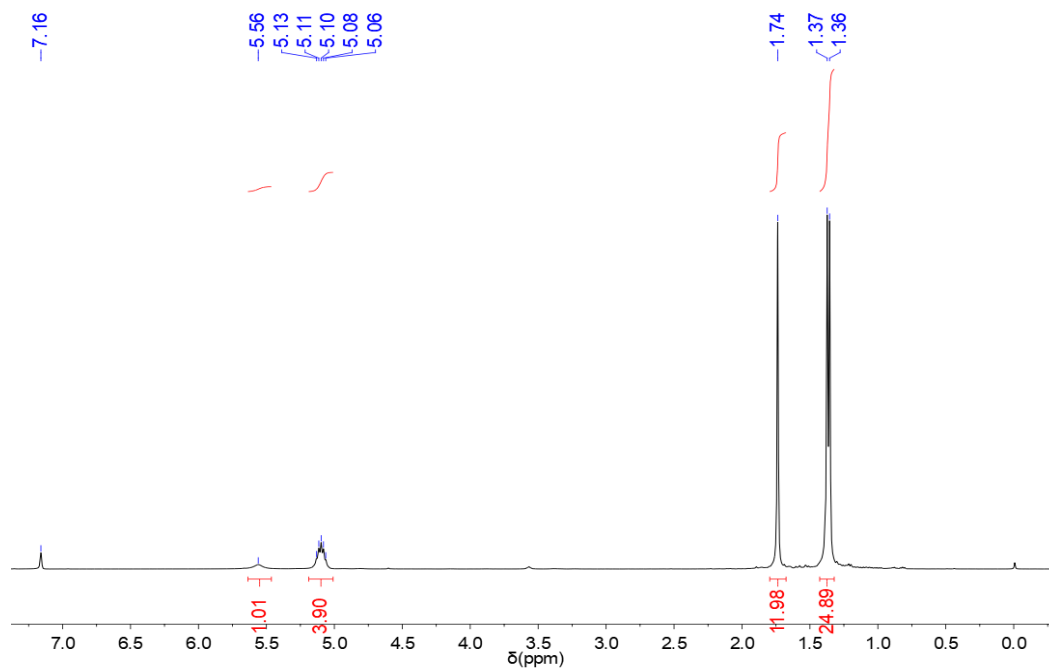
**Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS).** MALDI-TOF mass spectrometric measurements were performed on a Shimadzu Axima CFR MALDI-TOF MS mass spectrometer, equipped with a nitrogen laser delivering 3 ns laser pulses at 337 nm. Trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) (J&K, 97%), was used as a matrix. CF<sub>3</sub>COONa (J&K, 98%) was added for ion formation.

## 2. Synthesis of *N,N'*-bis(imidazolyl)guanidinylphosphines

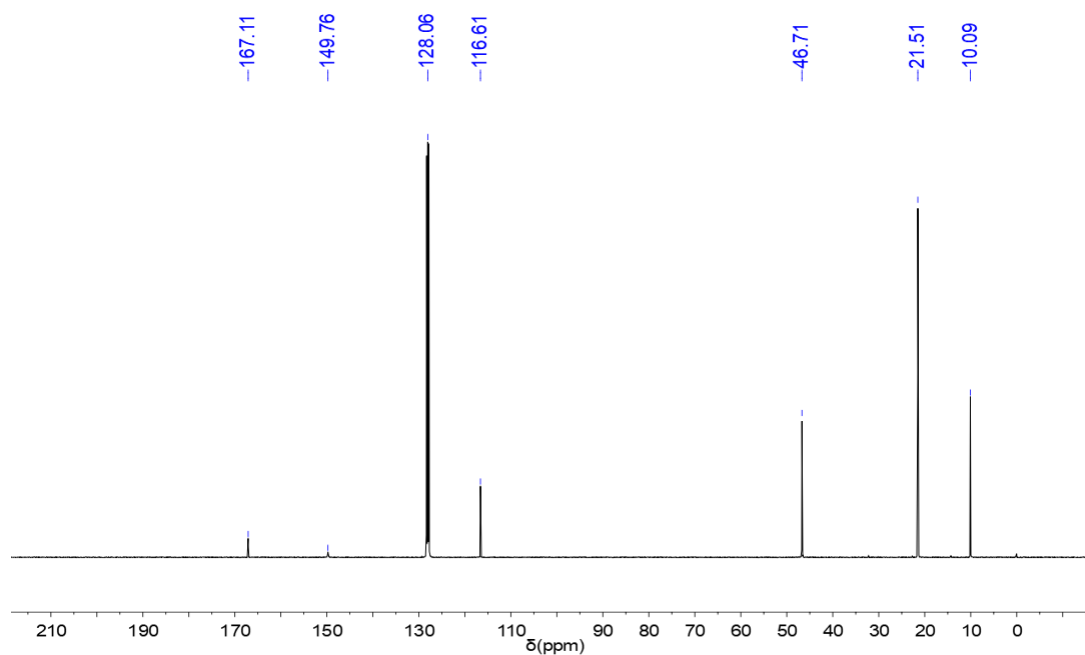
1,3-Bis(1,3-diisopropyl-4,5-dimethyl-1*H*-imidazol-2(3*H*)-ylidene)guanidine (**BIG**) was synthesized according to literature.<sup>[S1]</sup>



**<sup>1</sup>H NMR** (400 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  5.56 (s, 1H), 5.10 (dt,  $J = 13.5, 6.6$  Hz, 4H), 1.74 (s, 12H), 1.36 (d,  $J = 7.0$  Hz, 24H); **<sup>13</sup>C NMR** (101 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  167.1 (s), 149.8 (s), 116.6 (s), 46.7 (s), 21.5 (s), 10.1 (s).



**Figure S1** <sup>1</sup>H NMR spectrum of **BIG** in C<sub>6</sub>D<sub>6</sub>.

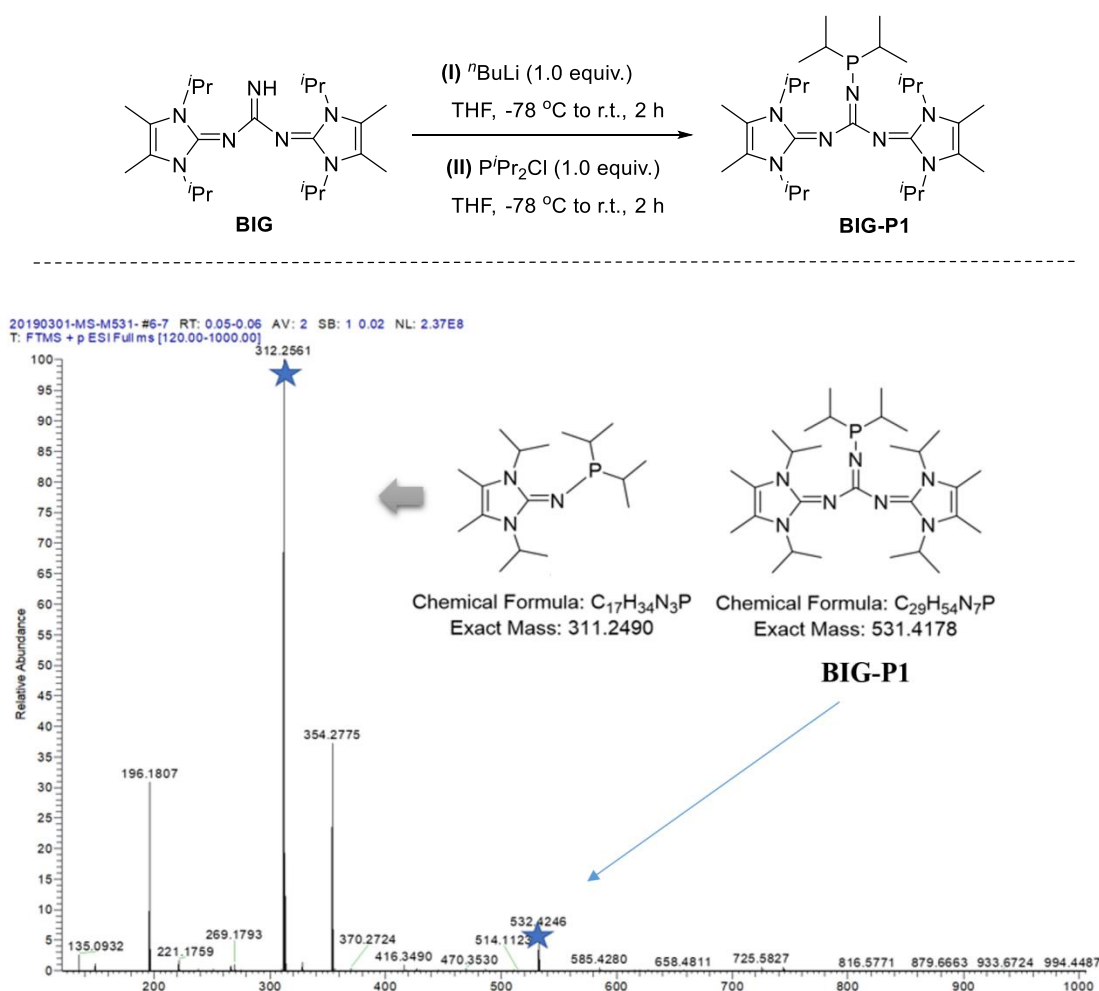


**Figure S2:** <sup>13</sup>C NMR spectrum of **BIG** in C<sub>6</sub>D<sub>6</sub>.

### 3. Preliminary attempt at the synthesis of BIG-Ps using <sup>n</sup>BuLi as base

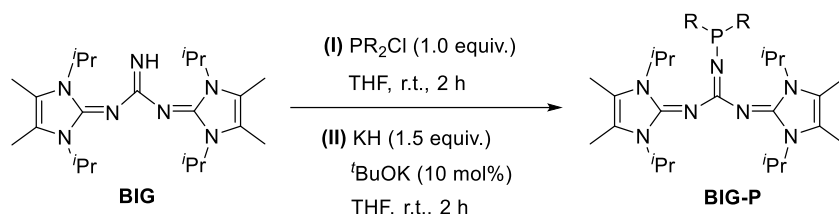
Firstly, the synthesis of BIG-P was attempted using <sup>n</sup>BuLi as base according to the reported synthetic procedures.<sup>[S2-S3]</sup> A solution of <sup>n</sup>BuLi (0.23 mL, 1.6 M in hexane) was added dropwise to a stirred solution of **BIG** (0.15 g, 0.36 mmol) in THF (5.0 mL) at -78 °C. After completing the addition, the cold bath was removed, and the solution was stirred at room temperature for 2 h. At -78 °C, P(<sup>i</sup>Pr)<sub>2</sub>Cl (0.36 mmol) was added and the stirred reaction mixture was allowed to warm up to room temperature for 2 h. The volatiles were subsequently removed under vacuum, and the solid components were analyzed using <sup>1</sup>H-NMR spectroscopy and MS.

It is hard to prove the formation of the desired **BIG-P1** from the data of <sup>1</sup>H-NMR spectroscopy, due to the presence of elusive side reactions. As shown in Figure S1, **BIG-P1** could be observed, along with the generation of imidazolin-2-ylidenamino-substituted phosphine.

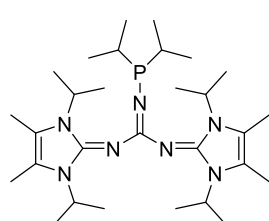


**Figure S3.** ESI-MS spectrum of the reaction crude mixture.

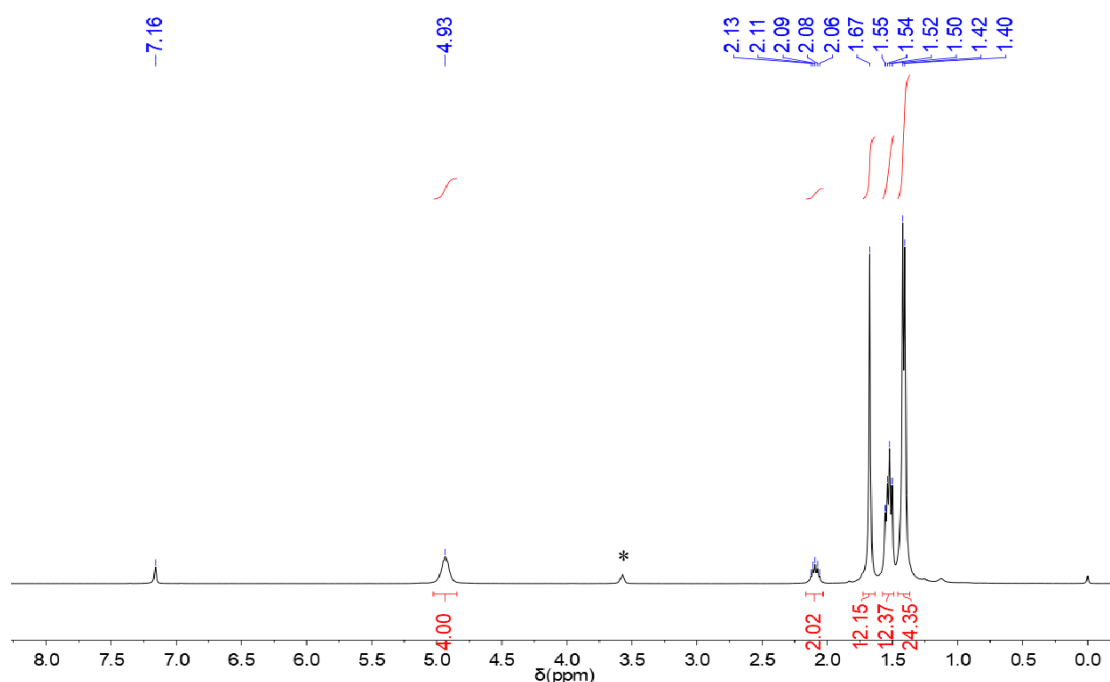
#### 4. General synthetic procedure for BIG-Ps



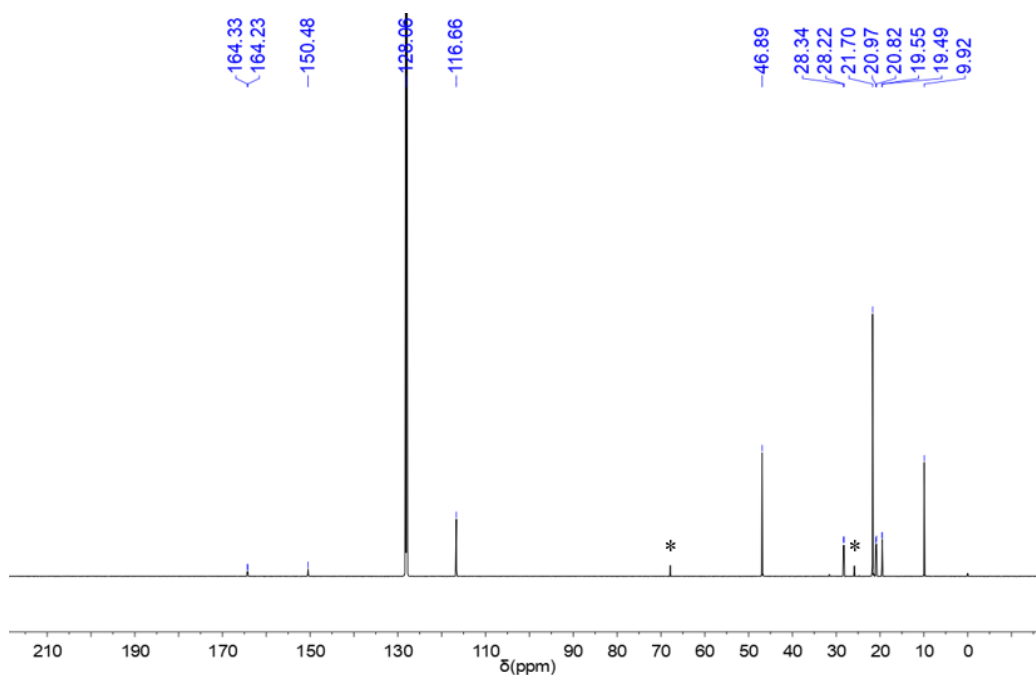
In an argon-filled glovebox, the corresponding disubstituted phosphine chloride (0.36 mmol) was added dropwise to a stirred solution of **BIG** (150 mg, 0.36 mmol) in THF (5 mL) at room temperature. After 2 h, KH (21.7 mg, 0.54 mmol) and <sup>t</sup>BuOK (4 mg, 0.036 mmol) were introduced to the reaction mixture, then stirred for 2 hours. The volatiles were removed under vacuum, and the residue was extracted with toluene (3×10 mL). The solid components were separated by filtration, and the filtrate was dried to obtain the desired phosphines (**BIG-Ps**).



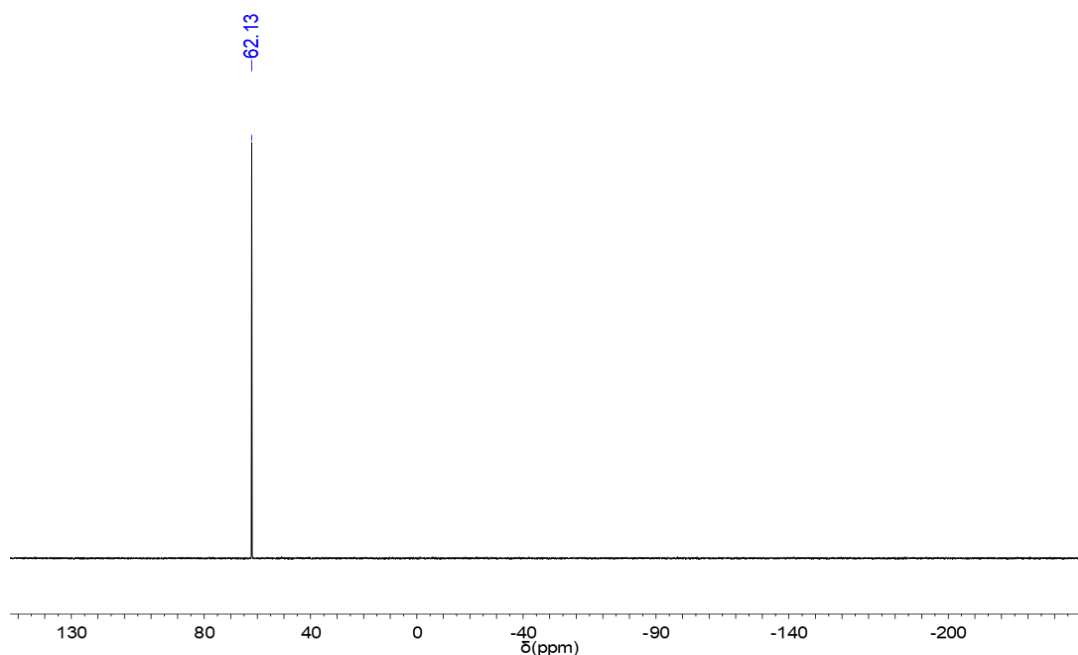
**BIG-P1** (yellowish solid, 156 mg, 82% yield). <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>) δ 4.93 (s, 4H), 2.09 (dt, *J* = 13.8, 6.9 Hz, 2H), 1.67 (s, 12H), 1.53 (dd, *J* = 13.8, 6.6 Hz, 12H), 1.41 (d, *J* = 6.9 Hz, 24H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, C<sub>6</sub>D<sub>6</sub>) δ 164.3 (d, *J* = 14.2 Hz), 150.5 (s), 116.7 (s), 46.9 (s), 28.3 (d, *J* = 17.5 Hz), 21.7 (s), 20.9 (d, *J* = 22.2 Hz), 19.5 (d, *J* = 9.8 Hz), 9.9 (s). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, C<sub>6</sub>D<sub>6</sub>) δ 62.1 (s). **HRMS** (ESI): [C<sub>29</sub>H<sub>55</sub>N<sub>7</sub>P]<sup>+</sup>[M+H]<sup>+</sup>: calcd. 532.4251, found 532.4244 m/z. **IR** (Film): 2977, 2939, 2878, 2157, 1567, 1514, 1466, 1351, 1248, 1216, 1113, 1056, 993, 950, 886, 812, 729, 673 cm<sup>-1</sup>.



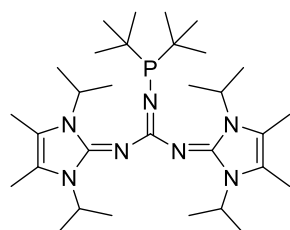
**Figure S4.** <sup>1</sup>H NMR spectrum of **BIG-P1** in C<sub>6</sub>D<sub>6</sub>. \* denote THF.



**Figure S5.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P1** in  $\text{C}_6\text{D}_6$ . \* denote THF.



**Figure S6.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P1** in  $\text{C}_6\text{D}_6$ .



**BIG-P2** (dark red solid, 168 mg, 83 % yield).  $^1\text{H}$  NMR (600 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  4.94 – 4.92 (m, 4H), 1.67 (s, 12H), 1.56 (d,  $J = 9.7$  Hz, 18H), 1.40 (d,  $J = 7.0$  Hz, 24H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  165.3 (d,  $J = 20.2$  Hz), 150.3 (s), 116.7 (s), 46.8 (s), 34.2 (d,  $J = 27.1$  Hz), 30.1 (d,  $J = 15.9$  Hz), 21.8 (s), 10.0 (s).  $^{31}\text{P}\{^1\text{H}\}$  NMR (162 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  77.9 (s). **HRMS** (ESI):  $[\text{C}_{31}\text{H}_{59}\text{N}_7\text{P}]^+[\text{M}+\text{H}]^+$ : calcd. 560.4564, found 560.4562 m/z. **IR** (Film): 2978, 2946, 2876, 2157, 1567, 1512, 1471, 1351, 1256, 1217, 1114, 1055, 989, 949, 813, 728, 635, 517  $\text{cm}^{-1}$ .

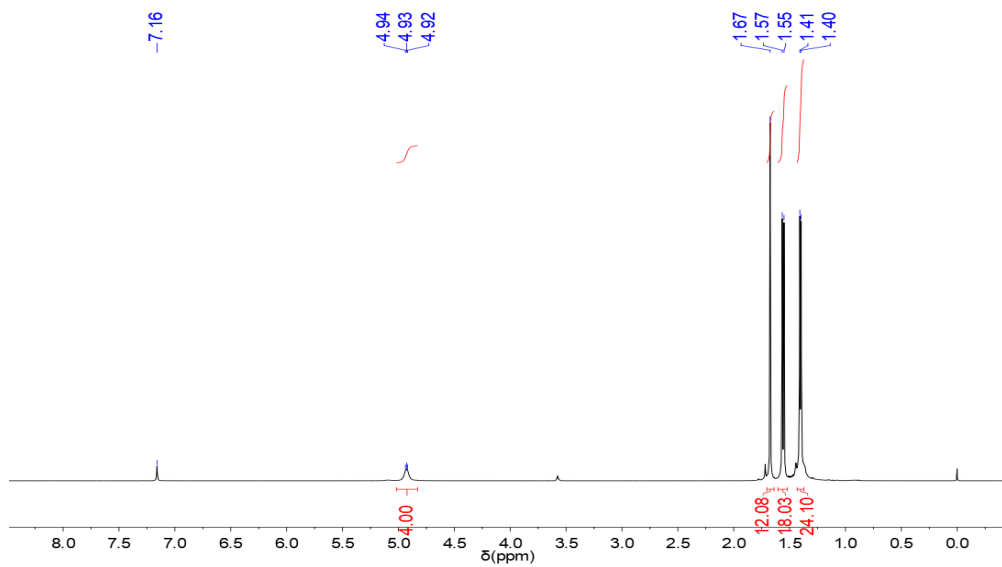


Figure S7.  $^1\text{H}$  NMR spectrum of **BIG-P2** in  $\text{C}_6\text{D}_6$ .

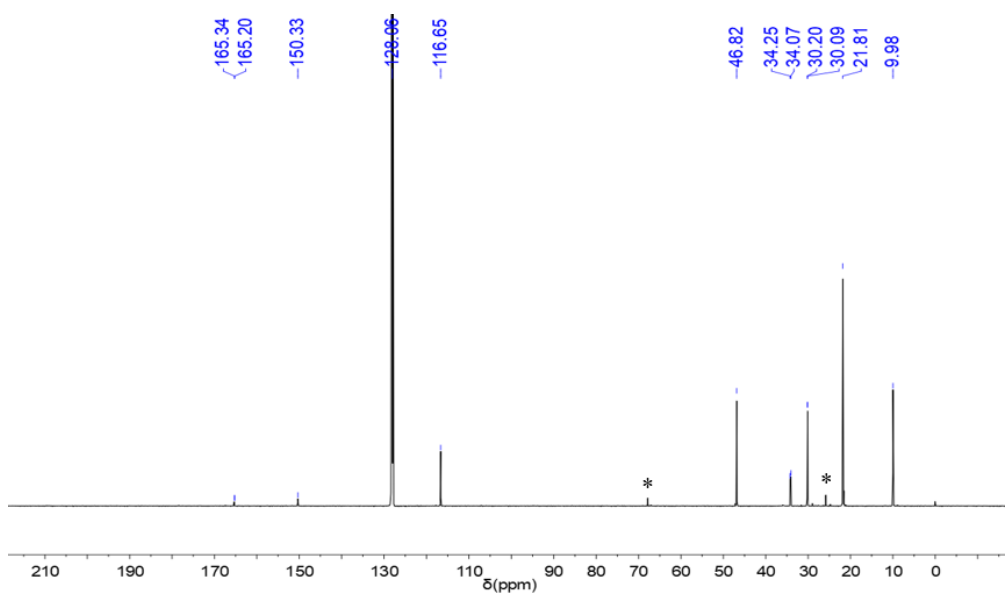


Figure S8.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P2** in  $\text{C}_6\text{D}_6$ . \* denote THF.

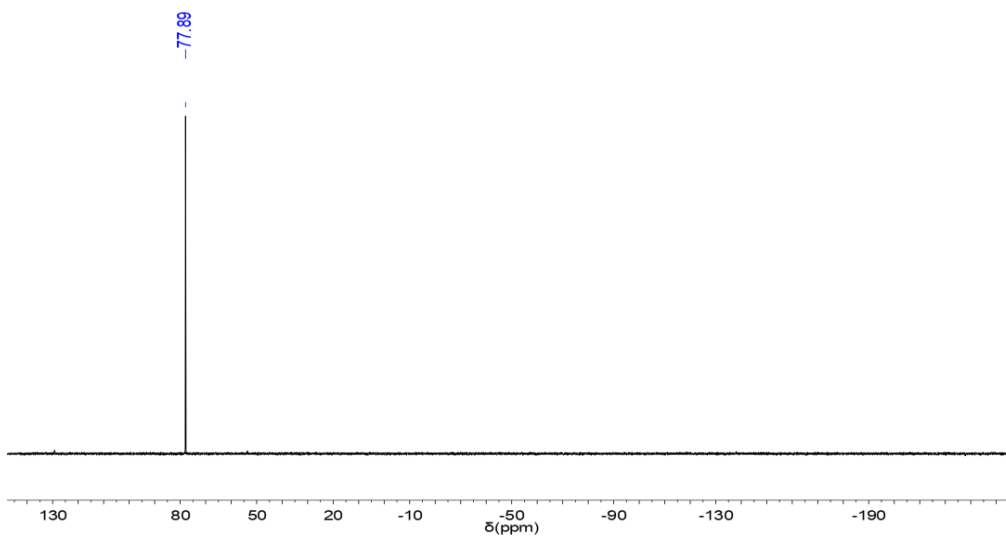
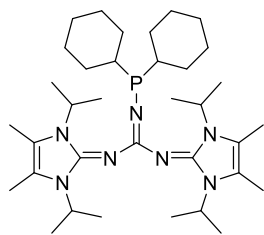
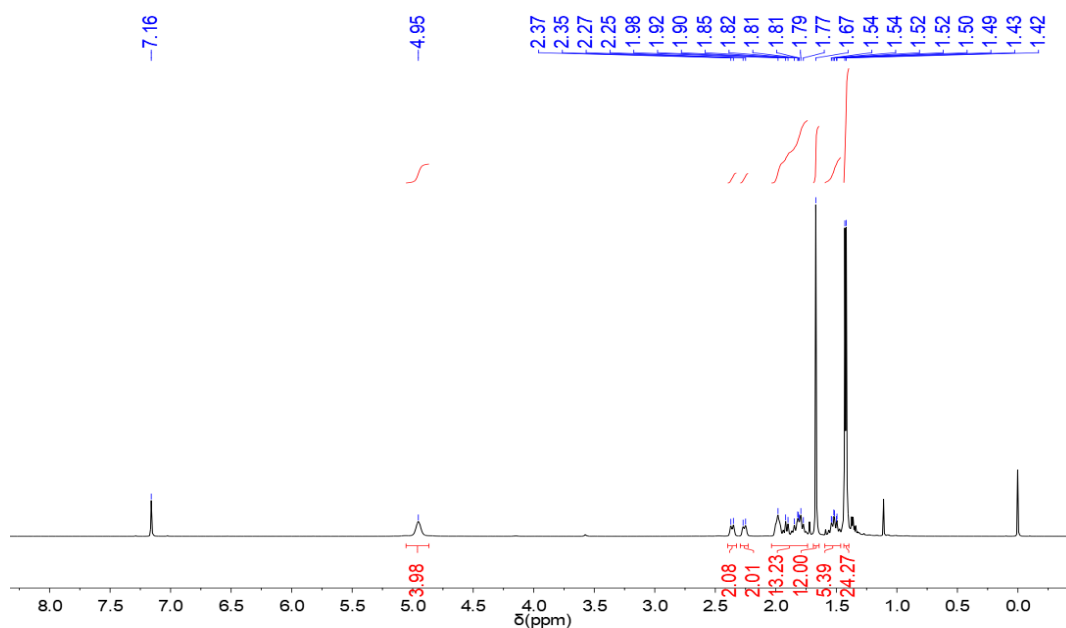


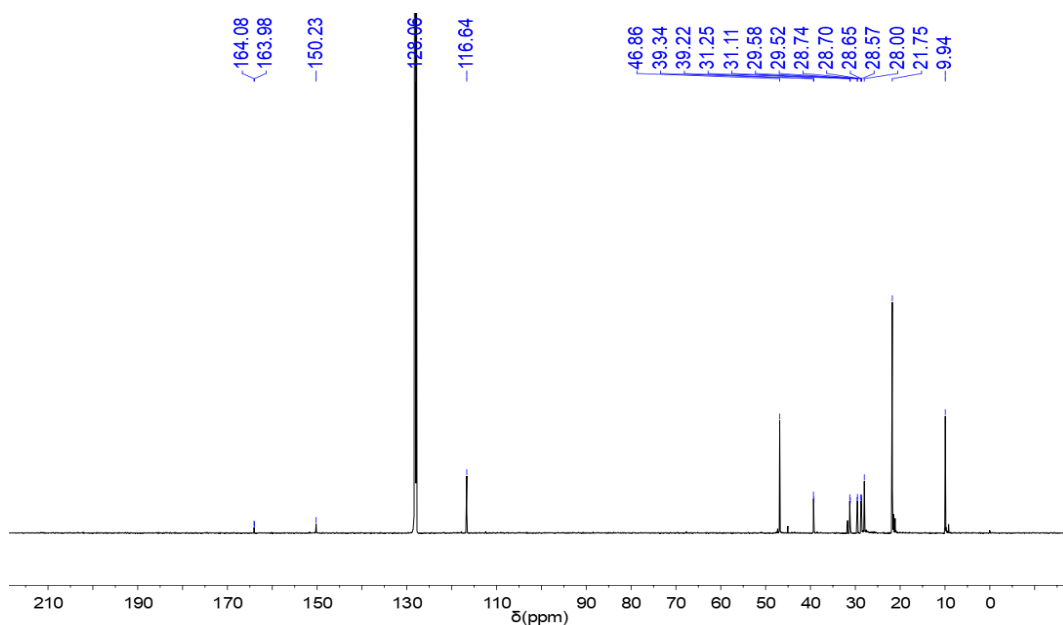
Figure S9.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P2** in  $\text{C}_6\text{D}_6$ .



**BIG-P3** (yellowish solid, 180 mg, 82% yield).  $^1\text{H NMR}$  (600 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  4.95 (s, 4H), 2.36 (d,  $J = 12.8$  Hz, 2H), 2.26 (d,  $J = 12.4$  Hz, 2H), 1.98 – 1.77 (m, 13H), 1.67 (s, 12H), 1.54 – 1.49 (m, 5H), 1.42 (d,  $J = 7.0$  Hz, 24H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  164.0 (d,  $J = 14.9$  Hz), 150.2 (s), 116.6 (s), 46.9 (s), 39.3 (d,  $J = 17.7$  Hz), 31.2 (d,  $J = 20.4$  Hz), 29.6 (d,  $J = 8.9$  Hz), 28.7 (dd,  $J = 16.8, 8.8$  Hz), 28.0 (s), 21.8 (s), 9.9 (s).  $^{31}\text{P}\{^1\text{H}\}$  NMR (162 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  54.9 (s). **HRMS** (ESI):  $[\text{C}_{35}\text{H}_{63}\text{N}_7\text{P}]^+[\text{M}+\text{H}]^+$ : calcd. 612.4877, found 612.4867 m/z. **IR** (Film): 2982, 2933, 2855, 1566, 1513, 1448, 1367, 1252, 1216, 1114, 1056, 1012, 951, 853, 806, 716, 574  $\text{cm}^{-1}$ .

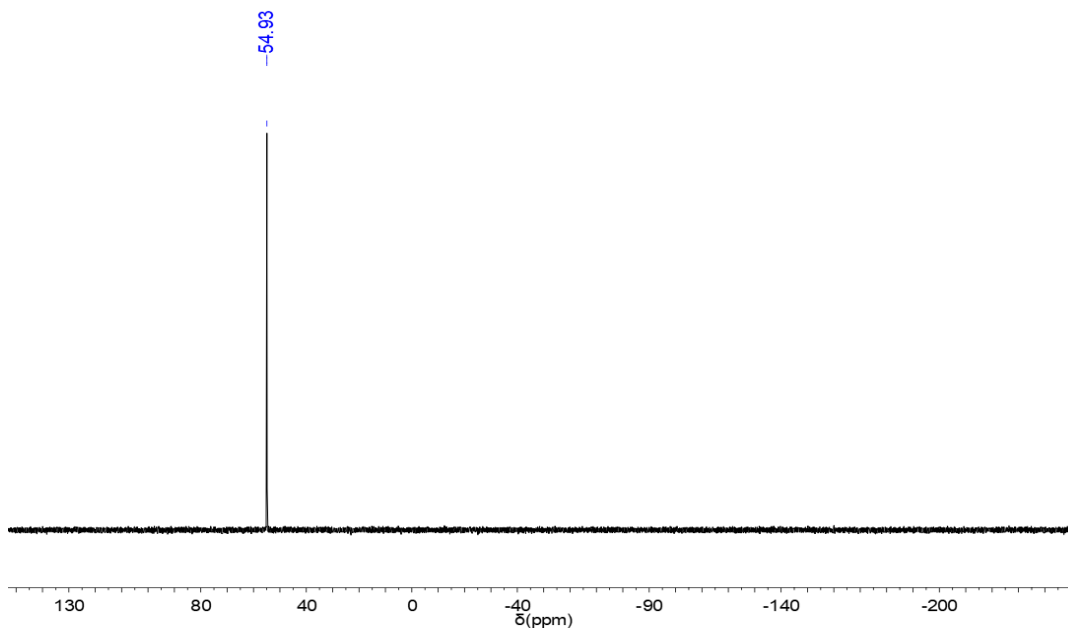


**Figure S10.**  $^1\text{H NMR}$  spectrum of **BIG-P3** in  $\text{C}_6\text{D}_6$ .

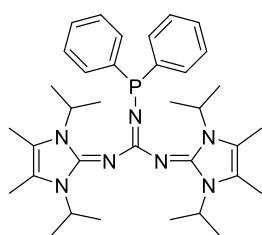


**Figure S11.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P3** in  $\text{C}_6\text{D}_6$ .

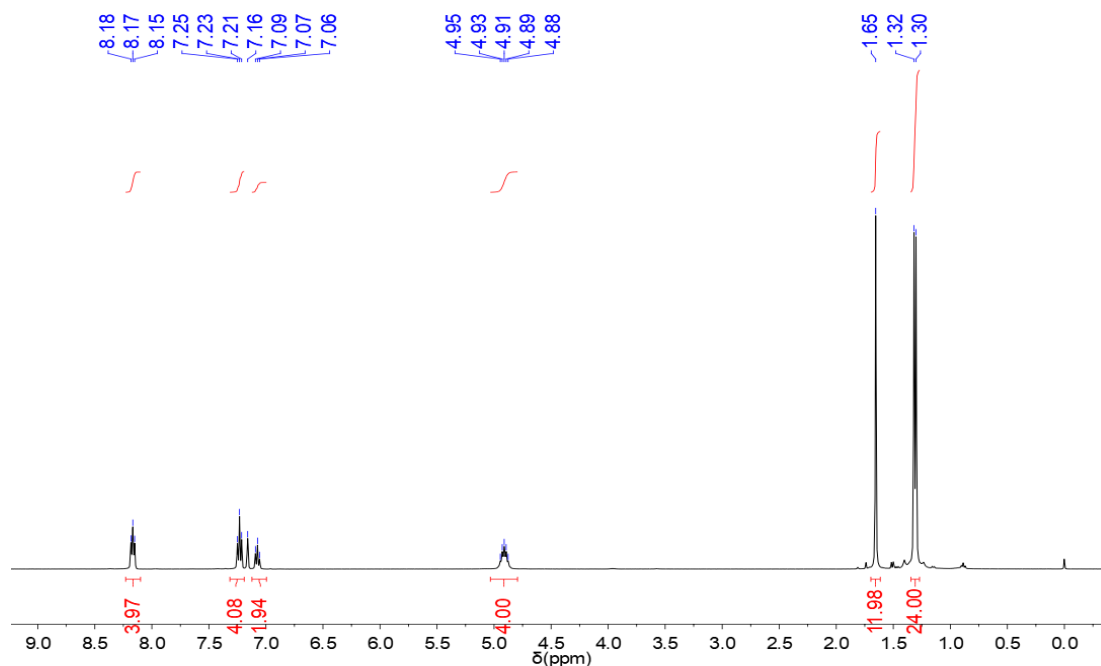




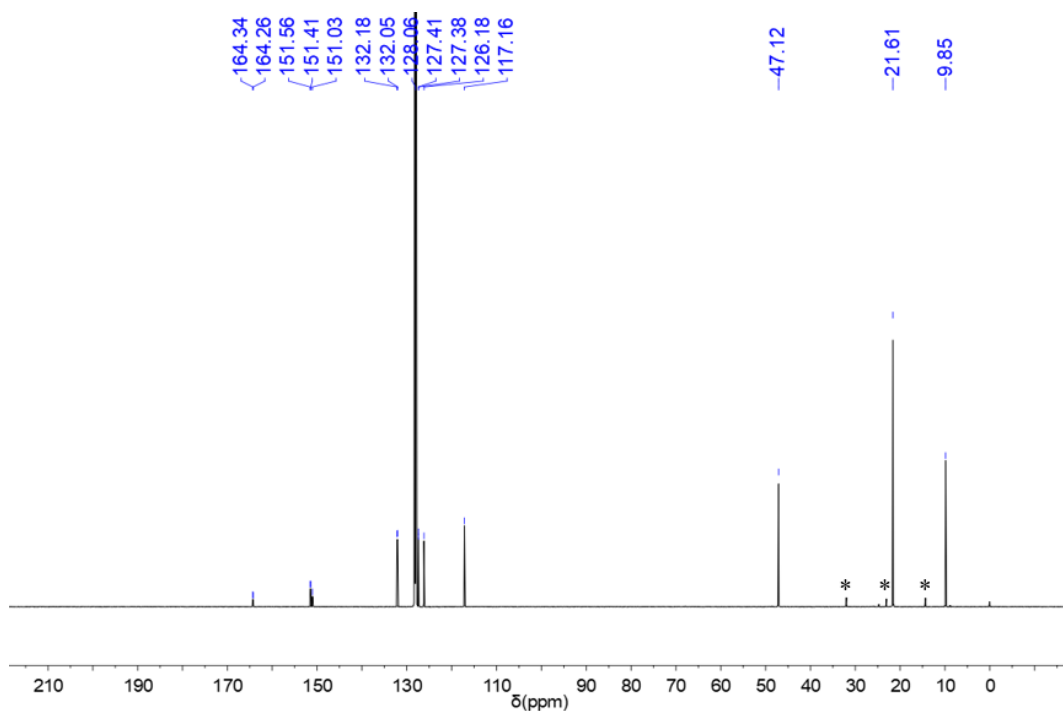
**Figure S12.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P3** in  $\text{C}_6\text{D}_6$ .



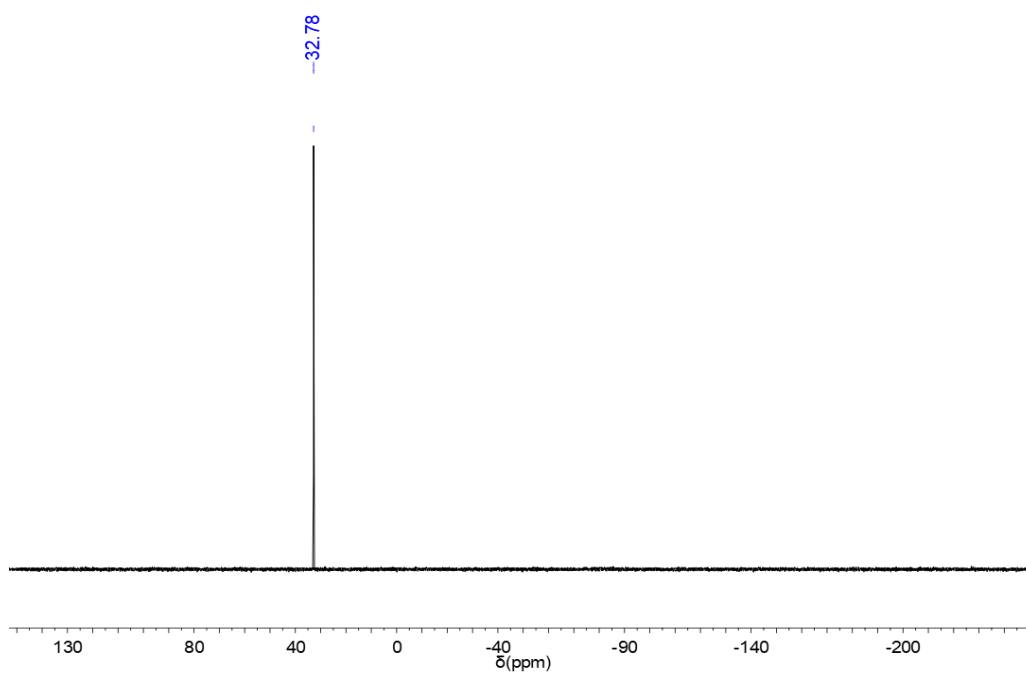
**BIG-P4** (orange red solid, 190 mg, 88% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  8.17 (t,  $J = 6.5$  Hz, 4H), 7.23 (t,  $J = 7.4$  Hz, 4H), 7.07 (t,  $J = 7.2$  Hz, 2H), 4.91 (dt,  $J = 13.7, 6.8$  Hz, 4H), 1.65 (s, 12H), 1.31 (d,  $J = 7.0$  Hz, 24H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  164.3 (d,  $J = 12.7$  Hz), 151.5 (d,  $J = 23.1$  Hz), 151.0 (s), 132.1 (d,  $J = 19.6$  Hz), 127.4 (d,  $J = 5.2$  Hz), 126.2 (s), 117.2 (s), 47.1 (s), 21.6 (s), 9.9 (s).  $^{31}\text{P}\{^1\text{H}\}$  NMR (162 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  32.8 (s). HRMS (ESI):  $[\text{C}_{35}\text{H}_{51}\text{N}_7\text{P}]^+[\text{M}+\text{H}]^+$ : calcd. 600.3938, found 600.3931 m/z. IR (Film): 3054, 2979, 2937, 1500, 1440, 1368, 1218, 1114, 997, 949, 914, 813, 733, 702, 585, 521  $\text{cm}^{-1}$ .



**Figure S13.**  $^1\text{H}$  NMR spectrum of **BIG-P4** in  $\text{C}_6\text{D}_6$ .



**Figure S14:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P4** in  $\text{C}_6\text{D}_6$ . \* denote n-hexane.



**Figure S15:**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P4** in  $\text{C}_6\text{D}_6$ .

## 5. Computational details for the electronic properties of BIG-Ps

### 5.1 Calculated TEP values of BIG-Ps

Geometry optimizations  $\text{PNi}(\text{CO})_3$  were performed using the Gaussian 16 package with the hybrid density functional B3LYP and the mixed basis set 6-31G(d) for C, N, O, P, H atoms and LANL2DZ for Ni atom. Based on the calculated infrared spectrum of nickel tricarbonyl phosphine complexes, the calculated TEP values were obtained by the following formula:

$$\text{Calculated TEP} = \nu(\text{CO}) \times \mathbf{A}$$

$\nu(\text{CO})$ : A1 symmetrical CO stretching frequency of nickel tricarbonyl phosphine complexes.

$\mathbf{A}$ : The fundamental vibrational frequency scale factor (0.9610).<sup>[S4]</sup>

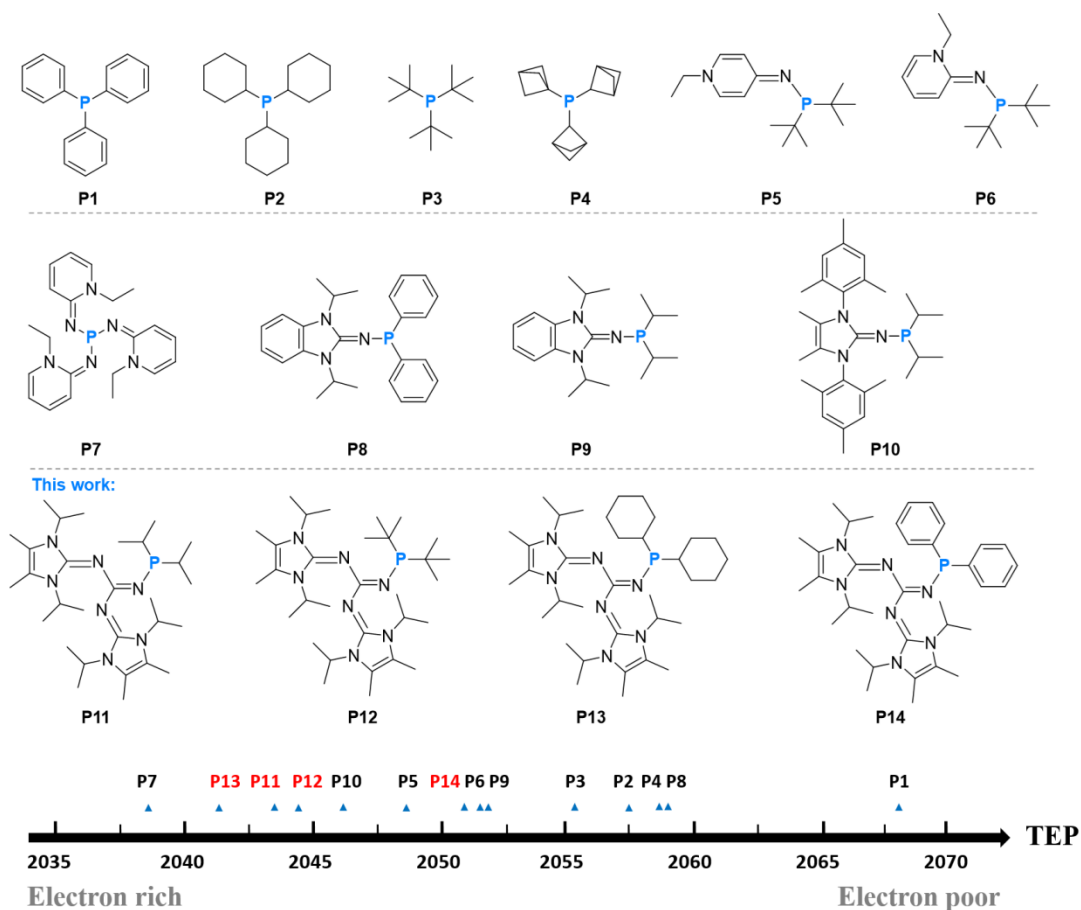
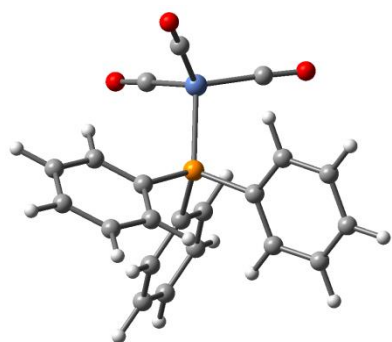


Figure S16. DFT-calculated TEP values of selected phosphines.

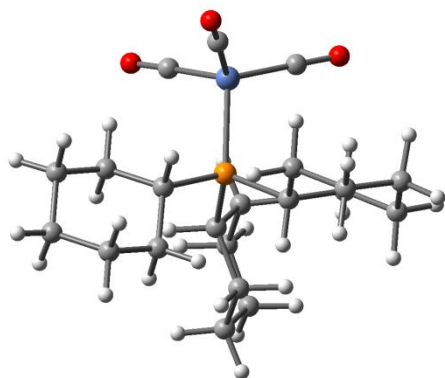
### Cartesian coordinates of PNi(CO)<sub>3</sub> complexes



#### P1

Ni	2.19024400	-0.00008100	-0.00019500
C	2.65722600	1.68796300	0.50128600
C	2.65676700	-1.27864700	1.21084800
C	2.65716100	-0.40963700	-1.71287800
O	2.91331700	2.76271200	0.82003000
O	2.91295200	-0.67050500	-2.80318800
O	2.91252700	-2.09231100	1.98208000
P	-0.09311400	0.00005500	-0.00045500
C	-0.86623800	1.57475000	-0.53589100
C	-0.24553500	2.29194200	-1.56955000
C	-2.04396100	2.07622700	0.03479400
C	-0.80132600	3.48243500	-2.03457600
H	0.67671000	1.91546800	-2.00259200
C	-2.59355200	3.27327400	-0.42676100
H	-2.52731400	1.53336500	0.84046300
C	-1.97576100	3.97627700	-1.46224200
H	-0.31295700	4.02904800	-2.83620100
H	-3.50412500	3.65695700	0.02489500
H	-2.40404300	4.90899800	-1.81805200
C	-0.86584700	-0.32323400	1.63118600
C	-2.04386700	-1.06768200	1.78073700
C	-0.24474000	0.21338200	2.76893100
C	-2.59337400	-1.26560800	3.04835600
H	-2.52751400	-1.49459800	0.90822400
C	-0.80045600	0.02174300	4.03259700
H	0.67783800	0.77604100	2.65929200
C	-1.97526900	-0.72010100	4.17461300
H	-3.50414800	-1.84821200	3.15518100
H	-0.31170000	0.44280300	4.90650400
H	-2.40352700	-0.87763000	5.16039700
C	-0.86642500	-1.25124200	-1.09598200

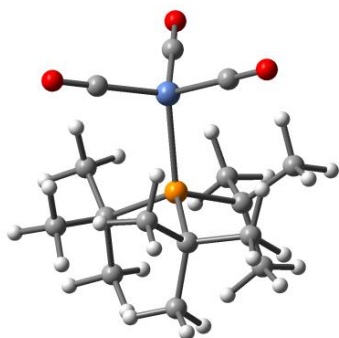
C	-2.04306900	-1.00791500	-1.81752400
C	-0.24650800	-2.50562200	-1.19754900
C	-2.59244600	-2.00722900	-2.62224700
H	-2.52573000	-0.03814400	-1.75326200
C	-0.80204600	-3.50456400	-1.99496500
H	0.67505200	-2.69189800	-0.65367000
C	-1.97555600	-3.25614900	-2.71043200
H	-3.50214100	-1.80817800	-3.18187500
H	-0.31421000	-4.47251900	-2.06544500
H	-2.40374000	-4.03139000	-3.33943800



**P2**

Ni	0.52953500	-0.96809900	1.90754100
C	-0.57028800	-0.27000400	3.17633400
C	0.23060200	-2.73072500	1.58322700
C	2.26520100	-0.54272600	2.24171200
O	-1.27067100	0.19628500	3.96255800
O	3.35836400	-0.25441400	2.46014600
O	0.01282700	-3.83221500	1.32606000
P	-0.08799500	0.01556500	-0.08435100
C	1.06056900	-0.31558000	-1.52005600
C	2.48711100	0.17901500	-1.21619300
C	1.08862400	-1.81285100	-1.88019900
H	0.68252200	0.23835500	-2.38933600
C	3.43372100	-0.08403200	-2.39526000
H	2.86169500	-0.34465400	-0.32929600
H	2.48529800	1.24603900	-0.96937400
C	2.04218600	-2.08786000	-3.05223700
H	1.41258600	-2.38535800	-1.00133200
H	0.08517300	-2.16925000	-2.13671000
C	3.45688300	-1.57210400	-2.76383500
H	4.44298500	0.26456100	-2.14457900
H	3.10344200	0.50261500	-3.26507400

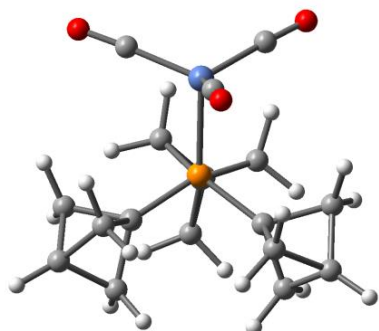
H	2.06231300	-3.16331500	-3.26687600
H	1.65331400	-1.59366100	-3.95462500
H	4.10887000	-1.74286000	-3.62916000
H	3.88514800	-2.14250000	-1.92705200
C	-0.33014800	1.87919200	-0.05402800
C	0.54448600	2.54220100	1.02870600
C	-0.15792200	2.61083400	-1.39943700
H	-1.37758700	1.99805100	0.26077900
C	0.23238200	4.03890500	1.16078100
H	1.60482500	2.41023700	0.77332300
H	0.39539700	2.03793800	1.98757000
C	-0.48753100	4.10493200	-1.26065100
H	0.88054300	2.51110100	-1.73908800
H	-0.78450200	2.16163300	-2.17497600
C	0.37466800	4.76852600	-0.18037700
H	0.88887500	4.49010500	1.91474200
H	-0.79720600	4.15703800	1.52930300
H	-0.34686800	4.60669700	-2.22615000
H	-1.54984400	4.21703500	-0.99893400
H	0.10387400	5.82582800	-0.07173600
H	1.42804900	4.74333600	-0.49574900
C	-1.72989200	-0.67188200	-0.66717000
C	-2.82490300	-0.49500400	0.40100000
C	-2.23572600	-0.18782400	-2.03646500
H	-1.53213300	-1.75080300	-0.73905600
C	-4.11586300	-1.22135800	-0.00395500
H	-3.04093800	0.57448000	0.53562600
H	-2.47021800	-0.87055300	1.36507400
C	-3.51675600	-0.93133100	-2.44426600
H	-2.45460600	0.88632500	-1.98178000
H	-1.46660800	-0.31732800	-2.80628700
C	-4.61247700	-0.77097500	-1.38331900
H	-4.88952000	-1.05399600	0.75525600
H	-3.92276600	-2.30362300	-0.02348000
H	-3.86772800	-0.56473700	-3.41691200
H	-3.28701900	-1.99891200	-2.57335400
H	-5.50741000	-1.33643400	-1.67020200
H	-4.91073200	0.28657200	-1.33245300



**P3**

Ni	-1.72698300	0.00007500	0.00014100
C	-2.25711900	-0.21041700	-1.72531000
C	-2.25743000	-1.38895500	1.04507600
C	-2.25721000	1.59967600	0.68044200
O	-2.59925700	-0.35254100	-2.81601500
O	-2.59948200	2.61535100	1.10251600
O	-2.59985400	-2.26249300	1.71333600
P	0.61867900	-0.00007100	0.00019400
C	1.30777900	1.19245000	-1.35238700
C	1.30802500	0.57490000	1.70905500
C	1.11784700	2.09702000	1.86876700
H	0.08765900	2.40384500	1.67620300
H	1.35001100	2.36424500	2.90724300
H	1.78242700	2.68092100	1.23034300
C	2.78907100	0.24564900	1.97245300
H	2.97440600	-0.82834900	2.03032800
H	3.45383300	0.66591600	1.21566400
H	3.07920900	0.67460000	2.94047900
C	0.44405100	-0.06855700	2.81650500
H	0.48053500	-1.15702400	2.81957700
H	0.81186400	0.27764400	3.79089600
H	-0.60153600	0.23357900	2.72252200
C	2.78842300	1.58617400	-1.19820000
H	2.97265200	2.17400600	-0.29725400
H	3.45352200	0.72097700	-1.18253800
H	3.07890500	2.20958600	-2.05390300
C	0.44300100	2.47275500	-1.34963100
H	0.47726000	3.01920100	-0.40818500
H	0.81182200	3.14417700	-2.13559600
H	-0.60200500	2.23970700	-1.56640900
C	1.11865900	0.56964000	-2.75059600
H	1.35092400	1.33559300	-3.50099900

H	1.78368700	-0.27486600	-2.93692000
H	0.08866900	0.24917300	-2.92077600
C	1.30772900	-1.76759500	-0.35661900
C	0.44308900	-2.40483400	-1.46716200
H	0.47850000	-1.86305400	-2.41123600
H	0.81105900	-3.42162700	-1.65507700
H	-0.60220400	-2.47488400	-1.15761900
C	1.11821400	-2.66745600	0.88149000
H	0.08805100	-2.65472400	1.24355500
H	1.35070500	-3.70020300	0.59317900
H	1.78284700	-2.40673800	1.70642400
C	2.78850400	-1.83085700	-0.77432000
H	3.07891000	-2.88360300	-0.88673600
H	2.97306700	-1.34411500	-1.73358700
H	3.45352000	-1.38511800	-0.03249100

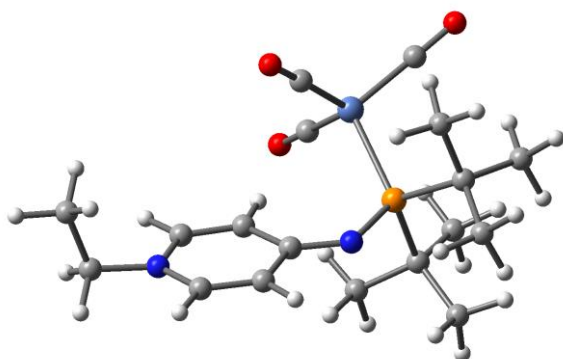


**P4**

P	0.29804100	-0.00003000	-0.00024300
C	1.06639500	0.30473000	1.63158700
C	2.54945000	0.60195800	2.03352900
H	3.26531100	-0.21297500	1.89161300
H	2.95925300	1.55990100	1.69948200
C	0.65445900	1.43815100	2.62185800
H	0.91916600	2.45872200	2.32848600
H	-0.36520700	1.38289500	3.01397400
C	1.01400300	-0.66423200	2.85554200
H	1.61307100	-1.57671000	2.77563300
H	0.02174200	-0.86852900	3.26740200
C	1.74291500	0.61130500	3.35989300
H	2.13672100	0.78970400	4.36433700
C	1.06591800	1.25906000	-1.08225100
C	0.65137600	1.55003400	-2.55822800
H	-0.36816700	1.91837400	-2.70454500
H	0.91377300	0.78516400	-3.29566600



C	2.54835400	1.45669100	-1.54370800
H	3.26618400	1.74065700	-0.76861000
H	2.95591200	0.68773300	-2.20689500
C	1.01573700	2.80361300	-0.85549400
H	0.02387400	3.26341400	-0.88269000
H	1.61673600	3.19026600	-0.02652900
C	1.74177100	2.60139500	-2.21369300
H	2.13521300	3.38139000	-2.87143200
C	1.06020800	-1.56857900	-0.55179700
C	0.64263500	-2.99095600	-0.06449400
H	0.90697700	-3.24778500	0.96594700
H	-0.37854000	-3.29867100	-0.30747400
C	1.00459100	-2.14438500	-2.00260600
H	1.60540800	-1.62160500	-2.75335200
H	0.01104100	-2.39481400	-2.38480000
C	2.54122600	-2.07138300	-0.49602200
H	3.25885300	-1.54433200	-1.13154800
H	2.95081100	-2.26216600	0.50049000
C	1.72948900	-3.22163700	-1.15013600
H	2.11911500	-4.18247300	-1.49769900
Ni	-1.97259300	0.00330500	0.00152200
C	-2.41996500	-1.10840300	1.36959900
C	-2.41747500	1.74450200	0.28107300
C	-2.42183900	-0.62465300	-1.64507200
O	-2.64288300	-1.81726300	2.24905200
O	-2.64597100	-1.03153900	-2.69855900
O	-2.63874100	2.86085900	0.45543500

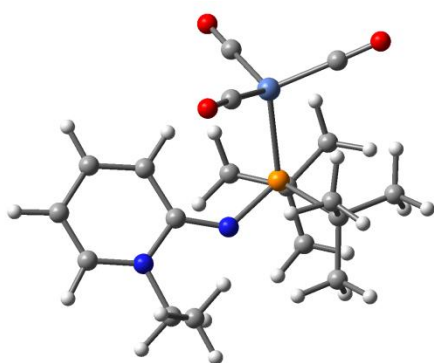


**P5**

P	1.08080000	0.68083600	-0.00412800
N	-0.37352500	1.51238300	-0.30446900
C	-1.59143300	1.09637000	-0.07281300
C	-3.99091800	1.55914400	-0.34969000
H	-4.82122000	2.16244000	-0.70009200

C	-3.33589000	-0.41306100	0.76517100
H	-3.66487100	-1.31615800	1.26838000
C	-2.02040800	-0.10803400	0.61832600
H	-1.28260200	-0.78642300	1.01874300
Ni	1.11724200	-1.66140900	-0.09570200
C	-0.13977600	-1.98827800	-1.37178500
C	2.79146500	-2.17626300	-0.58105700
C	0.69898700	-2.34406500	1.52687900
O	-0.94746000	-2.13758200	-2.17922200
O	0.42675600	-2.78352100	2.55900500
O	3.85149800	-2.52236100	-0.87107700
C	2.11676400	1.45251200	-1.40674400
C	1.69050300	0.68929100	-2.67809100
H	2.19955700	1.12189900	-3.54877800
H	1.95113900	-0.37066500	-2.62276500
H	0.61069900	0.76886100	-2.84303800
C	3.61933300	1.24180300	-1.17241100
H	4.16951500	1.50983200	-2.08348700
H	3.99839200	1.87566100	-0.36527000
H	3.86161600	0.20217500	-0.93632900
C	1.82592700	2.94551800	-1.63636200
H	2.21613200	3.57528300	-0.83523200
H	2.30971000	3.26160400	-2.56992200
H	0.75157300	3.12053100	-1.71726600
C	1.63284000	1.36350800	1.68626600
C	2.89532600	0.62122700	2.15467400
H	3.75350700	0.80895100	1.50516800
H	3.16196500	0.95867200	3.16487600
H	2.73071800	-0.45952000	2.18966600
C	0.48920400	1.05545700	2.67106300
H	0.78719800	1.37539900	3.67762900
H	-0.42638300	1.59081400	2.40476000
H	0.26646300	-0.01353600	2.71894100
C	1.87106200	2.88018100	1.68648800
H	2.00493800	3.22834200	2.71945800
H	2.77307900	3.15223700	1.13221600
H	1.02051900	3.41444400	1.25325900
N	-4.33927000	0.39928900	0.30217800
C	-5.73784800	-0.03745100	0.35382600
H	-5.86987900	-0.61871900	1.27144600

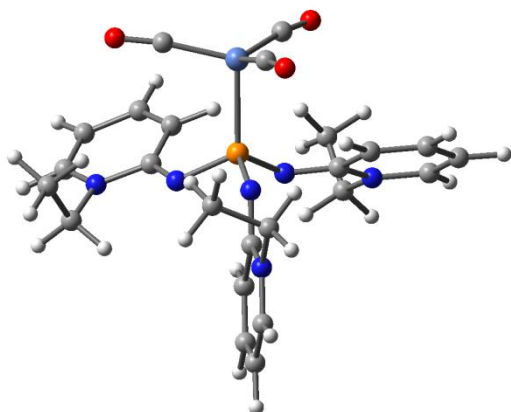
H	-6.36191900	0.85677400	0.44668600
C	-6.13832100	-0.85756700	-0.87253300
H	-7.18620200	-1.16689200	-0.79677000
H	-6.01620600	-0.27132000	-1.78908600
H	-5.51761600	-1.75524500	-0.95877200
C	-2.69586600	1.91986300	-0.53358700
H	-2.45707900	2.84653700	-1.04216400



**P6**

P	0.53101900	0.64466900	0.27799700
N	-3.38552000	0.15086800	0.11328600
N	-1.16119100	0.75884700	0.22191600
C	-3.70244100	1.56157600	-0.16034100
H	-3.01639100	2.16329400	0.43631400
H	-4.72386400	1.73871100	0.18880200
C	-2.03174800	-0.21007000	0.28310300
C	-4.40171100	-0.76047900	0.13934600
H	-5.39267400	-0.34659400	-0.00925300
C	-3.56337700	1.89631900	-1.64370000
H	-4.25259900	1.29588600	-2.24740400
H	-2.54270300	1.70036300	-1.97985500
H	-3.78749600	2.95492700	-1.81341900
C	-4.18450800	-2.09208900	0.34036800
H	-5.01665000	-2.78455800	0.35976400
C	-2.84353400	-2.51891000	0.52897800
H	-2.62892100	-3.57128100	0.69354300
C	-1.81754300	-1.61754300	0.51274500
H	-0.79622100	-1.93718700	0.65352600
Ni	1.58294700	-1.25521000	-0.59202800
C	0.45740800	-1.68208000	-1.95967600
C	3.24456100	-0.77037600	-1.14509500
C	1.70460100	-2.53650900	0.68365800
O	-0.29188000	-1.89467600	-2.80755300
O	1.78628700	-3.35599900	1.49134000

O	4.30717900	-0.48332800	-1.48549300
C	0.94557100	2.19868500	-0.74498800
C	0.77533600	1.76970500	-2.21716700
H	0.91687700	2.64106500	-2.86899000
H	1.50309100	1.00684400	-2.50400000
H	-0.22624100	1.36757500	-2.40318100
C	2.39907600	2.64143500	-0.52082100
H	2.66749300	3.39553900	-1.27158000
H	2.54004800	3.09766500	0.46332500
H	3.10514700	1.81301200	-0.62119400
C	-0.00217100	3.38220600	-0.48740200
H	0.10786500	3.79910000	0.51454800
H	0.22505100	4.18103100	-1.20544700
H	-1.04273100	3.08327900	-0.61960000
C	0.93056000	0.93694500	2.11759000
C	2.43801700	0.74519000	2.35407600
H	3.04011600	1.50157300	1.84557100
H	2.64939900	0.81907300	3.42875100
H	2.77146600	-0.23776500	2.00922000
C	0.17229500	-0.15068000	2.90182100
H	0.42312800	-0.06455900	3.96656300
H	-0.91102000	-0.03970400	2.80233500
H	0.44961300	-1.15748300	2.57961400
C	0.47586200	2.30760600	2.63783600
H	0.57453200	2.33476700	3.73111100
H	1.08474900	3.12172100	2.23611400
H	-0.57206700	2.49797900	2.38690100

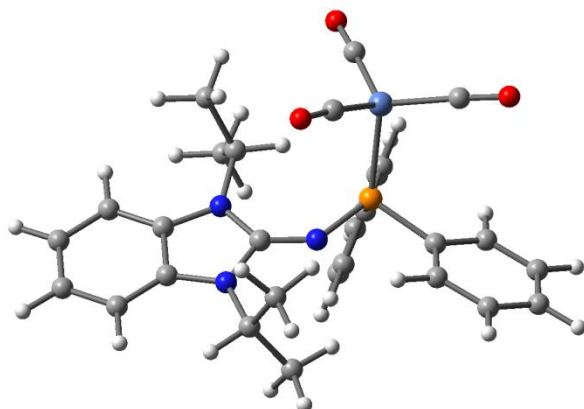


**P7**

P	-0.02003400	-0.09816100	0.23934100
N	1.20686200	-1.25631100	0.33243700
N	1.65164900	2.92317300	-1.64034600

N	-1.26448900	-0.91180900	-0.56372400
N	0.43430700	1.10274100	-0.88469600
N	2.67745700	-2.87889600	-0.38124900
C	1.68050400	-1.92968100	-0.67877600
N	-3.42433700	-1.23618000	-1.31860000
C	0.56245200	3.18911900	-2.59155200
H	0.15528900	2.22062100	-2.88287900
H	1.00232900	3.67268300	-3.46927400
C	1.49743800	1.84162300	-0.74696800
C	-2.81667500	1.00882500	-0.70738700
H	-2.06645500	1.69961400	-0.34998100
C	-2.41700500	-0.37385200	-0.83788600
C	2.71707300	3.77346700	-1.58936800
H	2.70915200	4.56409200	-2.33166100
C	-0.52579100	4.05983100	-1.96596400
H	-0.13736200	5.05121500	-1.70820900
H	-0.90213600	3.59305300	-1.05346700
H	-1.35921700	4.18385600	-2.66595800
C	-3.11454100	-2.67257800	-1.39167800
H	-2.09090400	-2.75990000	-1.75887800
H	-3.79662200	-3.11552000	-2.12382000
C	3.71668300	3.63716100	-0.67083800
H	4.54961500	4.32910000	-0.66439500
C	3.24416900	-3.67288100	-1.33421900
H	3.99174800	-4.36848800	-0.96969500
C	2.89467900	-3.59119000	-2.65129000
H	3.37031000	-4.23371500	-3.38190900
C	3.61969700	2.56629200	0.25989200
H	4.39542100	2.43247900	1.00909300
C	2.56458000	1.70087600	0.21934800
H	2.48965500	0.87225400	0.91132000
C	3.06760600	-3.04362400	1.03109300
H	3.12236800	-2.04678500	1.46940600
H	4.06459200	-3.49403100	1.03791400
C	-5.04957700	0.50727900	-1.49897600
H	-6.05389600	0.81707900	-1.75973800
C	1.90631400	-2.63760700	-3.01744200
H	1.61256800	-2.54259400	-4.05960400
C	1.32532300	-1.83662600	-2.07537000
H	0.57396600	-1.10408600	-2.33632900

C	-4.67858800	-0.79988100	-1.62827200
H	-5.35770900	-1.56721900	-1.98310200
C	-4.07920400	1.42721800	-1.01542200
H	-4.34337900	2.47414100	-0.89204800
C	2.06641100	-3.89601500	1.80701900
H	1.98552500	-4.90055800	1.37654600
H	1.08539500	-3.41646600	1.79074700
H	2.38991400	-3.98856300	2.84916500
C	-3.24780800	-3.34755000	-0.02773800
H	-2.99718700	-4.41089100	-0.11061200
H	-4.27037000	-3.26039300	0.35520600
H	-2.56473800	-2.88153700	0.68566700
Ni	-0.51901700	0.69677400	2.31752200
C	-0.51392200	2.48723000	2.05720600
C	-2.13986600	-0.06055800	2.62618300
C	0.87691300	-0.00379600	3.24625600
O	-0.49356400	3.59344700	1.72476900
O	1.82035600	-0.49808600	3.68971500
O	-3.15631900	-0.60213800	2.68825400

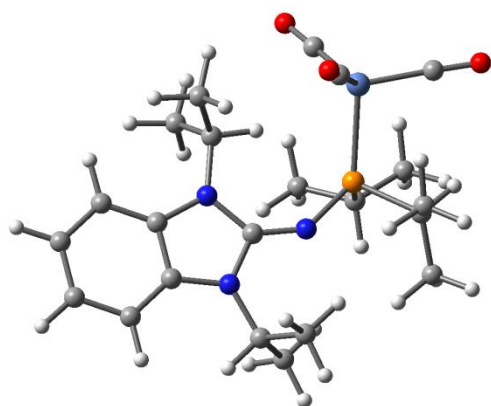


### P8

C	-1.50215100	0.66038400	-0.00033900
C	-3.74401100	1.08351300	0.00887000
C	-5.01251300	1.65393000	0.01837500
H	-5.15155600	2.72945600	0.00557100
C	-6.11461200	0.79244300	0.04427400
H	-7.11543600	1.21288200	0.05221500
C	-5.94440600	-0.59457700	0.06117700
H	-6.81402200	-1.24394100	0.08211100
C	-4.66752600	-1.16814400	0.05338100
H	-4.55139900	-2.24392300	0.07057000
C	-3.56864500	-0.31432100	0.02563100
C	-2.20272300	3.09818900	-0.06504300

H	-3.19141800	3.56472600	-0.04030800
C	-1.43263700	3.57844300	1.16993500
H	-1.96567900	3.29592900	2.08421100
H	-1.34785300	4.67039500	1.14641000
H	-0.43100100	3.14814900	1.20121300
C	-1.53850500	3.47423900	-1.39382800
H	-0.58269000	2.95961800	-1.50647700
H	-1.36767700	4.55538000	-1.43477600
H	-2.17990500	3.19249400	-2.23514300
C	-1.57342900	-1.87451800	-0.20350600
H	-0.50571000	-1.68187400	-0.27110000
C	-1.79743200	-2.81656600	0.98147800
H	-1.48295500	-2.34161500	1.91368700
H	-1.19602400	-3.71966500	0.83771000
H	-2.84412900	-3.11892400	1.07922500
C	-1.99949200	-2.46635200	-1.55106600
H	-3.06927500	-2.68912800	-1.58438500
H	-1.45036400	-3.39515800	-1.72947500
H	-1.76821300	-1.76962200	-2.36169700
C	2.20888300	2.67727800	0.10909800
H	1.30575300	2.94533600	-0.42583200
C	3.19035800	3.63630800	0.36284500
H	3.04569200	4.65774600	0.02130500
C	4.35303900	3.28650400	1.05090000
H	5.11712900	4.03331500	1.24707700
C	4.53143800	1.97063900	1.48414700
H	5.43340600	1.69137400	2.02158700
C	3.55210000	1.01123900	1.23251400
H	3.69557900	-0.00852700	1.57851900
C	2.37904800	1.35978400	0.54947800
C	1.06702800	-0.89610400	1.67947500
C	0.35344900	-0.37951800	2.77059400
H	-0.12588900	0.59091700	2.68213400
C	0.25335400	-1.11017200	3.95308000
H	-0.30413800	-0.70652400	4.79386400
C	0.86932500	-2.36117400	4.05789700
H	0.78734100	-2.93151800	4.97882900
C	1.58631700	-2.87694800	2.97800100
H	2.06414800	-3.84956200	3.05448500
C	1.68119000	-2.14778400	1.79059700

H	2.22488200	-2.55336500	0.94318000
N	-0.24315700	0.95214300	0.03173300
N	-2.47638100	1.65447900	-0.01069500
N	-2.19029900	-0.55655600	0.01215900
P	1.16614300	0.05697200	0.10668100
Ni	1.79647100	-1.03841100	-1.80731400
C	3.55876800	-0.58445500	-1.99662500
C	1.50809500	-2.81452300	-1.62860100
C	0.65505100	-0.22129400	-2.96366600
O	4.66452000	-0.27840900	-2.05791400
O	-0.13845600	0.32920000	-3.59046100
O	1.28028200	-3.93361400	-1.46499300



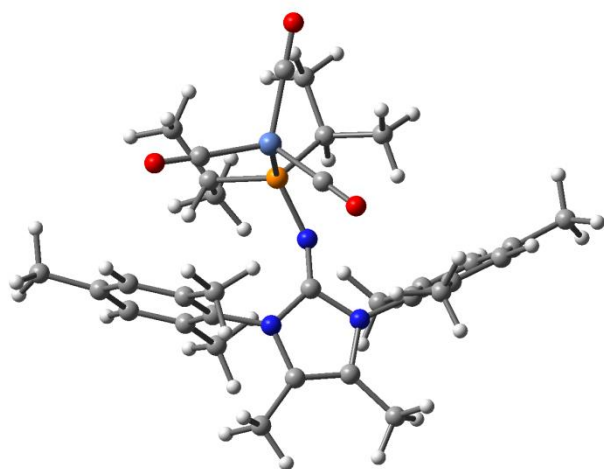
### P9

C	-1.44440500	0.46052800	0.02423000
C	-3.71904100	0.26135500	-0.14058700
C	-5.08871300	0.46663900	-0.27162900
H	-5.50633000	1.46101800	-0.38561700
C	-5.92168600	-0.65726300	-0.25812600
H	-6.99416500	-0.52309000	-0.35942500
C	-5.39259400	-1.94333200	-0.12130100
H	-6.05669000	-2.80201500	-0.11882300
C	-4.01470600	-2.14938600	0.01226700
H	-3.62082700	-3.15196400	0.11290300
C	-3.18353600	-1.03234100	0.00700300
C	-2.79423500	2.61278100	-0.16515400
H	-3.87179100	2.77792000	-0.24740700
C	-2.32713000	3.24767400	1.14893500
H	-2.88701700	2.83139000	1.99312400
H	-2.49791500	4.32928500	1.12159500
H	-1.26458400	3.06116100	1.30977500
C	-2.13858000	3.21421200	-1.41053800
H	-1.06015800	3.06007000	-1.39062500



H	-2.34236600	4.28966600	-1.45501900
H	-2.54037800	2.74854800	-2.31642500
C	-0.84531100	-1.99979500	0.24174100
H	0.12885900	-1.52247700	0.32121400
C	-1.07777900	-2.82027100	1.51542300
H	-1.14092300	-2.17078900	2.39209100
H	-0.23733100	-3.50606200	1.65715700
H	-1.99321500	-3.41546600	1.46633500
C	-0.82881300	-2.86170500	-1.02404100
H	-1.76601400	-3.41008000	-1.15680100
H	-0.01336800	-3.58891000	-0.95965200
H	-0.66525400	-2.24342800	-1.90968700
N	-0.31437500	1.08206400	0.06219200
N	-2.64997800	1.15047800	-0.12929900
N	-1.79740100	-0.89100200	0.11969900
P	1.32404400	0.78098200	0.28407200
Ni	2.59776000	-0.99842500	-0.52301500
C	4.26550000	-0.26826400	-0.56067800
C	2.50670900	-2.39994600	0.61983100
C	1.97085600	-1.32356600	-2.19677300
O	5.30768300	0.22092400	-0.56344700
O	1.57775100	-1.47956300	-3.26805600
O	2.43731200	-3.29197100	1.34842300
C	2.06481900	2.34160900	-0.44069800
H	3.13841600	2.24023900	-0.23749500
C	1.52426000	1.04621300	2.12635800
H	1.05666700	2.01370600	2.34558000
C	0.77072700	-0.03420000	2.90626100
H	1.17190600	-1.03059000	2.69288200
H	0.86718500	0.13845900	3.98490900
H	-0.29569300	-0.03065500	2.66142200
C	3.00449700	1.09109500	2.52053900
H	3.54654200	1.89394800	2.01065300
H	3.10238500	1.25635000	3.60020800
H	3.50036000	0.14502000	2.27895800
C	1.87169500	2.33623500	-1.96304900
H	2.32940700	3.22783100	-2.40753500
H	2.32966900	1.45498100	-2.42080400
H	0.80837300	2.33625300	-2.22341400
C	1.56490100	3.64785300	0.18281400

H	2.02750800	4.50431800	-0.32284400
H	0.48138600	3.74231200	0.07945800
H	1.81313400	3.72158500	1.24616700

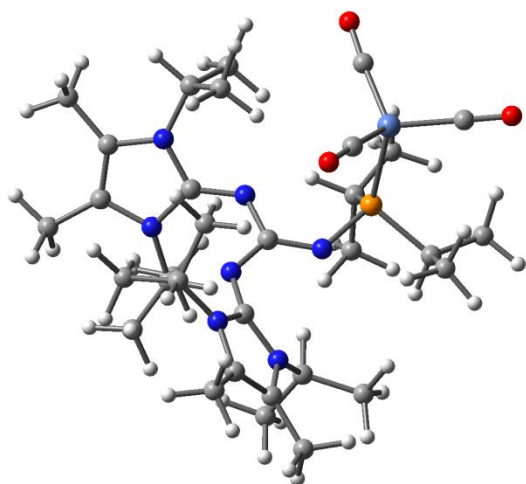


**P10**

C	1.45905832	-0.78145813	5.75511050
H	1.91247432	-1.63011213	5.23485350
C	2.53168032	0.31008687	5.85308850
H	2.86367532	0.63671087	4.86465550
H	3.40518032	-0.07954213	6.39134750
H	2.17879632	1.19223787	6.39441150
C	0.99686532	-1.25715613	7.13584250
H	0.64592932	-0.42058813	7.75033850
H	1.82520332	-1.73732813	7.67180650
H	0.18104632	-1.98077413	7.05537550
C	-1.13472068	0.69637087	5.61634950
H	-1.46116268	0.03874787	6.43244550
C	-2.35926268	1.03159587	4.75425950
H	-2.08207468	1.69677387	3.92829450
H	-3.11849568	1.54263787	5.35950950
H	-2.80682868	0.12787087	4.33460650
C	-0.50979068	1.96264587	6.20883450
H	0.23305632	1.73778487	6.97866750
H	-1.28935368	2.57849287	6.67417950
H	-0.02692168	2.57471187	5.44137850
C	-1.07745168	-2.81469413	3.89417350
C	-2.20148768	-4.63269613	3.03575650
C	-3.39710568	-5.44654213	2.67960650
H	-4.08097968	-5.53453513	3.53210550
H	-3.09529568	-6.45305113	2.37906250
H	-3.96654968	-5.00513413	1.85357950

C	-0.87562568	-4.90152813	2.94093550
C	-0.14573768	-6.09923213	2.44039250
H	0.46772232	-5.86502513	1.56146250
H	-0.85299168	-6.88234013	2.15595850
H	0.52863332	-6.50884613	3.20211650
C	-3.54369568	-2.65091313	3.86000650
C	-3.99489368	-2.55198213	5.18803150
C	-5.15765668	-1.82447813	5.43794150
H	-5.51255868	-1.73696013	6.46240250
C	-5.87135168	-1.19979213	4.40838950
C	-5.40162368	-1.33062913	3.10125850
H	-5.94282468	-0.85035013	2.28926450
C	-4.23814068	-2.04908513	2.80157350
C	-3.22328468	-3.18752513	6.31394650
H	-2.93735668	-4.21840613	6.07676450
H	-3.81100168	-3.19526413	7.23643950
H	-2.29763468	-2.62778413	6.49021050
C	-7.10032368	-0.37912913	4.71460150
H	-6.82436068	0.61696187	5.08442350
H	-7.71560168	-0.85238313	5.48778150
H	-7.72056268	-0.23862613	3.82386550
C	-3.76473668	-2.15692813	1.37417750
H	-3.96608168	-1.23106213	0.82842750
H	-4.28402168	-2.96696013	0.84495350
H	-2.69353168	-2.35318313	1.31411150
C	1.20944732	-3.76444413	3.76643850
C	2.13693332	-3.31354413	2.81772550
C	3.48019532	-3.24576713	3.19752750
H	4.20781532	-2.86928113	2.48422650
C	3.90456832	-3.63136013	4.47315550
C	2.95672932	-4.13125813	5.37258950
H	3.27565432	-4.45646713	6.35998550
C	1.60280732	-4.20748213	5.03886850
C	1.69697532	-2.94227313	1.42543850
H	0.85497032	-2.24740413	1.44560850
H	1.37327232	-3.82926413	0.86683950
H	2.51300932	-2.47389913	0.87073850
C	5.35126732	-3.48534313	4.87645150
H	5.61003432	-4.16337913	5.69597150
H	5.55827832	-2.46232113	5.21646550

H	6.02403532	-3.68911913	4.03688850
C	0.58257932	-4.74122413	6.01155050
H	0.07722632	-5.62941213	5.61329950
H	-0.19555068	-3.99982113	6.21550750
H	1.05354132	-5.01330713	6.96005350
N	-0.91569868	-1.71566113	4.54037350
N	-2.32660468	-3.35068313	3.59917350
N	-0.18120068	-3.77852813	3.44291450
P	0.04071632	-0.35444313	4.60341650
Ni	0.70906132	0.65308987	2.63349350
C	2.41985432	0.14918687	2.31103650
C	-0.48139668	0.07471387	1.39631850
C	0.61213332	2.45149487	2.87177750
O	3.51899432	-0.14263313	2.11688250
O	0.55686432	3.59538187	3.00009450
O	-1.23508068	-0.30968513	0.61270550



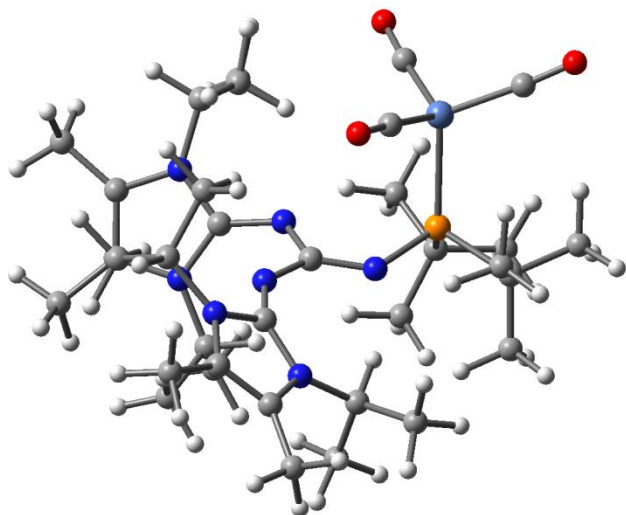
**P11 (BIG-P1)**

P	-2.22820400	-0.55501800	0.76415800
N	2.28936500	2.27301000	0.93692500
N	1.57882100	-0.41642900	-0.22633300
N	0.11769600	1.31161800	0.31975600
N	1.89648500	-2.82391200	0.23202100
N	2.73725900	-1.93109800	-1.59194500
N	0.96343200	3.40069000	-0.40645500
N	-0.60584000	-0.92635700	0.47404100
C	1.07710000	2.21166800	0.27042500
C	1.97578700	-1.64527200	-0.48365300
C	4.01818100	0.79774500	1.97319300
H	4.18505600	0.34163900	0.99393800
H	4.14009100	0.02704400	2.74081400

H	4.78562000	1.55430100	2.15047600
C	1.44131900	-2.84934300	1.63474100
H	0.83436600	-1.95055000	1.72567500
C	3.95543100	-3.88320100	-2.65351900
H	4.92109100	-3.37725400	-2.77827000
H	3.43965000	-3.85197500	-3.62169800
H	4.16087600	-4.93156900	-2.42603300
C	2.07334200	4.21154500	-0.14167000
C	3.14045300	-3.27018800	-1.56515200
C	2.89899400	3.51864000	0.68723900
C	2.59882500	1.36059300	2.05180900
H	1.92087700	0.52279900	1.91279000
C	0.33806800	-0.04134400	0.22674900
C	0.51435900	-4.02555300	1.94635400
H	-0.24457800	-4.13172900	1.16964400
H	0.00212200	-3.82627200	2.89352500
H	1.05021900	-4.97173300	2.05733800
C	-1.37003900	4.14754200	-0.18650500
H	-2.23472600	4.53928100	-0.72832200
H	-1.04811800	4.89389800	0.54865500
H	-1.67641100	3.24177500	0.34040200
C	2.63629600	-2.77030400	2.58953000
H	3.25131100	-3.67627800	2.55297100
H	2.28229600	-2.64780600	3.61942000
H	3.27248900	-1.91760900	2.33921000
C	-2.25568800	0.59709800	2.24853800
H	-1.63377000	1.41692100	1.87316600
C	-2.73416200	-2.23492200	1.41703800
H	-1.97013700	-2.49626900	2.15934000
C	2.73267400	-5.24095000	0.03136500
H	3.13983100	-5.32141000	1.04511800
H	3.40037600	-5.79577800	-0.63233600
H	1.76212000	-5.74943800	0.02470900
C	2.62700900	-3.82661700	-0.43458800
C	1.78891000	-0.41301700	-3.31821900
H	1.14187900	-1.22584100	-3.65883500
H	2.06736000	0.19631700	-4.18561800
H	1.22181300	0.20288600	-2.61968000
C	4.24945000	3.91336600	1.18720400
H	4.33420000	3.84953600	2.27710000

H	4.45479800	4.94922600	0.90635500
H	5.04385800	3.29153400	0.75774600
C	-0.62197800	2.82047900	-2.24146400
H	0.23235300	2.59629400	-2.88902500
H	-1.42309300	3.24419500	-2.85626000
H	-0.97912600	1.89400400	-1.79462300
C	-0.23108800	3.82837300	-1.15892300
H	0.07080600	4.75431700	-1.65543600
C	2.24156700	5.55968400	-0.75728200
H	2.26544300	5.51143900	-1.85340300
H	3.18029300	6.01059000	-0.42782500
H	1.43090500	6.24311700	-0.47598400
C	3.97065700	0.15376500	-2.12625800
H	3.44356200	0.74397600	-1.37435700
H	4.26994400	0.80797000	-2.95278800
H	4.87681900	-0.26883200	-1.67713100
C	3.05584000	-0.95826800	-2.65293600
H	3.61095900	-1.53291200	-3.39893900
C	2.26713400	2.01681200	3.39657400
H	2.90526600	2.88119700	3.60624300
H	2.40448000	1.29232300	4.20676000
H	1.22358100	2.34701800	3.40698900
Ni	-3.47286800	0.05086800	-1.09846100
C	-4.99956100	-0.92598000	-1.10308100
C	-3.89031000	1.80956900	-1.08431800
C	-2.29523300	-0.46013100	-2.38513000
O	-5.97486300	-1.54246800	-1.11083200
O	-1.50702800	-0.80980500	-3.14961200
O	-4.22487400	2.91464400	-1.09417800
C	-3.64363100	1.16167000	2.56744100
H	-4.32203800	0.40104800	2.96506300
H	-3.56409300	1.95704200	3.32007700
H	-4.11000300	1.58726500	1.67393800
C	-1.55342000	0.00622100	3.47535300
H	-1.41774700	0.77364800	4.24883100
H	-2.13052800	-0.81137600	3.92259600
H	-0.56497400	-0.38361400	3.20818300
C	-2.65913900	-3.25244700	0.27064500
H	-1.70397400	-3.17710400	-0.25594600
H	-2.77186600	-4.27300900	0.65946000

H	-3.45989400	-3.08100800	-0.45555500
C	-4.11160500	-2.25907500	2.08600300
H	-4.40198000	-3.29341300	2.30993500
H	-4.12297400	-1.70293200	3.02737200
H	-4.88300300	-1.83649900	1.43465400



**P12 (BIG-P2)**

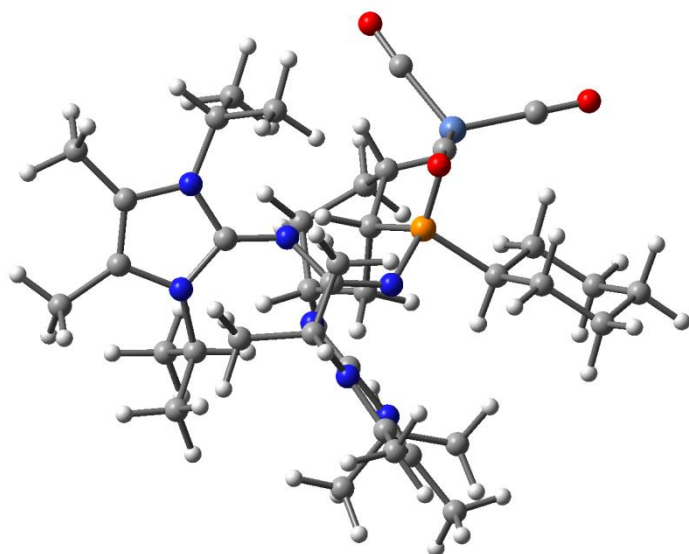
P	-2.40904000	-0.55112400	0.61849300
N	2.28873700	1.95295700	1.25225400
N	1.43204700	-0.43578100	-0.33416800
N	0.09631400	1.28833600	0.40208400
N	2.03880100	-2.83535100	-0.07473300
N	3.06273200	-1.56307500	-1.55050800
N	1.27629000	3.28941800	-0.16465200
N	-0.76799600	-0.91274000	0.40128000
C	1.15305300	2.07737200	0.46921000
C	2.04303900	-1.55677600	-0.61114900
C	3.74990100	0.15025400	2.17310900
H	3.89865500	-0.21200200	1.15343600
H	3.72747500	-0.71336400	2.84499800
H	4.60612200	0.76381800	2.46250600
C	1.11667900	-3.26122700	0.99133900
H	0.30447600	-2.53211300	0.93427400
C	4.86175400	-3.10212600	-2.45228700
H	5.68829400	-2.39469800	-2.30870200
H	4.58155000	-3.06890900	-3.51301500
H	5.24579300	-4.10437100	-2.24976700
C	2.45592600	3.92651100	0.24157900
C	3.70713000	-2.80206900	-1.55666700
C	3.09020100	3.09939600	1.11455000

C	2.42337000	0.90637800	2.27829200
H	1.63104500	0.19755500	2.04993300
C	0.22017400	-0.06734000	0.19233500
C	0.51401600	-4.64564900	0.72710200
H	0.19809900	-4.74097200	-0.31584800
H	-0.37155100	-4.76959600	1.35464800
H	1.19919600	-5.46273900	0.96482600
C	-0.84161100	4.54796700	-0.25917900
H	-1.53335500	5.07387300	-0.92374600
H	-0.43660500	5.26525100	0.46368200
H	-1.40651200	3.78899600	0.28223400
C	1.76351900	-3.15958900	2.37500000
H	2.62409200	-3.83008400	2.48143900
H	1.03040600	-3.42584000	3.14465800
H	2.09887200	-2.13748000	2.56782100
C	-2.62749400	0.36222300	2.29912000
C	-3.03641200	-2.34519700	0.83361100
C	3.43487200	-4.99121300	-0.25432200
H	3.51187800	-5.11524500	0.83095600
H	4.40657400	-5.25360900	-0.68042200
H	2.70774100	-5.72483300	-0.61931000
C	3.08829600	-3.59019700	-0.63930200
C	2.16511400	-0.06521500	-3.31307900
H	1.78375200	-0.93469900	-3.85736900
H	2.45631800	0.69928100	-4.04245300
H	1.36124800	0.32384000	-2.68937000
C	4.42890500	3.28149200	1.75051300
H	4.40989400	3.12717600	2.83371600
H	4.78186500	4.30037400	1.57372700
H	5.17655800	2.59733200	1.33209700
C	-0.20513600	2.93665900	-2.14319100
H	0.63836600	2.51503500	-2.69794700
H	-0.84868400	3.47707300	-2.84521800
H	-0.77435500	2.12184500	-1.70109300
C	0.28663700	3.90657500	-1.07027300
H	0.83915300	4.70328100	-1.57539200
C	2.87206500	5.25614200	-0.29099100
H	3.05000400	5.23064600	-1.37378100
H	3.80080400	5.57788900	0.18543700
H	2.11777500	6.02888600	-0.09963100



C	3.97600200	0.74910700	-1.70963500
H	3.24282200	1.17428700	-1.02616800
H	4.28504800	1.51613800	-2.42875800
H	4.85789000	0.44380200	-1.13474000
C	3.37650300	-0.44644600	-2.45815700
H	4.14592000	-0.84249500	-3.12579400
C	2.14725000	1.46962200	3.67688500
H	2.91272400	2.18293800	3.99736400
H	2.12487900	0.65124600	4.40468300
H	1.17512600	1.97087700	3.69850600
Ni	-3.32509100	0.39644400	-1.33000300
C	-4.94376200	-0.29702400	-1.76024900
C	-3.51304900	2.19130000	-1.20877800
C	-2.01591200	-0.15072400	-2.46656100
O	-5.97805700	-0.68562700	-2.09269100
O	-1.16342700	-0.52465100	-3.14542600
O	-3.69247700	3.33143100	-1.19240800
C	-3.97493900	0.04600200	2.96548200
H	-4.02512400	-0.96868700	3.36667100
H	-4.12574900	0.73655300	3.80613400
H	-4.80993100	0.18854500	2.27097400
C	-1.46811000	0.03552400	3.25377800
H	-1.59816600	0.59587100	4.19007100
H	-1.41442900	-1.02622100	3.50407700
H	-0.51519200	0.33105100	2.81144100
C	-2.59163300	-3.08937900	-0.44255200
H	-1.51437300	-3.01781700	-0.59462000
H	-2.87477100	-4.14739600	-0.36340500
H	-3.08501400	-2.67243500	-1.32602300
C	-4.56995500	-2.43935900	0.90480400
H	-4.86216000	-3.49619700	0.84555700
H	-4.98069500	-2.04033400	1.83263700
H	-5.04640400	-1.92056800	0.07209600
C	-2.43755300	-3.03663500	2.06900300
H	-2.64447100	-4.11476700	2.02793900
H	-1.35733300	-2.89690300	2.12343500
H	-2.87353700	-2.66032300	2.99830700
C	-2.61096800	1.87229800	2.00833800
H	-1.71627500	2.14158500	1.44723000
H	-3.49289800	2.17324200	1.43679300

H	-2.61869000	2.42535100	2.95816000
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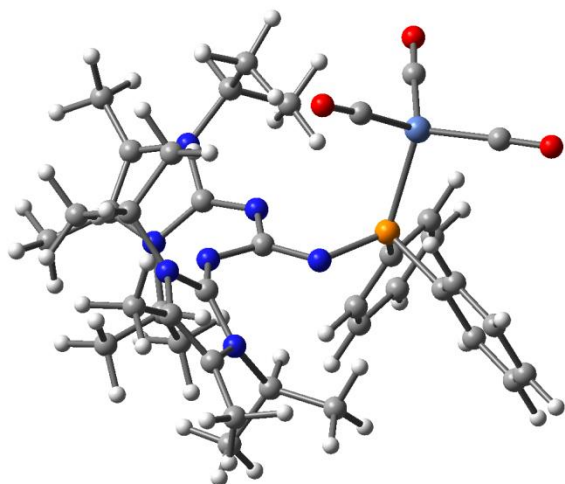
**P13 (BIG-P3)**

P	1.91787200	-0.25881300	0.09715100
N	-3.23464300	-1.47364100	0.88784600
N	-1.81549900	0.94768100	-0.17471100
N	-0.95350500	-1.21001100	0.01013500
N	-1.23613100	3.24230100	0.52365400
N	-2.54687700	2.92448700	-1.21069200
N	-2.51656000	-2.85083200	-0.66905200
N	0.49360500	0.64835300	0.12985300
C	-2.15362900	-1.74822800	0.06566800
C	1.86619400	-3.27963400	3.65434200
H	2.01660000	-3.82570800	4.59311700
H	1.18060900	-3.88851400	3.04903300
C	1.22895000	-1.89697400	3.93463300
H	0.13653800	-1.99563900	3.94962500
H	1.52095000	-1.54533400	4.93262800
C	-1.79998900	2.26137100	-0.26717800
C	-4.21838500	0.39097300	2.22586800
H	-4.28665900	0.99107200	1.31533900
H	-3.99907600	1.05638800	3.06687300
H	-5.18832600	-0.07048500	2.42395200
C	-0.61411100	2.92926100	1.82315300
H	-0.36587900	1.87286300	1.74411700
C	-3.14126400	5.29077300	-1.89639300
H	-4.22899600	5.14693000	-1.90969500
H	-2.78756400	5.22473700	-2.93318600
H	-2.94858500	6.30837500	-1.54932000
C	-3.79791700	-3.27456900	-0.29915100

C	-2.45905700	4.30598300	-1.00803500
C	-4.24948600	-2.42526800	0.66158600
C	5.39021100	1.70807600	1.55261200
H	6.38681900	1.31538400	1.79108600
H	4.99577900	2.15086900	2.47965200
C	-3.09261100	-0.63433800	2.09070700
H	-2.17351900	-0.07795100	1.92604400
C	5.48621200	2.79747100	0.47844000
H	6.13421400	3.61488900	0.81978100
H	5.95382100	2.37467200	-0.42235500
C	-0.71975200	0.14477600	0.02285300
C	2.92818800	-2.55049800	1.48190400
H	3.85887100	-2.14580000	1.07183800
H	2.63132300	-3.35711000	0.80288700
C	0.70751700	3.66547800	2.04585800
H	1.33115300	3.60276600	1.15354100
H	1.24576100	3.18378100	2.86883600
H	0.56881500	4.71592200	2.31464300
C	-0.52809200	-4.29457400	-0.81148900
H	0.08656300	-4.89814700	-1.48426200
H	-0.96874500	-4.95215200	-0.05347400
H	0.11698300	-3.56640200	-0.31639800
C	-1.60970600	3.14285800	2.96717500
H	-1.85227300	4.20167300	3.10855500
H	-1.18228400	2.77019500	3.90492000
H	-2.54037500	2.60399600	2.77340300
C	1.80179500	-1.48618500	1.50003900
H	0.85309300	-1.98196200	1.26981900
C	3.07529400	1.06955400	0.71957300
H	2.59408500	1.48644800	1.61447700
C	-1.20201900	5.80324200	0.65978800
H	-1.41763600	5.87502400	1.73126200
H	-1.71999500	6.62993000	0.16740100
H	-0.12576300	5.96240300	0.52898200
C	-1.65138300	4.50822500	0.06842700
C	-2.36984700	1.43072200	-3.18951400
H	-1.53037600	2.03121500	-3.55038600
H	-2.93280500	1.06602700	-4.05615500
H	-1.96725300	0.57638700	-2.64449300
C	-5.59682100	-2.39147800	1.30467800

H	-5.54874300	-2.40326100	2.39848500
H	-6.17118600	-3.26848200	0.99644900
H	-6.16796500	-1.50312100	1.00972400
C	-1.08320300	-2.65797300	-2.69671000
H	-1.90020800	-2.13567800	-3.20613500
H	-0.54069700	-3.25931300	-3.43384700
H	-0.39935100	-1.92187300	-2.27818900
C	4.47045900	0.55843600	1.11344900
H	4.39616400	-0.17397900	1.92372400
H	4.92681300	0.03883500	0.26294000
C	1.63971400	-0.84134200	2.88411400
H	0.89004400	-0.04298600	2.83774700
H	2.57996700	-0.36650700	3.18784900
C	-1.62613400	-3.57236600	-1.59740600
H	-2.26576800	-4.32345000	-2.06802400
C	4.09282700	3.32752700	0.11912600
H	4.16311100	4.08740300	-0.66997100
H	3.66093000	3.82596100	0.99980100
C	-4.47435000	-4.43334900	-0.95076400
H	-4.59523800	-4.28480000	-2.03132400
H	-5.46994800	-4.57725200	-0.52522100
H	-3.91682700	-5.36719300	-0.80762500
C	-4.46310600	1.43795400	-1.73422100
H	-4.08235200	0.61241700	-1.12994400
H	-5.05857100	1.03415300	-2.56067600
H	-5.11573100	2.06282000	-1.11377000
C	-3.29489400	2.25860000	-2.29295000
H	-3.70618900	3.07643500	-2.89038100
C	3.18504900	-3.13121700	2.88676600
H	3.69985600	-4.09578600	2.80389900
H	3.85769900	-2.47010600	3.45080900
C	3.17191100	2.18795400	-0.33458700
H	3.56572100	1.76592200	-1.26716500
H	2.16597100	2.55361800	-0.56363500
C	-2.89975000	-1.50388000	3.33849700
H	-3.79501500	-2.08203500	3.58773000
H	-2.66002000	-0.86908700	4.19857700
H	-2.07047000	-2.20200900	3.18785300
Ni	2.61298400	-1.06960200	-1.96676100
C	4.33976400	-0.58465500	-2.22568200

C	2.48473300	-2.87255000	-2.00813600
C	1.47247900	-0.16029100	-3.04947900
O	5.43825600	-0.27691700	-2.40167100
O	0.73275100	0.45168700	-3.68729200
O	2.46937000	-4.02650800	-2.04533000

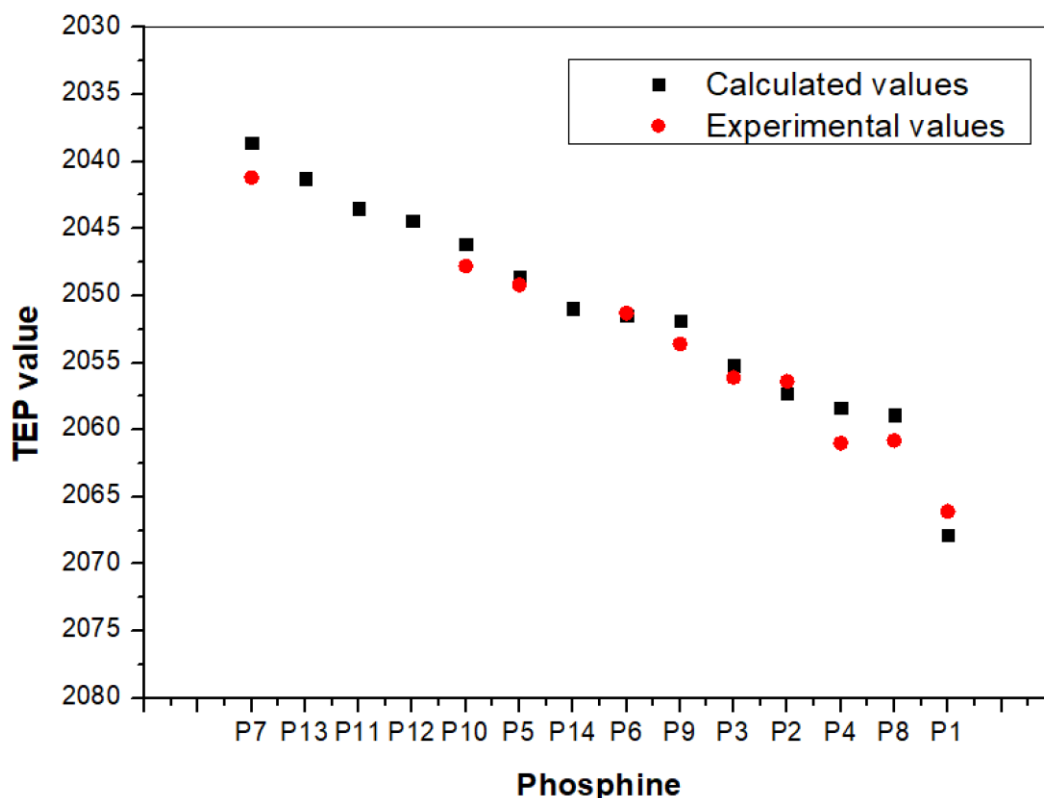


**P14 (BIG-P4)**

P	0.17631282	1.98748946	2.17775347
N	-4.84551295	0.57508292	1.45752531
N	-3.07919641	2.64046127	0.11920062
N	-2.39823935	0.79477467	1.38104204
N	-2.71331167	5.08085196	0.14352458
N	-3.24462262	4.07637971	-1.73495116
N	-3.61443853	-1.18348191	0.97005560
N	-1.07998734	2.73248881	1.34721379
C	-3.54060797	0.15858829	1.24986037
C	-2.96795158	3.84556665	-0.41061322
C	-6.21422821	2.66469878	1.48643626
H	-5.92239014	2.84407912	0.44901992
H	-6.29776919	3.63060274	1.99548322
H	-7.20309630	2.20027416	1.50620130
C	-2.62750550	5.28979694	1.60234114
H	-2.48308101	4.28840810	1.99880710
C	-3.38055661	6.00455187	-3.37471167
H	-4.38092550	5.76886436	-3.75908872
H	-2.65054512	5.62226008	-4.09955508
H	-3.28370484	7.09240291	-3.35598268
C	-4.94652057	-1.60943918	1.01677752
C	-3.16128961	5.44561802	-2.00948431
C	-5.71377893	-0.52711061	1.31394792
C	-5.15017247	1.81948304	2.18684183

H	-4.22489758	2.38762172	2.15102169
C	-2.17237157	2.08221601	0.97854588
C	-1.39270016	6.09123708	2.01522933
H	-0.50800777	5.70821275	1.50533096
H	-1.22663977	5.96536619	3.08962531
H	-1.49740121	7.16171536	1.81699559
C	-1.72240114	-2.20958471	2.16456313
H	-0.89682674	-2.92064744	2.07680264
H	-2.41607778	-2.57057569	2.93237916
H	-1.32162313	-1.24589572	2.48360944
C	-3.93844094	5.86438029	2.14822523
H	-4.11488613	6.89153769	1.81245645
H	-3.90531603	5.87509044	3.24347573
H	-4.78953172	5.25278321	1.83441289
C	-2.56345750	7.52360489	-0.61933148
H	-3.15981515	7.94059109	0.19858377
H	-2.80830569	8.08781185	-1.52267454
H	-1.50949818	7.71145764	-0.38613698
C	-2.83203692	6.07266948	-0.84667299
C	-2.36764035	2.02837400	-2.83885351
H	-1.42518333	2.55124256	-3.02291911
H	-2.55445140	1.34548681	-3.67530194
H	-2.26073612	1.44459062	-1.92367156
C	-7.20298315	-0.43428655	1.36872358
H	-7.57099871	-0.01671764	2.31168146
H	-7.63649506	-1.43199825	1.26493369
H	-7.60258504	0.18544942	0.55700495
C	-1.52813301	-1.61195028	-0.32003700
H	-2.09771410	-1.49444439	-1.24853615
H	-0.74930573	-2.36422603	-0.48191471
H	-1.05038193	-0.66373838	-0.07599298
C	-2.44269809	-2.06737833	0.81994173
H	-2.86178873	-3.03908937	0.54550183
C	-5.34397260	-3.01579290	0.71895143
H	-5.03896615	-3.32431744	-0.28902559
H	-6.42914693	-3.12308141	0.78235652
H	-4.90061105	-3.72560667	1.42820100
C	-4.86383533	2.32255044	-2.41095911
H	-4.79353465	1.78755240	-1.46195401
H	-5.10145221	1.60985932	-3.20857897

H	-5.67803157	3.05359092	-2.34917670
C	-3.53209011	3.01616263	-2.71891445
H	-3.63228081	3.54208093	-3.67193501
C	-5.46202433	1.52538443	3.65867528
H	-6.39492406	0.96756613	3.78568164
H	-5.55948359	2.46842755	4.20867326
H	-4.64795041	0.94907479	4.10778668
Ni	1.65403032	0.69075339	0.95673950
C	3.28788217	1.35126288	1.42196926
C	1.54066622	-1.07236812	1.34061292
C	1.11605489	1.11038225	-0.72559621
O	4.30546603	1.78063872	1.74584296
O	0.72227617	1.40394643	-1.76794482
O	1.52066085	-2.20265726	1.57258205
C	1.05172668	3.50370168	2.75642680
C	1.05476265	3.94667453	4.08322319
C	1.73336398	4.25953931	1.78963502
C	1.71427932	5.12820732	4.43454897
H	0.53790123	3.37453366	4.84613989
C	2.38636206	5.43945038	2.13781845
H	1.74142291	3.91837440	0.75851092
C	2.37716991	5.87919295	3.46461398
H	1.70821031	5.45971844	5.46977214
H	2.90691426	6.01429497	1.37634673
H	2.89059892	6.79655224	3.73959467
C	-0.47683069	1.30047099	3.75753591
C	0.20189492	0.26057975	4.40064078
C	-1.65407415	1.80119653	4.33019559
C	-0.28415994	-0.27199825	5.59717177
H	1.10880094	-0.13745429	3.95449267
C	-2.14037664	1.27341073	5.52468173
H	-2.18481444	2.60448189	3.82800509
C	-1.45700513	0.23167351	6.15994675
H	0.25071387	-1.08256644	6.08472005
H	-3.05215557	1.67171985	5.96248137
H	-1.83933426	-0.18387327	7.08836575



**Figure S17.** Comparison of calculated and experimental TEP values of selected phosphines.

**5.2 Gas phase basicity (GB)** was calculated as the Gibbs free energy  $\Delta G_{298.15}$  of the gas phase reaction:  $PR_3 + H^+ = HPR_3^+$ .

$$GB = \Delta G_{298.15} = G(HPR_3^+) - [G(PR_3) + G(H^+)].$$

The geometry optimizations were performed with Gaussian 16 package at the TPSS-D3BJ/def2-TZVP level of theory.<sup>[S5]</sup> The electronic energy  $E_{el}$  were calculated with ORCA program15 at the PW6B95-D3(BJ)/def2-TZVP level based on the geometries optimized of the gas-phase molecules above.  $G^{298.15}(H^+) = H^{298.15}(H^+) - T \times S^{298.15}(H^+) = 5/2 RT - T \times S^{298.15}(H^+) = 1.48 \text{ kcal/mol} - 298.15 \times 25.85 \text{ J/(Kmol)} = -6.22 \text{ kcal/mol}$ .  $G_{298.15} = E_{el} + G_{therm}^{298.15}$ .

**5.3 Proton affinities (PA)** were calculated as the enthalpy  $\Delta H^{298.15}$  of the gas phase reaction:  $PR_3 + H^+ = HPR_3^+$ .

$$PA = \Delta H_{298.15} = H(HPR_3^+) - [H(PR_3) + H(H^+)] = H(HPR_3^+) - [H(PR_3) + 1.48 \text{ kcal/mol}]$$

**5.4 pKa values** of the listed phosphines are estimated by calculating the Gibbs free energy of the reactions of proton exchange equilibrium:  $HPR_3^+ + PPh_3 = PR_3 + HPPH_3^+$ . The experimental pKa value of  $HPPH_3^+$  (7.64) in  $CH_3CN$  was chosen as the reference. Free energies of  $CH_3CN$  were obtained with the SMD model at at PW6B95-D3 level of theory with ORCA program.<sup>[S5]</sup> Relative pKa values was then obtained from  $\Delta pKa = \Delta G^{298.15} / (RT \ln(10))$ .

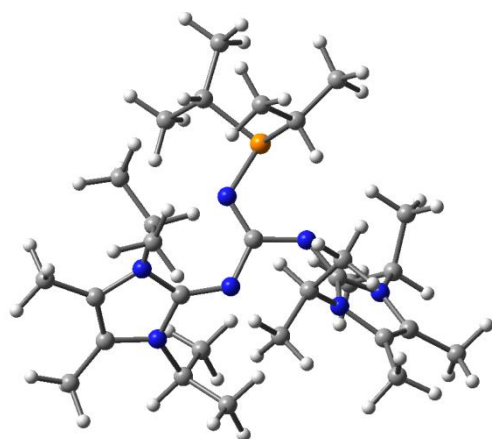
$$pKa(H(HPR_3^+)) = pKa(HPPH_3^+) - \Delta pKa.$$



**Table S1** Calculated electronic energies at TPSS-D3BJ and PW6B95-D3BJ level, enthalpic and free energy corrections for 298.15 K.

	$E_{\text{el}}(\text{TPSS-D3BJ})$	$G_{\text{therm}}(298.15 \text{ K})$	$H_{\text{therm}}(298.15 \text{ K})$
<b>BIG-P1</b>	-1865.110382	0.712772	0.841455
<b>BIG-P2</b>	-1943.862033	0.765994	0.898953
<b>BIG-P3</b>	-2098.974518	0.83878	0.975563
<b>BIG-P4</b>	-2091.737676	0.70312	0.835698
<b>PPh<sub>3</sub></b>	-1037.798855	0.22217	0.286054
<b>BIG-P1+H<sup>+</sup></b>	-1865.569085	0.725404	0.854503
<b>BIG-P2+H<sup>+</sup></b>	-1944.325525	0.779351	0.911993
<b>BIG-P3+H<sup>+</sup></b>	-2099.435676	0.850488	0.988677
<b>BIG-P4+H<sup>+</sup></b>	-2092.190129	0.715789	0.848519
<b>PPh<sub>3</sub>+H<sup>+</sup></b>	-1038.185897	0.232144	0.297510

**Cartesian coordinates of BIG-Ps and BIG-Ps+H<sup>+</sup>**

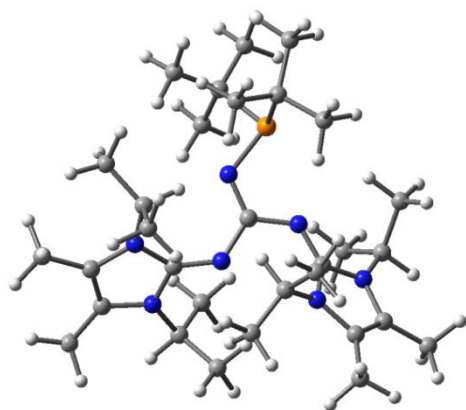


**BIG-P1**

P	-0.24183800	2.97210800	-0.73725500
N	2.34484700	-1.11280100	1.06785500
N	-0.42701000	-0.90767100	-0.24746100
N	1.31588800	0.64630300	-0.30581500
N	-2.81203000	-0.96440300	0.41139300
N	-2.01889600	-2.47782800	-0.97175600
N	3.44309000	-0.30317400	-0.66199100
N	-0.89170300	1.41324700	-0.42068000
C	2.24275000	-0.22247200	0.00748600
C	-1.66688900	-1.34655500	-0.26479600
C	0.85303500	-2.39161800	2.60993900
H	0.39877300	-2.87012200	1.73939200
H	0.08110200	-2.25208500	3.37367400
H	1.61536800	-3.05323700	3.02943500

C	-2.78011800	0.04768600	1.48682300
H	-1.81337900	0.53250300	1.34646500
C	-4.03693200	-3.94889600	-1.39727200
H	-3.54084200	-4.89919800	-1.16316800
H	-4.05988600	-3.84679300	-2.48997900
H	-5.07031800	-4.01891800	-1.05063500
C	4.28920000	-1.21742000	-0.02387200
C	-3.36199400	-2.79389800	-0.74071800
C	3.61706400	-1.71924400	1.04991400
C	1.41946600	-1.02756300	2.21515300
H	0.59171600	-0.43000900	1.83396000
C	-0.04179400	0.41732700	-0.28438600
C	-3.83783200	1.13343200	1.29121200
H	-3.75967300	1.54021300	0.28091700
H	-3.64892500	1.94492500	2.00126800
H	-4.85350700	0.76796800	1.46539800
C	3.83645300	1.97559500	-1.56864500
H	4.19057300	2.51139100	-2.45606100
H	4.53184200	2.17054600	-0.74527900
H	2.84484200	2.34857700	-1.30088600
C	-2.82629800	-0.61027000	2.86996800
H	-3.79887400	-1.06517400	3.08378100
H	-2.63617000	0.14791300	3.63724500
H	-2.05926400	-1.38536300	2.95264200
C	0.44651700	3.46305500	0.95673500
H	1.10602700	2.60519600	1.14438800
C	-1.88439200	3.87321900	-0.80634200
H	-2.44645500	3.63168600	0.10487900
C	-5.25435600	-1.71939700	0.62455200
H	-5.29991900	-1.62771200	1.71445100
H	-5.82940400	-2.60517800	0.34343700
H	-5.75774000	-0.84444200	0.19699900
C	-3.85787900	-1.85944100	0.11787200
C	-0.70595300	-2.23452100	-3.06109300
H	-1.58377100	-1.81488500	-3.56224000
H	-0.11894100	-2.79454400	-3.79711300
H	-0.09999400	-1.41610700	-2.66929900
C	4.04875400	-2.78858500	1.99644500
H	3.96402500	-2.48487000	3.04535500
H	5.09687300	-3.03463000	1.80920400

H	3.46205900	-3.70665300	1.86930400
C	2.78601600	0.16304200	-3.01269200
H	2.72962100	-0.91543300	-3.19308500
H	3.12942900	0.65257400	-3.93016000
H	1.79146900	0.53848000	-2.76472400
C	3.76586000	0.47509300	-1.87594200
H	4.76098200	0.12607500	-2.16766000
C	5.64553800	-1.54624000	-0.54582400
H	5.60503100	-1.97206000	-1.55674000
H	6.12529300	-2.28051500	0.10508400
H	6.29259000	-0.66121500	-0.58497200
C	0.07087300	-3.80638800	-1.20934400
H	0.69748900	-3.02718200	-0.77057300
H	0.65979400	-4.38388400	-1.93039300
H	-0.26565200	-4.48410400	-0.41741100
C	-1.12797600	-3.17084800	-1.92305200
H	-1.74373500	-3.97169100	-2.34290400
C	2.05983500	-0.26682800	3.38237700
H	2.90200200	-0.81239400	3.81936300
H	1.31416700	-0.11049300	4.16917000
H	2.41564500	0.71177700	3.04693400
C	-0.58472900	3.53280500	2.08557300
H	-1.24968400	4.39700800	1.97157100
H	-1.20363400	2.62970800	2.10062500
H	-0.09086000	3.62506200	3.06316700
C	1.32825200	4.71741200	0.89371700
H	2.06273500	4.63862800	0.08509600
H	0.73737900	5.62289200	0.71830300
H	1.87108800	4.85713600	1.83862200
C	-1.70094300	5.39237600	-0.90398900
H	-1.02618200	5.65188700	-1.72917200
H	-2.66400600	5.88551000	-1.09037800
H	-1.28365300	5.81526500	0.01515700
C	-2.66610600	3.33870300	-2.01484500
H	-2.13992500	3.57402700	-2.94858600
H	-2.77386000	2.25176900	-1.95211700
H	-3.66392700	3.79547200	-2.06346400

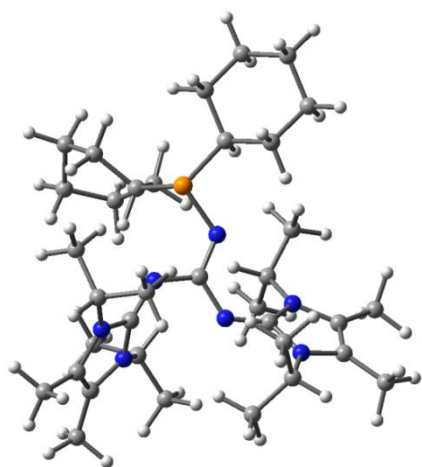


**BIG-P2**

P	1.26951500	-2.61476600	-0.45579500
N	-2.81123300	0.37665100	0.99341000
N	-0.05078800	1.05512400	-0.18525900
N	-1.08445300	-1.02449900	-0.05476100
N	2.05612900	2.19876900	0.43669900
N	0.74344200	3.06539000	-1.09869200
N	-3.36396500	-0.98205400	-0.64840100
N	1.25492100	-0.92305200	-0.16172400
C	-2.28819100	-0.52906800	0.08113000
C	0.89151200	1.96816700	-0.27426100
C	-2.04293500	2.31434000	2.36826600
H	-1.71305500	2.81193300	1.45369000
H	-1.35418300	2.57998700	3.17689300
H	-3.03276400	2.68646000	2.64492200
C	2.46133200	1.32209000	1.55463500
H	1.99060600	0.36774300	1.30014000
C	1.88792200	5.26170000	-1.63022600
H	0.99285500	5.88447700	-1.50803700
H	2.03471100	5.09873300	-2.70578100
H	2.74412500	5.83275600	-1.26448200
C	-4.54267800	-0.38306300	-0.19139400
C	1.77884000	3.97901400	-0.87939400
C	-4.20794900	0.45689300	0.82865700
C	-2.02679900	0.79826900	2.17030200
H	-1.00716900	0.51210000	1.91111600
C	0.08659400	-0.30999400	-0.09166500
C	3.96948700	1.06779500	1.60097100
H	4.35798100	0.85528800	0.60184900
H	4.14992300	0.18864800	2.22641100
H	4.52821300	1.90275900	2.03221200

C	-2.80859800	-3.33412900	-1.22654300
H	-2.87068300	-4.06767100	-2.03794100
H	-3.45168600	-3.66932200	-0.40577400
H	-1.77389200	-3.27643700	-0.87840800
C	1.91426700	1.84802700	2.88430300
H	2.37031500	2.80599800	3.15985100
H	2.12815900	1.12797900	3.68131400
H	0.83179500	1.98606900	2.82516800
C	1.47444100	-3.34308900	1.30495400
C	2.95717000	-2.69664000	-1.33273400
C	3.82291800	4.04541400	0.67368100
H	3.77769200	4.08436700	1.76763400
H	3.93532300	5.07019800	0.31108900
H	4.72683000	3.49143600	0.39764600
C	2.58959900	3.45148400	0.08033400
C	-0.17807800	2.03424000	-3.15371500
H	0.82806500	1.99497400	-3.58262300
H	-0.89742800	2.18695400	-3.96550600
H	-0.38896900	1.08114500	-2.66674200
C	-5.09092100	1.38753300	1.59041600
H	-4.99645200	1.26721200	2.67485300
H	-6.13339500	1.19186800	1.32756100
H	-4.87815500	2.43727600	1.35381700
C	-2.35470600	-1.45129700	-2.87131000
H	-2.66829600	-0.45578900	-3.20188400
H	-2.41343700	-2.13629200	-3.72375900
H	-1.31943300	-1.40889300	-2.52736200
C	-3.26128900	-1.96546400	-1.74763100
H	-4.28191900	-2.04979100	-2.13294300
C	-5.86853200	-0.65223400	-0.81603900
H	-5.88975000	-0.36525000	-1.87528400
H	-6.64393300	-0.08057400	-0.30126200
H	-6.13945400	-1.71348000	-0.75504400
C	-1.69712900	3.30043500	-1.54265100
H	-1.95486900	2.38190200	-1.01207200
H	-2.42277700	3.47287800	-2.34515900
H	-1.74897300	4.14302900	-0.84479200
C	-0.29208700	3.18223700	-2.14449400
H	-0.05815900	4.11917600	-2.65848900
C	-2.44368300	0.01289600	3.41945900

H	-3.46116000	0.25696100	3.74045700
H	-1.76372100	0.25169100	4.24414800
H	-2.38720200	-1.06256100	3.22822900
C	2.14593500	-4.72285900	1.26273100
H	3.21631300	-4.65124600	1.04715300
H	2.03514300	-5.21645900	2.23877100
H	1.68341200	-5.36835700	0.50704700
C	2.21008500	-2.42701500	2.29102600
H	2.20775000	-2.88293500	3.29223800
H	3.24864000	-2.25362500	1.99984700
H	1.70686500	-1.45820400	2.35748700
C	2.78553900	-1.74586500	-2.53590800
H	2.65036200	-0.71561200	-2.19586500
H	3.67565000	-1.80375300	-3.17816900
H	1.91052600	-2.02576500	-3.13583800
C	3.18083800	-4.11556600	-1.88341700
H	4.03398900	-4.11345400	-2.57623300
H	3.39602700	-4.84001600	-1.09382900
H	2.29756800	-4.46305600	-2.43178600
C	4.16790300	-2.23539900	-0.51574500
H	5.05340400	-2.14824200	-1.16300900
H	3.97025800	-1.25673100	-0.07142000
H	4.41388700	-2.94143000	0.28401500
C	0.02867200	-3.52829500	1.81088500
H	-0.51546900	-2.57937300	1.79931800
H	-0.52104500	-4.23210700	1.17690800
H	0.04304000	-3.92173100	2.83799900



**BIG-P3**

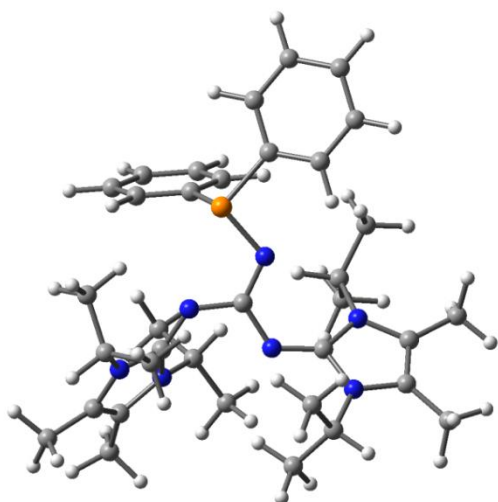
P	1.91393400	-1.23948000	-0.99484300
N	-2.95153700	-1.06135100	0.68592600
N	-1.05508900	1.18787400	-0.20114000

N	-0.88879800	-1.09898200	-0.65042900
N	0.33835100	2.95427700	0.83315000
N	-1.30717300	3.50218700	-0.51809100
N	-2.92793900	-2.11654300	-1.24805900
N	1.06909900	0.17197000	-0.49450200
C	-2.15157200	-1.34534400	-0.41269600
C	1.68295800	-4.00559800	2.74829200
H	1.80616900	-4.61695500	3.64991600
H	0.63578400	-4.11715600	2.43584500
C	1.98089500	-2.52037000	3.06289500
H	1.07399500	-2.03978100	3.45097800
H	2.73629200	-2.45353200	3.85679800
C	-0.64474300	2.41787400	0.01979100
C	-3.08741000	0.61541500	2.53224500
H	-3.14539300	1.40753800	1.78251500
H	-2.53109600	0.99255800	3.39648500
H	-4.09552000	0.36568200	2.87323700
C	1.09941500	2.12511800	1.78979400
H	0.90473600	1.10711300	1.45050200
C	-1.23249700	6.03416600	-0.48098100
H	-2.29467700	6.17849800	-0.24662600
H	-1.10660300	6.19013100	-1.56024400
H	-0.66909100	6.81593400	0.03316600
C	-4.18968500	-2.32204500	-0.67835600
C	-0.74556800	4.69404600	-0.04786400
C	-4.20972700	-1.67491400	0.52060300
C	6.13683100	-0.88746600	-0.98945100
H	6.91570100	-1.64174400	-1.16132100
H	6.30283100	-0.48337900	0.02012600
C	-2.35373100	-0.59413100	1.95260300
H	-1.35771700	-0.26174300	1.65978900
C	6.26322700	0.25081100	-2.01018200
H	7.24976200	0.72535300	-1.93138200
H	6.19045800	-0.16689600	-3.02504800
C	-0.24152300	0.09213700	-0.40612600
C	2.23941100	-3.77774700	0.29417500
H	3.09742600	-3.82170600	-0.38639500
H	1.42009800	-4.30009200	-0.21405100
C	2.60811100	2.33702400	1.66533600
H	2.90779900	2.22039300	0.62183900

H	3.12376300	1.57259800	2.25541300
H	2.92866800	3.31484900	2.03468900
C	-1.33372600	-3.64931700	-2.37927100
H	-1.10022100	-4.10282000	-3.34868300
H	-1.62757100	-4.44500700	-1.68626600
H	-0.44068200	-3.14848500	-1.99746100
C	0.57338700	2.29729800	3.21857300
H	0.79669200	3.28700600	3.62995900
H	1.04335100	1.55116600	3.86843900
H	-0.50959900	2.14905000	3.24975200
C	1.80741500	-2.31311900	0.54817700
H	0.72280000	-2.30784800	0.71985600
C	3.62974600	-0.50587300	-0.84792600
H	3.72676800	-0.06412800	0.15409900
C	1.22003500	5.26866500	1.50258100
H	1.29347200	5.04708300	2.57208100
H	0.87190400	6.29971300	1.40219300
H	2.23124400	5.21500900	1.08263700
C	0.27384700	4.35982300	0.79182800
C	-1.85239400	2.71380700	-2.80505400
H	-0.96933300	3.23169900	-3.19209600
H	-2.63159500	2.73059800	-3.57479100
H	-1.58612200	1.67789200	-2.58912000
C	-5.35125700	-1.51326200	1.46753300
H	-5.09871600	-1.81061000	2.49097700
H	-6.18395100	-2.14019000	1.13933600
H	-5.70724900	-0.47632200	1.50259000
C	-2.08769400	-1.49328700	-3.50161400
H	-2.90399900	-0.76866300	-3.58786200
H	-1.87858900	-1.90293200	-4.49549000
H	-1.19373500	-0.98538900	-3.13504200
C	4.74730100	-1.54181200	-1.04084200
H	4.68396900	-2.32205400	-0.27376000
H	4.61234600	-2.04149500	-2.01134300
C	2.47628700	-1.75995100	1.81106200
H	2.26604900	-0.69003200	1.91030300
H	3.56566300	-1.85857000	1.72499000
C	-2.47074400	-2.63557200	-2.55384600
H	-3.34441800	-3.15093800	-2.96407900
C	5.14844100	1.28678000	-1.81611100



H	5.22782600	2.07788600	-2.57333000
H	5.27311000	1.77061600	-0.83574600
C	-5.26323100	-3.08545600	-1.37475000
H	-5.54021500	-2.62529400	-2.33205300
H	-6.15890400	-3.11912900	-0.75057600
H	-4.95996300	-4.11957300	-1.57993800
C	-3.62670200	2.72538200	-0.97384700
H	-3.40476200	1.68891200	-0.71151300
H	-4.42104100	2.74769700	-1.72801900
H	-3.98284400	3.25259100	-0.08228100
C	-2.37085500	3.40116500	-1.53655700
H	-2.61739500	4.43872600	-1.78035600
C	2.58566600	-4.50438200	1.61321000
H	2.49132600	-5.58913000	1.48368900
H	3.63351400	-4.31295400	1.88216000
C	3.76514700	0.62673900	-1.88074000
H	3.60757200	0.20986600	-2.88706100
H	2.96863300	1.35952700	-1.71346900
C	-2.19928500	-1.75152100	2.94647800
H	-3.16563200	-2.13145700	3.29209400
H	-1.63916600	-1.40842500	3.82275000
H	-1.64600200	-2.57557500	2.48710600



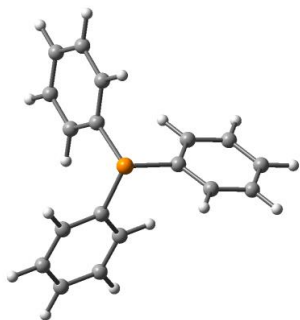
**BIG-P4**

P	1.37088500	-1.91312200	-1.21957300
N	-2.90612800	-0.24367700	0.83849600
N	-0.45934200	1.38301200	-0.27203500
N	-1.10921800	-0.81676600	-0.73311100
N	1.52428900	2.46480500	0.73670300
N	0.16407600	3.63629700	-0.53205800
N	-3.41769600	-1.09028600	-1.12745600

N	1.16138800	-0.27565000	-0.76015400
C	-2.35622000	-0.66926300	-0.35950200
C	0.38916300	2.36680000	-0.04762400
C	-2.35754700	1.32835200	2.69291300
H	-2.26611300	2.13418600	1.96030800
H	-1.63181500	1.49980800	3.49382800
H	-3.35377200	1.36017600	3.14134600
C	1.92762800	1.38875000	1.66872000
H	1.33908500	0.53136500	1.34168200
C	1.18287800	5.95392400	-0.44364500
H	0.26342000	6.47912500	-0.15617700
H	1.31789700	6.08798000	-1.52468200
H	2.01822700	6.44804900	0.05719500
C	-4.61323500	-0.94598200	-0.41480600
C	1.14413200	4.51497900	-0.05829100
C	-4.30238400	-0.42502100	0.80560500
C	-2.06193500	-0.01695500	2.02880800
H	-1.05214200	0.03216400	1.62217100
C	-0.09359900	0.08636200	-0.55279400
C	3.39630000	1.00102500	1.50856200
H	3.59366300	0.70972900	0.47548800
H	3.60820600	0.14052300	2.15120900
H	4.07558900	1.80447900	1.80448100
C	-2.52189500	-2.90669400	-2.56917300
H	-2.55568800	-3.30439100	-3.58930300
H	-2.97072500	-3.64373100	-1.89478800
H	-1.47919400	-2.74473100	-2.28424600
C	1.54885000	1.74048600	3.11193200
H	2.18013700	2.53278900	3.52662800
H	1.66989700	0.85238300	3.74125200
H	0.50689700	2.06580200	3.16962700
C	3.23388500	4.25704900	1.41060400
H	3.25955400	3.98789200	2.47107400
H	3.29438300	5.34623100	1.34480000
H	4.13393700	3.84317800	0.94127700
C	1.98980100	3.79315400	0.72947100
C	-0.76609400	3.20831700	-2.79124900
H	0.22367800	3.37248400	-3.22839900
H	-1.52348000	3.54952800	-3.50519600
H	-0.89930900	2.14019900	-2.61317200

C	-5.23086400	-0.01944500	1.90086000
H	-4.95176000	-0.44658800	2.86949900
H	-6.23938300	-0.36809100	1.66524500
H	-5.27371900	1.07017700	2.01857700
C	-2.67804900	-0.51581400	-3.42619000
H	-3.23381800	0.42477800	-3.35477600
H	-2.71034600	-0.86275600	-4.46433100
H	-1.63803200	-0.33819500	-3.14662100
C	-3.29333000	-1.58330800	-2.51448300
H	-4.32421500	-1.76226900	-2.83419300
C	-5.93847300	-1.29288600	-1.00095800
H	-6.16673900	-0.68972900	-1.88924200
H	-6.72675900	-1.11286600	-0.26669000
H	-5.99018200	-2.34852800	-1.29498800
C	-2.29619900	3.80595900	-0.83915200
H	-2.46271900	2.75216300	-0.60595800
H	-3.06790900	4.15120100	-1.53578900
H	-2.37474900	4.39313800	0.08205900
C	-0.91416000	3.98516600	-1.47843500
H	-0.76427600	5.04866900	-1.68605600
C	-2.12658000	-1.20925900	2.98885900
H	-3.11803300	-1.32531900	3.43806900
H	-1.40355200	-1.06244800	3.79785200
H	-1.86335600	-2.13180900	2.46556500
C	3.20851400	-1.93869900	-1.26149200
C	3.92571400	-3.11679500	-1.00110000
C	3.91815600	-0.80562100	-1.68760700
C	5.31201300	-3.15558200	-1.14080400
H	3.39438500	-4.00605800	-0.66932600
C	5.30521500	-0.84547000	-1.83209700
H	3.36455300	0.10815200	-1.88573600
C	6.00931100	-2.01881000	-1.55680500
H	5.85107600	-4.07380700	-0.91999700
H	5.83950200	0.04471300	-2.15685800
H	7.09030900	-2.04882500	-1.66552400
C	1.08899500	-2.81684100	0.37700400
C	0.07959900	-3.78361100	0.44863500
C	1.80181600	-2.50521500	1.54382600
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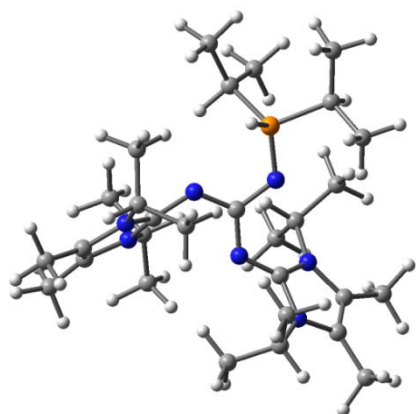
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H	2.59600500	-1.76653800	1.49249800
C	0.50221300	-4.10512600	2.80784000
H	-0.99855700	-5.17758400	1.69243200
H	2.07830100	-2.89238200	3.64528400
H	0.27700900	-4.60385500	3.74705500



**PPh<sub>3</sub>**

P	-0.00082400	-0.00002200	-1.26892800
C	0.90744000	1.36970500	-0.44295800
C	0.75554700	2.65665000	-0.98355300
C	1.73720000	1.19982700	0.67344700
C	1.39861400	3.75039300	-0.40819800
H	0.12625800	2.79684600	-1.85964200
C	2.39290500	2.29368700	1.24007500
H	1.86929000	0.20992500	1.09973100
C	2.22219300	3.57071700	0.70520500
H	1.26602700	4.74119700	-0.83434300
H	3.03497300	2.14699700	2.10466700
H	2.73258400	4.42113000	1.14874600
C	0.73258000	-1.47117600	-0.44379300
C	0.16762100	-2.11016300	0.66794600
C	1.92739000	-1.97736000	-0.98035600
C	0.78806900	-3.22478700	1.23389900
H	-0.75871300	-1.73373100	1.09127700
C	2.55439600	-3.08040700	-0.40509800
H	2.36608500	-1.49825200	-1.85282800
C	1.98381600	-3.70936300	0.70358400
H	0.33742700	-3.71175700	2.09475200
H	3.48225900	-3.45625000	-0.82780500
H	2.46606600	-4.57619300	1.14682500
C	-1.64097800	0.10093200	-0.44275200
C	-2.67955400	-0.67373500	-0.98378700
C	-1.90876300	0.90413500	0.67382200
C	-3.94837300	-0.66372300	-0.40856500

H	-2.48621200	-1.28857300	-1.86002100
C	-3.18405000	0.92528800	1.24016000
H	-1.11729800	1.51285900	1.10055300
C	-4.20465200	0.13919900	0.70493900
H	-4.74018700	-1.27363600	-0.83505100
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H	-5.19646300	0.15623600	1.14816600

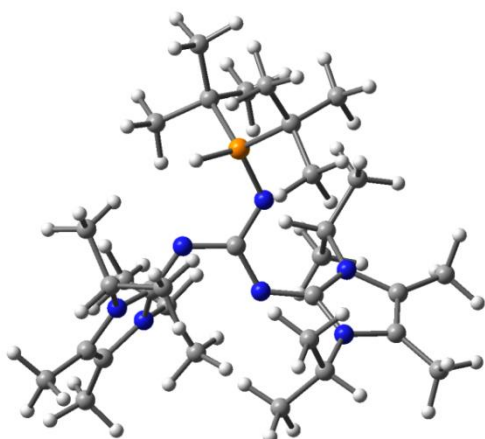


**BIG-P1+H<sup>+</sup>**

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N	-2.77142300	-1.02019000	0.56403500
N	-2.13814200	-2.25098000	-1.13275500
N	3.36039900	-0.35525000	-0.70304700
N	-0.91879100	1.35662300	-0.28705400
C	2.24885000	-0.27613800	0.08472100
C	-1.69964100	-1.31860300	-0.23775100
C	0.95760500	-2.66025900	2.49222100
H	0.49781500	-3.03812100	1.57608600
H	0.19272200	-2.61035100	3.27289100
H	1.72381200	-3.36157700	2.82955700
C	-2.63913000	-0.18664600	1.78023500
H	-1.62680400	0.21133700	1.70574400
C	-4.26138800	-3.49392600	-1.74186200
H	-3.82331200	-4.49851200	-1.71785300
H	-4.31297300	-3.17388700	-2.78943900
H	-5.28453700	-3.56912500	-1.36911500
C	4.22696600	-1.33579800	-0.20605300
C	-3.48919500	-2.53329200	-0.90384600
C	3.63935000	-1.87074100	0.90392200
C	1.51794400	-1.25775300	2.25780500
H	0.68685200	-0.61271700	1.97370000

C	-0.02250900	0.33843000	-0.14013500
C	-3.60418500	0.99901600	1.76624800
H	-3.50090400	1.54959300	0.82863000
H	-3.36059200	1.66909400	2.59667100
H	-4.64304400	0.68593200	1.89242300
C	3.85594300	1.94352400	-1.48283800
H	4.11874900	2.53645800	-2.36423000
H	4.67162900	2.02110300	-0.75763700
H	2.94649700	2.35072000	-1.03638000
C	-2.73710100	-1.03777300	3.05071800
H	-3.75020700	-1.40967100	3.22366900
H	-2.45630900	-0.42723100	3.91493200
H	-2.05958000	-1.89383300	2.99576400
C	0.43770300	3.48550200	1.17248100
H	1.00608000	2.59906900	1.48239100
C	-1.76515000	3.89993900	-0.88529800
H	-2.50230800	3.80284400	-0.07759700
C	-5.25155300	-1.66060500	0.75341800
H	-5.24356100	-1.77844200	1.84049800
H	-5.88703900	-2.44794700	0.34278700
H	-5.72336300	-0.69927000	0.52216200
C	-3.88932100	-1.76884400	0.15376700
C	-0.90415900	-1.72570000	-3.21556400
H	-1.77917000	-1.18978500	-3.59537800
H	-0.37976100	-2.17728000	-4.06340900
H	-0.23744700	-1.01161200	-2.72952700
C	4.12521000	-2.99362300	1.75838400
H	4.10837900	-2.74824400	2.82395000
H	5.15794500	-3.22694800	1.49127000
H	3.53027000	-3.90198500	1.61267800
C	2.53388500	0.32552100	-2.95221600
H	2.38587200	-0.72937100	-3.20073300
H	2.83325800	0.85580600	-3.86143500
H	1.58878700	0.74095500	-2.59762400
C	3.62742400	0.48641500	-1.89384300
H	4.55965300	0.08831600	-2.30169400
C	5.51824200	-1.67622400	-0.86796600
H	5.36955400	-2.04672200	-1.88937700
H	6.02614500	-2.46024200	-0.30337800
H	6.19147600	-0.81257300	-0.91767200

C	-0.13861000	-3.62737700	-1.68763600
H	0.56003600	-2.97197600	-1.16382800
H	0.37776800	-4.11359500	-2.52128100
H	-0.48366700	-4.40411500	-0.99798000
C	-1.32223100	-2.82135500	-2.23147800
H	-2.00110800	-3.50759700	-2.74355400
C	2.19941800	-0.65049300	3.48838800
H	3.04010300	-1.25536400	3.83825000
H	1.47405700	-0.58368500	4.30545900
H	2.56540500	0.35667600	3.26782100
C	-0.61383400	3.80580300	2.24540800
H	-1.19413000	4.69763600	1.98736200
H	-1.30881500	2.97214600	2.38470000
H	-0.11766100	3.99764600	3.20223600
C	1.43047400	4.63388100	0.93897600
H	2.16749100	4.37794300	0.17168500
H	0.92836600	5.55660700	0.63675700
H	1.97158700	4.83948200	1.86874600
C	-1.38932900	5.37986300	-1.05688800
H	-0.57120000	5.50323700	-1.77491100
H	-2.25403100	5.92940000	-1.44209100
H	-1.09319600	5.84468500	-0.11328300
C	-2.36369200	3.30974100	-2.17498400
H	-1.65005500	3.38277100	-3.00375100
H	-2.63061200	2.25959800	-2.03907700
H	-3.25890500	3.87588200	-2.45242600
P	-0.35332600	2.86519700	-0.36815700
H	0.62316000	3.08941400	-1.36681800



**BIG-P2+H<sup>+</sup>**

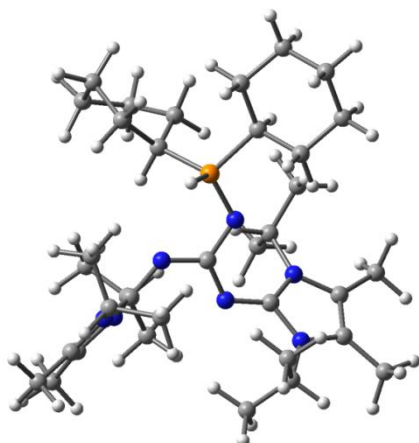
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N	1.20367400	2.78053900	-1.26124700
N	-3.40948800	-0.67149900	-0.69674600
N	1.15601700	-0.91285600	0.01674700
C	-2.37453600	-0.30238500	0.11576600
C	1.06626300	1.87537300	-0.24738600
C	-2.04533000	2.61569400	2.25807500
H	-1.65151100	3.02540900	1.32497100
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H	-3.01410000	3.07152700	2.47303800
C	2.24306900	1.39630600	1.89860800
H	1.46511600	0.63256900	1.85721200
C	2.80752700	4.58363900	-2.03693900
H	2.05780100	5.37671500	-2.14026500
H	3.00288200	4.17313300	-3.03489900
H	3.73167600	5.04447900	-1.68335500
C	-4.56447900	0.03989800	-0.35041900
C	2.37065300	3.53004300	-1.07745900
C	-4.23799700	0.86148900	0.68894200
C	-2.12715200	1.09219100	2.16921900
H	-1.11940400	0.71704000	1.99298400
C	-0.01445100	-0.21662000	0.03653700
C	3.58240700	0.68636200	2.09210500
H	3.77793900	0.01734800	1.25140400
H	3.54089800	0.08932100	3.00757600
H	4.41145900	1.38927800	2.19546700
C	-3.14703000	-3.09554700	-1.12562300
H	-3.15605900	-3.85779800	-1.91085300
H	-3.95076700	-3.31871100	-0.41752400
H	-2.19199100	-3.13524200	-0.59718000
C	1.91289000	2.38033400	3.02563700
H	2.68695100	3.14349500	3.14374600
H	1.83506600	1.83523100	3.97174300
H	0.96081500	2.88133000	2.83346600
C	1.26961700	-3.42917300	1.44744300
C	2.58737700	-2.86781400	-1.35684000
C	4.24864900	3.53083700	0.67891200
H	4.14948300	3.76341100	1.74302700
H	4.58757500	4.43835600	0.17492600



H	5.03607200	2.77685000	0.57079400
C	2.96167100	3.08464100	0.06927900
C	0.26851100	1.62839000	-3.24484600
H	1.27983200	1.36903600	-3.57206900
H	-0.35518900	1.77346200	-4.13238100
H	-0.13710400	0.80005800	-2.66201300
C	-5.09700300	1.87043600	1.37538100
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H	-6.13260500	1.73653600	1.05598200
H	-4.80087400	2.89505100	1.12442900
C	-2.28240900	-1.37586700	-2.80437300
H	-2.44478900	-0.37495400	-3.21436500
H	-2.34839300	-2.09938600	-3.62282400
H	-1.28116300	-1.42164300	-2.37206200
C	-3.33993600	-1.71055400	-1.75021300
H	-4.32148900	-1.67668500	-2.22918500
C	-5.85537100	-0.12371000	-1.07717200
H	-5.76513300	0.14260400	-2.13725100
H	-6.61168100	0.52830500	-0.63640300
H	-6.22894800	-1.15274000	-1.01940800
C	-1.11868500	3.34735900	-1.95881400
H	-1.57949100	2.57005100	-1.34614100
H	-1.74124300	3.53002700	-2.84036100
H	-1.06596500	4.27367400	-1.37819800
C	0.27859200	2.91253400	-2.41188900
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C	-2.67516000	0.42822700	3.43683300
H	-3.68523300	0.76887300	3.67967700
H	-2.02677000	0.67644300	4.28312800
H	-2.69388700	-0.65970200	3.32362600
C	1.68702500	-4.89931400	1.28385200
H	2.73702100	-4.99783700	0.99563700
H	1.55821900	-5.40599300	2.24724900
H	1.06775200	-5.42324800	0.54862900
C	2.21713600	-2.70248200	2.41643200
H	2.17692300	-3.20385500	3.39010300
H	3.25418700	-2.71451300	2.07113500
H	1.90873500	-1.66285900	2.54781000
C	2.37116900	-1.87498900	-2.52032400
H	2.45737000	-0.84290500	-2.17572000

H	3.13102800	-2.06752900	-3.28640100
H	1.38571000	-2.00507300	-2.98253000
C	2.48212100	-4.30295000	-1.90608600
H	3.20049800	-4.41479000	-2.72590700
H	2.71494700	-5.05924500	-1.15514300
H	1.48420300	-4.50754800	-2.30916300
C	3.96488400	-2.62071400	-0.72079000
H	4.73784900	-2.72119400	-1.49108200
H	4.02911200	-1.61131900	-0.30452100
H	4.18550100	-3.34429900	0.06939700
C	-0.16808400	-3.36597800	2.00802900
H	-0.52417400	-2.33581500	2.08534400
H	-0.86956300	-3.91802300	1.37461700
H	-0.17211700	-3.82381900	3.00417400
P	1.21538300	-2.50966400	-0.16502900
H	0.09637500	-3.07784600	-0.81310100



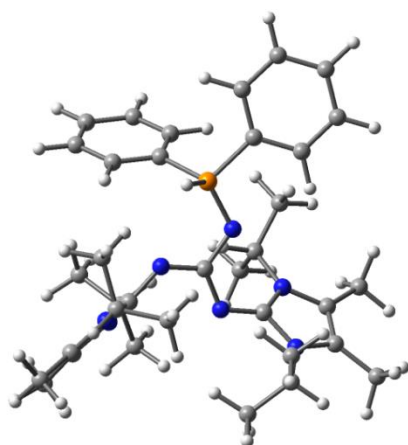
**BIG-P3+H<sup>+</sup>**

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N	-0.12004300	2.97381300	1.05828900
N	-1.50511700	3.41387400	-0.58017100
N	-2.62983400	-2.26666100	-1.38054400
N	1.01426600	0.41392000	-0.34196500
C	-1.99135800	-1.53075200	-0.42511400
C	2.15328000	-4.01791300	2.73541000
H	2.39968800	-4.71388800	3.54302800
H	1.08840800	-4.16689500	2.51139600
C	2.39680500	-2.56112400	3.19691100
H	1.49782700	-2.17649100	3.69308100
H	3.20324000	-2.53136900	3.93774200

C	-0.91458100	2.39024600	0.10377900
C	-3.35993700	0.17640900	2.46946600
H	-3.48525800	0.95305100	1.71121100
H	-2.91774800	0.62745800	3.36273200
H	-4.33933000	-0.21576500	2.75149300
C	0.53642500	2.19026300	2.12877500
H	0.37147300	1.15677700	1.82402600
C	-1.52176700	5.94771700	-0.62969300
H	-2.61062900	6.06248700	-0.57543000
H	-1.22255500	6.06631500	-1.67798700
H	-1.07329600	6.76634000	-0.06383900
C	-3.89833200	-2.64263000	-0.92272400
C	-1.07423300	4.64192800	-0.06749200
C	-4.04508800	-2.12813200	0.33312300
C	6.14498100	-0.45780800	-1.21495100
H	6.90576900	-1.21323700	-1.44026700
H	6.43034100	0.00722900	-0.26092300
C	-2.42493000	-0.91573100	1.95108000
H	-1.46280300	-0.45111500	1.73612000
C	6.10821500	0.61249500	-2.31157900
H	7.08343200	1.10518400	-2.38990700
H	5.91600000	0.13197000	-3.28121900
C	-0.31941800	0.13888500	-0.29215200
C	2.45804900	-3.49346300	0.28458500
H	3.23784300	-3.42523000	-0.48151500
H	1.60229200	-3.99174300	-0.18385900
C	2.04676700	2.42575600	2.16101200
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H	2.29955900	3.42855700	2.51281300
C	-0.89836000	-3.62733300	-2.51708700
H	-0.53785500	-3.95027900	-3.49853100
H	-1.22228300	-4.51166400	-1.95969700
H	-0.07909600	-3.14851300	-1.97682200
C	-0.14460400	2.41538900	3.48288100
H	0.05047900	3.41258800	3.88543700
H	0.24029100	1.68649200	4.20350500
H	-1.22630300	2.28229600	3.39888700
C	2.00541700	-2.08652700	0.75636300
H	0.93748800	-2.13029400	1.00248200

C	3.68036100	-0.09841500	-0.76778000
H	3.89478400	0.39558500	0.19095900
C	0.56705000	5.33989100	1.78474500
H	0.46100500	5.15491300	2.85725500
H	0.20545500	6.35152800	1.58921700
H	1.63537300	5.31718700	1.54296100
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C	-1.67845800	2.57694100	-2.90604500
H	-0.77795200	3.13849600	-3.17215900
H	-2.33624200	2.54282200	-3.78011400
H	-1.39245600	1.55795500	-2.64077400
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H	-4.98921500	-2.52415000	2.23756000
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C	4.77999100	-1.14191700	-1.04594200
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H	-2.66813700	4.26771700	-2.03275900

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H	4.02661900	-4.11014600	1.66341400
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H	-1.50796400	-2.79995700	2.52793600
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H	1.82050600	-1.56574200	-1.75591700

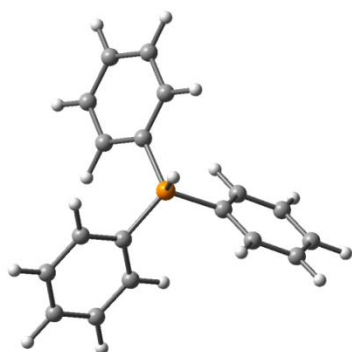


**BIG-P4+H<sup>+</sup>**

N	-3.00763800	-0.34308800	0.80410700
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N	1.37433200	2.47247800	1.02345400
N	0.28267700	3.61351700	-0.49417000
N	-3.36939000	-0.94303800	-1.27001700
N	1.15534800	-0.15195400	-0.62772900
C	-2.38193600	-0.65027600	-0.37523800
C	0.35371700	2.39266400	0.11024600
C	-2.59793300	1.16975200	2.74227400
H	-2.47374400	1.99619300	2.03785300
H	-1.91997200	1.32346400	3.58652900
H	-3.61672800	1.18014400	3.13526900
C	1.62213400	1.41249400	2.02791500
H	0.96950300	0.59979400	1.70775800
C	1.46285300	5.85624000	-0.45983400
H	0.56153600	6.46479100	-0.32207900
H	1.73043900	5.88671100	-1.52282000

H	2.27197400	6.33106100	0.09813600
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H	-0.98637000	3.44286400	-3.66397100
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H	-2.36704600	-0.50248300	-4.51208200
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C	-3.15669900	-1.32793900	-2.68583600
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H	-6.03399100	-0.35149300	-2.21012300

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C	-2.10643300	3.87788100	-1.14360100
H	-2.37065500	2.84735300	-0.89873900
H	-2.75325900	4.23602000	-1.95066200
H	-2.27547800	4.50626100	-0.26352100
C	-0.64586600	3.96314600	-1.59656700
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C	3.23813600	-1.80180700	-1.26102300
C	3.89633200	-3.04011500	-1.25745600
C	3.93755900	-0.63421000	-1.59450100
C	5.24850400	-3.10682600	-1.58418000
H	3.35685800	-3.94489700	-0.99002300
C	5.29106500	-0.70934500	-1.91803800
H	3.40936600	0.31393300	-1.59074100
C	5.94548400	-1.94222200	-1.91315400
H	5.75914800	-4.06495900	-1.57910500
H	5.83581200	0.19437600	-2.17488400
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C	1.15440300	-2.84564200	0.48193300
C	0.03721100	-3.68989700	0.44480100
C	1.98500800	-2.83563600	1.61164100
C	-0.24480300	-4.51868900	1.52899300
H	-0.61030700	-3.68621200	-0.42632000
C	1.69427000	-3.65968200	2.69647500
H	2.86264400	-2.19591700	1.63157400
C	0.57957400	-4.50020500	2.65572000
H	-1.10675000	-5.17871300	1.49601400
H	2.34191300	-3.65601400	3.56825100
H	0.35850100	-5.14736900	3.49938600
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H	0.80566700	-2.32099900	-1.95382600



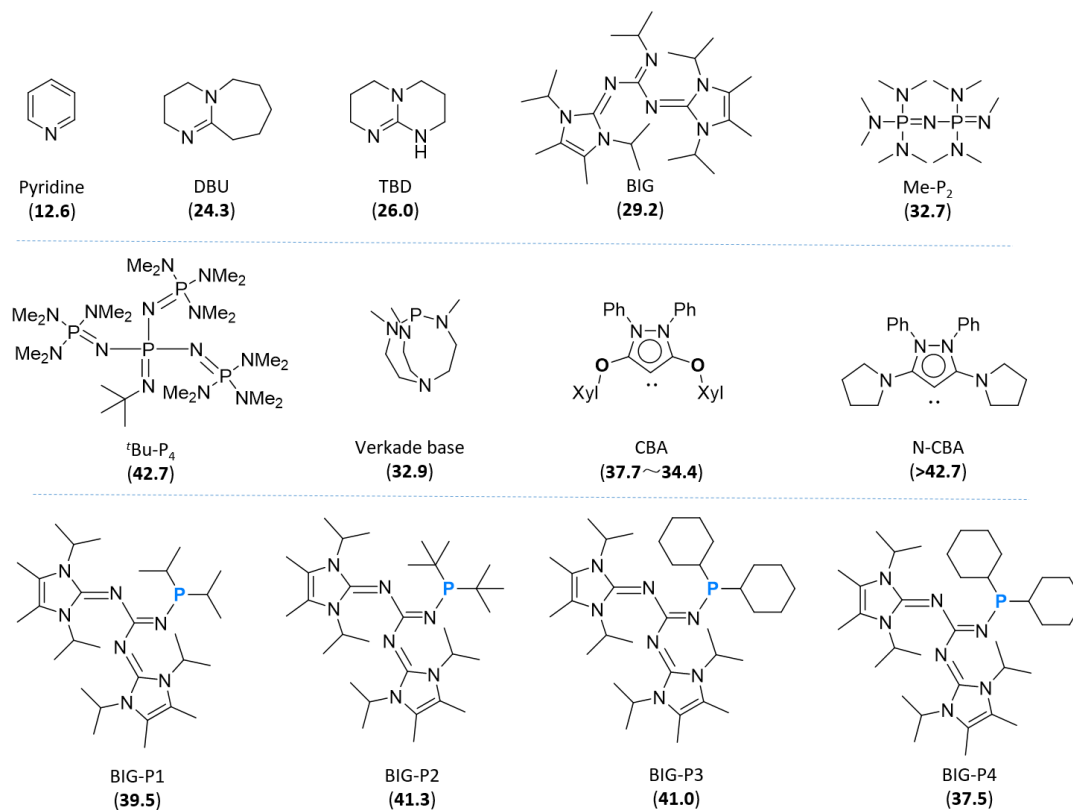
**PPh<sub>3</sub>+H<sup>+</sup>**

C	-0.39946100	1.65867900	-0.32757000
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C	-1.79984500	3.61558000	-0.51040900
H	-2.01503100	1.87793200	-1.76080400
C	-0.03587700	3.52944800	1.15187400
H	1.14183600	1.72301100	1.18931700
C	-1.08948800	4.20771100	0.53777800
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C	2.75737300	0.10202000	-0.94220700
C	3.07835700	-1.73945000	1.14592000
H	0.92526200	-1.86142100	1.18125600
C	4.03248900	-0.24221400	-0.50621800
H	2.63368700	0.81727900	-1.75114900
C	4.19160800	-1.15956500	0.53634500
H	3.20763200	-2.45424500	1.95227500
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C	-1.23741000	-1.17673300	-0.32734000
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C	-3.04903200	-1.79041500	1.14315300
H	-2.07546400	0.13399800	1.17592500
C	-3.10380100	-3.04563100	0.53616500
H	-2.27893800	-4.34600500	-0.97605100
H	-3.73437300	-1.54215600	1.94722100



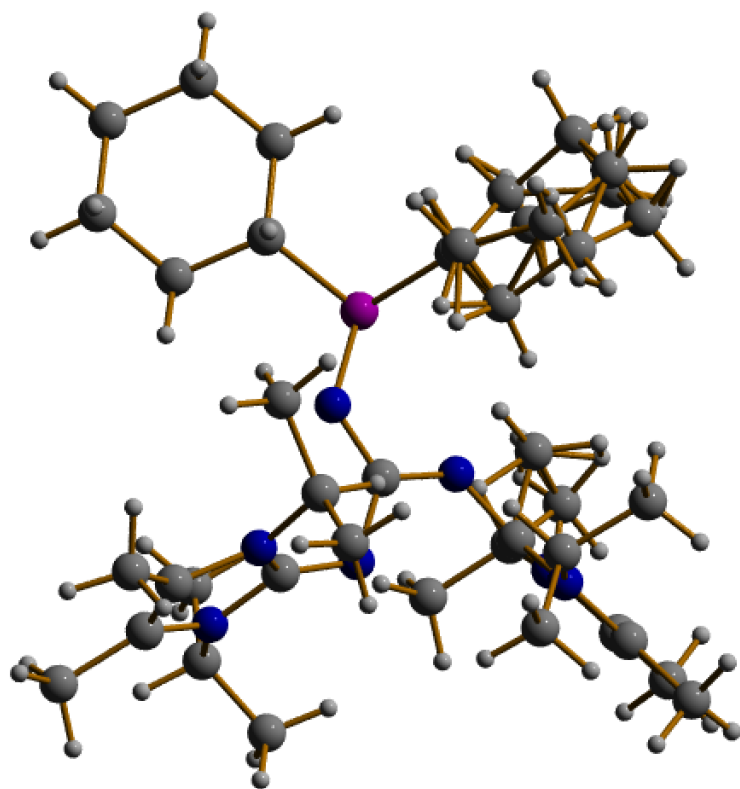
H	-3.83527500	-3.77483700	0.87059700
P	0.00048300	-0.00099100	-0.85314700
H	0.00044700	-0.00048200	-2.25767300

### 5.5 The $pK_{BH^+}$ of representative organobases in $CH_3CN$ .

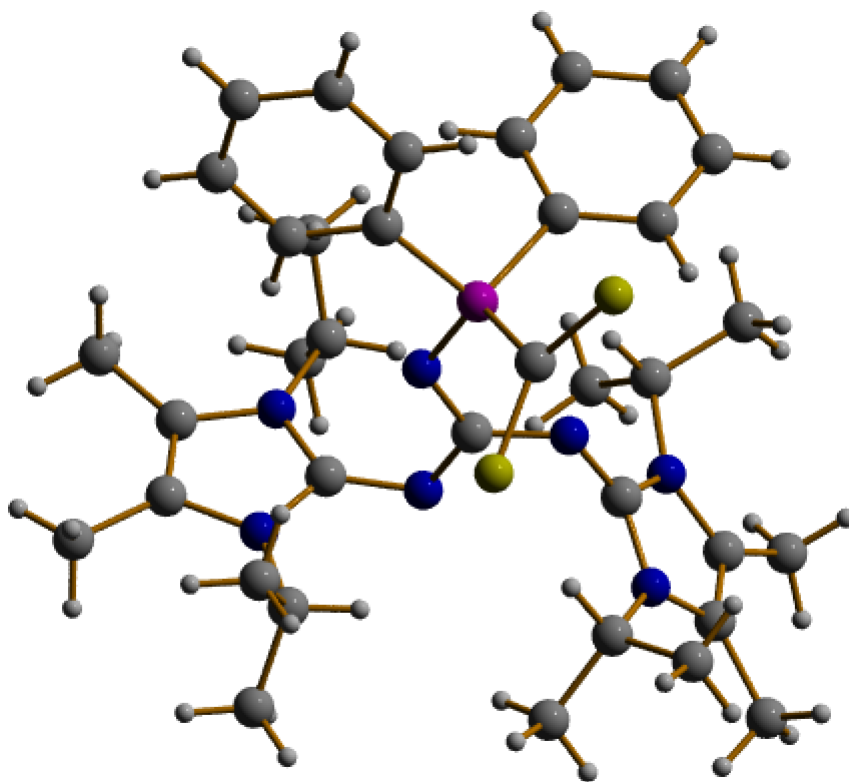


**Figure S18.** The  $pK_{BH^+}$  of representative organobases in  $CH_3CN$ .

## 6. X-ray single-crystal structure



A



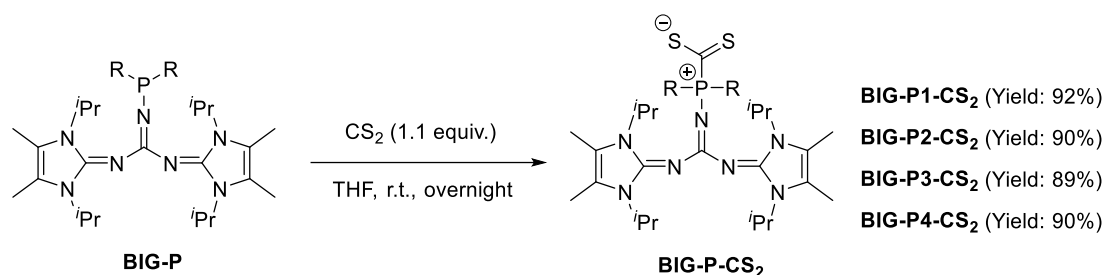
B

**Figure S19.** Solid-state structure of **BIG-P3** (A) and **BIG-P4-CS<sub>2</sub>** (B).

**Table S2.** Crystallographic data and structure refinement for **BIG-P3** and **BIG-P4-CS<sub>2</sub>**.

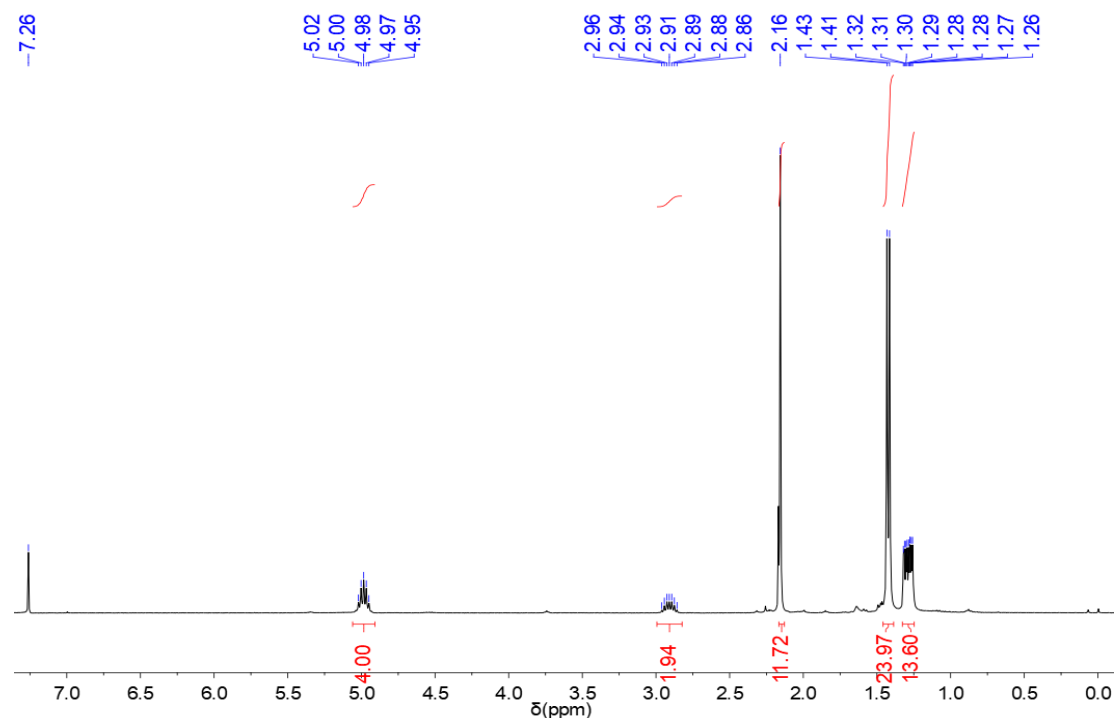
Identification code	<b>BIG-P3</b>	<b>BIG-P4-CS<sub>2</sub></b>
CCDC number	<b>2164342</b>	<b>2272051</b>
Empirical formula	C <sub>35</sub> H <sub>62</sub> N <sub>7</sub> P	C <sub>36</sub> H <sub>50</sub> N <sub>7</sub> PS <sub>2</sub>
Formula weight	611.88	675.92
Temperature/K	150	272
Crystal system	monoclinic	monoclinic
Space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /n
<i>a</i> /Å	11.1956(5)	11.3245(15)
<i>b</i> /Å	16.7938(7)	18.881(3)
<i>c</i> /Å	21.6192(10)	17.927(2)
<i>α</i> /°	90	90
<i>β</i> /°	94.677(2)	98.208(4)
<i>γ</i> /°	90	90
Volume/Å <sup>3</sup>	4051.2(3)	3794.0(9)
Z	4	4
$\rho_{\text{calc}}/\text{cm}^3$	1.003	1.183
$\mu/\text{mm}^{-1}$	0.098	0.217
F(000)	1344	1448
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)	MoK $\alpha$ ( $\lambda$ = 0.71073)
2 $\theta$ range for data collection/°	4.382 to 49.996	4.012 to 49.98
Index ranges	-13 ≤ <i>h</i> ≤ 13, -19 ≤ <i>k</i> ≤ 19, -25 ≤ <i>l</i> ≤ 25	-13 ≤ <i>h</i> ≤ 13, -22 ≤ <i>k</i> ≤ 22, -21 ≤ <i>l</i> ≤ 21
Reflections collected	49880	36147
Independent reflections	7117 [R <sub>int</sub> = 0.1430, R <sub>sigma</sub> = 0.0865]	6578 [R <sub>int</sub> = 0.0591, R <sub>sigma</sub> = 0.0611]
Data/restraints/parameters	7117/148/456	6578/0/427
Goodness-of-fit on F <sup>2</sup>	1.037	1.098
Final R indexes [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )]	R <sub>1</sub> = 0.0661, wR <sub>2</sub> = 0.1802	R <sub>1</sub> = 0.0671, wR <sub>2</sub> = 0.1510
Final R indexes [all data]	R <sub>1</sub> = 0.1179, wR <sub>2</sub> = 0.2055	R <sub>1</sub> = 0.1229, wR <sub>2</sub> = 0.1720
Largest diff. peak/hole / e Å <sup>-3</sup>	0.31/-0.30	0.38/-0.31

## 7. General synthetic procedure for BIG-Ps-CS<sub>2</sub>

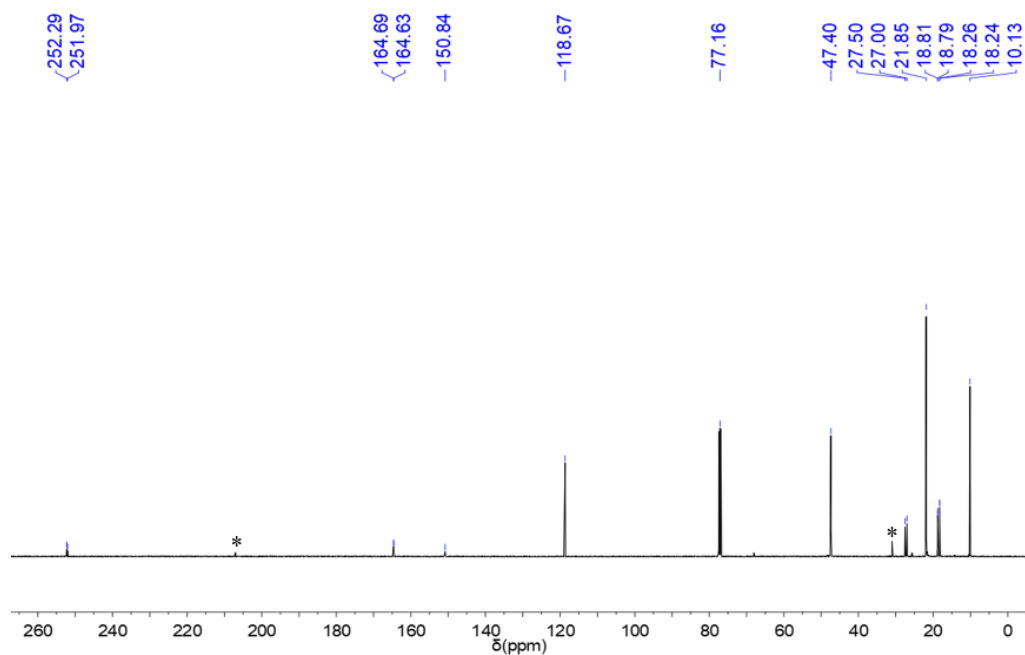


In an argon-filled glovebox, **BIG-Ps** (0.1 mmol) was dissolved in THF (2 mL). CS<sub>2</sub> (8.4 mg, 0.11 mmol, 1.1 eq) was added dropwise and the reaction mixture was stirred overnight. All volatiles were removed in vacuo. The residue was washed with *n*-hexane (5 mL) and dried under vacuum for 2 h to obtain the pink product.

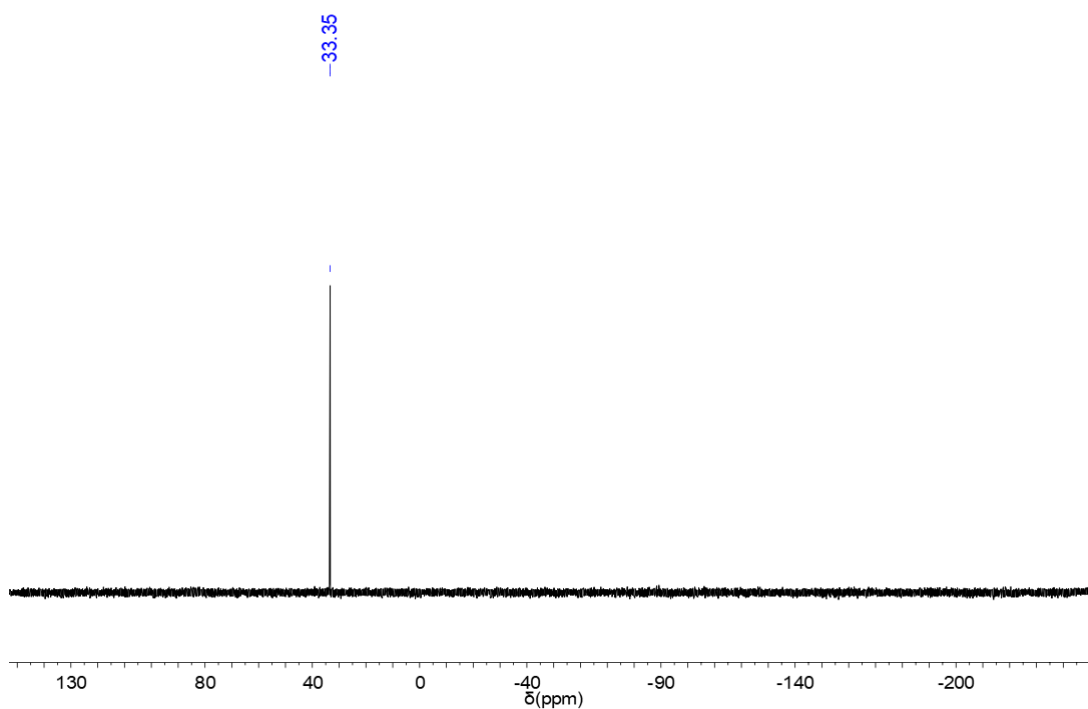
**BIG-P1-CS<sub>2</sub>** (56 mg, 92% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 4.98 (dt, *J* = 14.2, 7.1 Hz, 4H), 2.91 (tt, *J* = 14.3, 7.1 Hz, 2H), 2.16 (s, 12H), 1.42 (d, *J* = 7.1 Hz, 24H), 1.29 (ddd, *J* = 14.6, 7.1, 3.3 Hz, 12H). <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, CDCl<sub>3</sub>) δ 252.1 (d, *J* = 40.2 Hz), 164.7 (d, *J* = 7.4 Hz), 150.8 (s), 118.7 (s), 47.4 (s), 27.3 (d, *J* = 62.3 Hz), 21.9 (s), 18.8 (d, *J* = 2.1 Hz), 18.3 (d, *J* = 2.6 Hz), 10.1 (s). <sup>31</sup>P{<sup>1</sup>H} NMR (162 MHz, CDCl<sub>3</sub>) δ 33.4 (s). HRMS (ESI): [C<sub>29</sub>H<sub>55</sub>N<sub>7</sub>P]<sup>+</sup>[M-CS<sub>2</sub>+H]<sup>+</sup>: calcd. 532.4251, found 532.4254 *m/z*. IR (Film): 2974, 2933, 2870, 2055, 1550, 1497, 1418, 1216, 1105, 1024, 998, 913, 729, 684, 547 cm<sup>-1</sup>.



**Figure S20:** <sup>1</sup>H NMR spectrum of **BIG-P1-CS<sub>2</sub>** in CDCl<sub>3</sub>.

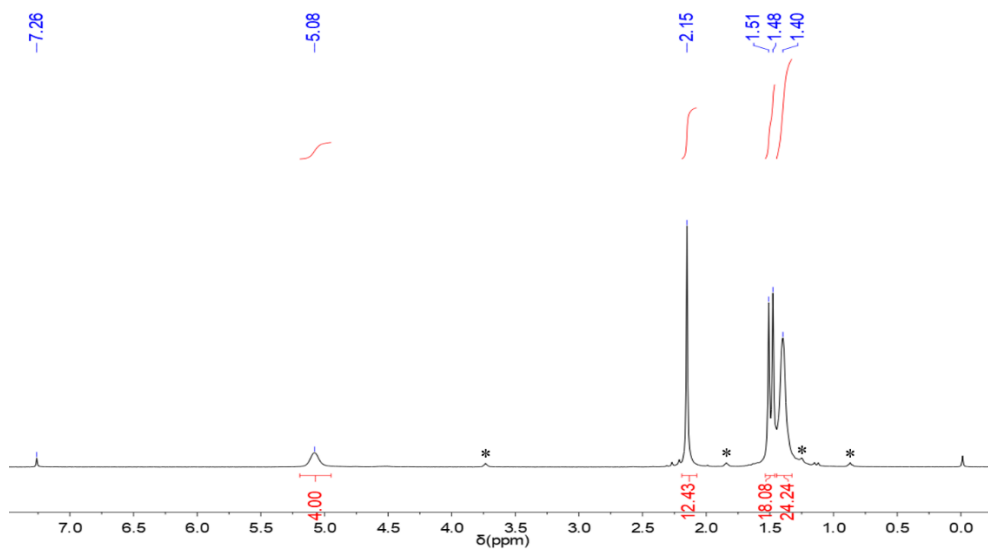


**Figure S21:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P1-CS<sub>2</sub>** in  $\text{CDCl}_3$ . \* denote acetone.

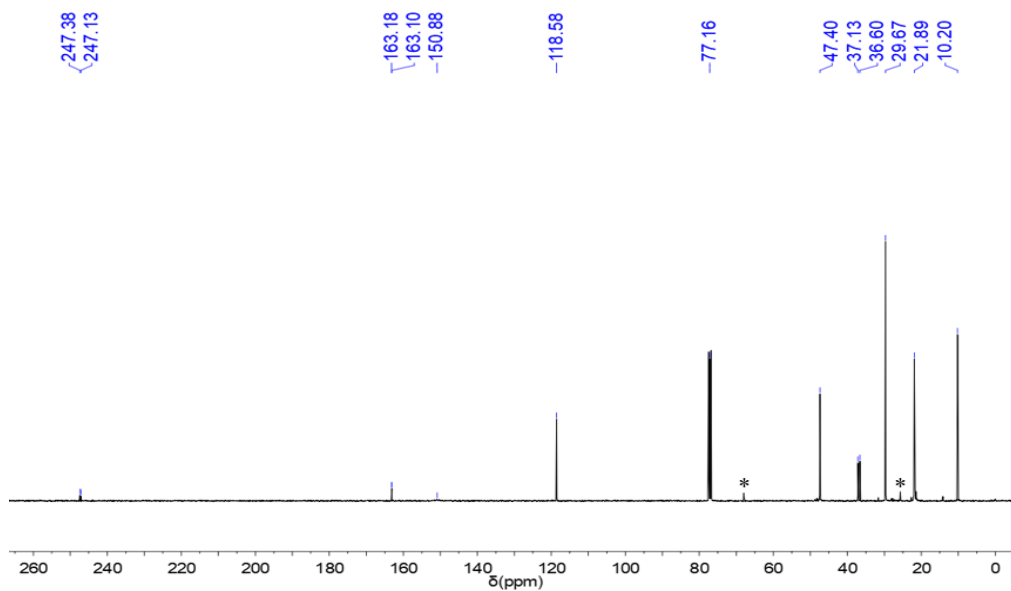


**Figure S22:**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P1-CS<sub>2</sub>** in  $\text{CDCl}_3$ .

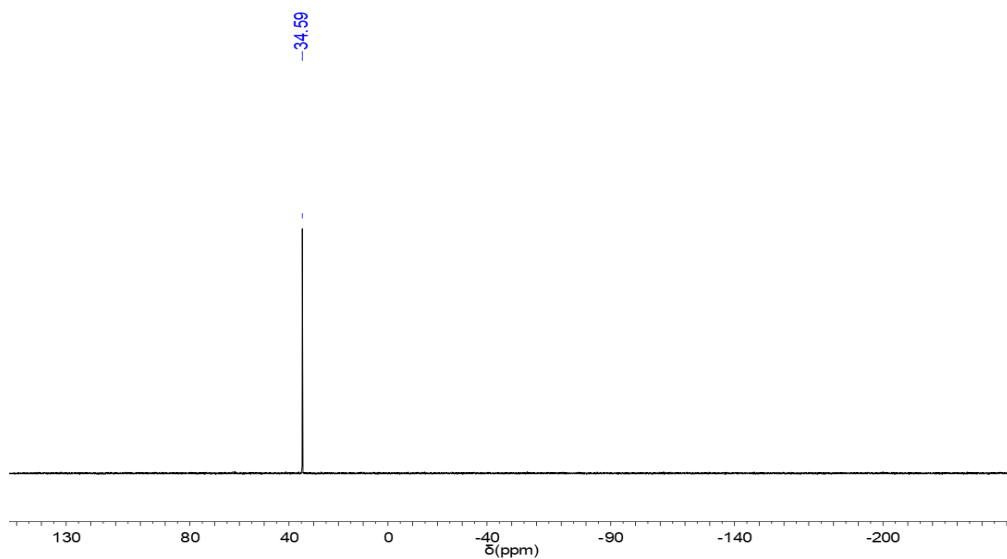
**BIG-P2-CS<sub>2</sub>** (57 mg, 90% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  5.08 (s, 4H), 2.15 (s, 12H), 1.49 (d,  $J = 13.1$  Hz, 18H), 1.40 (s, 24H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  247.3 (d,  $J = 24.9$  Hz), 163.1 (d,  $J = 8.5$  Hz), 150.9 (s), 118.6 (s), 47.4 (s), 36.9 (d,  $J = 52.9$  Hz), 29.7 (s), 21.9 (s), 10.2 (s).  $^{31}\text{P}\{^1\text{H}\}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  34.6 (s). **HRMS** (ESI):  $[\text{C}_{31}\text{H}_{59}\text{N}_7\text{P}]^+[\text{M-CS}_2+\text{H}]^+$ : calcd. 560.4564, found 560.4568 m/z. **IR** (Film): 2969, 2932, 2876, 2055, 1552, 1497, 1417, 1214, 1104, 1016, 911, 813, 724, 628, 590, 522  $\text{cm}^{-1}$ .



**Figure S23:**  $^1\text{H}$  NMR spectrum of **BIG-P2-CS<sub>2</sub>** in  $\text{CDCl}_3$ . \* denote THF and *n*-hexane.

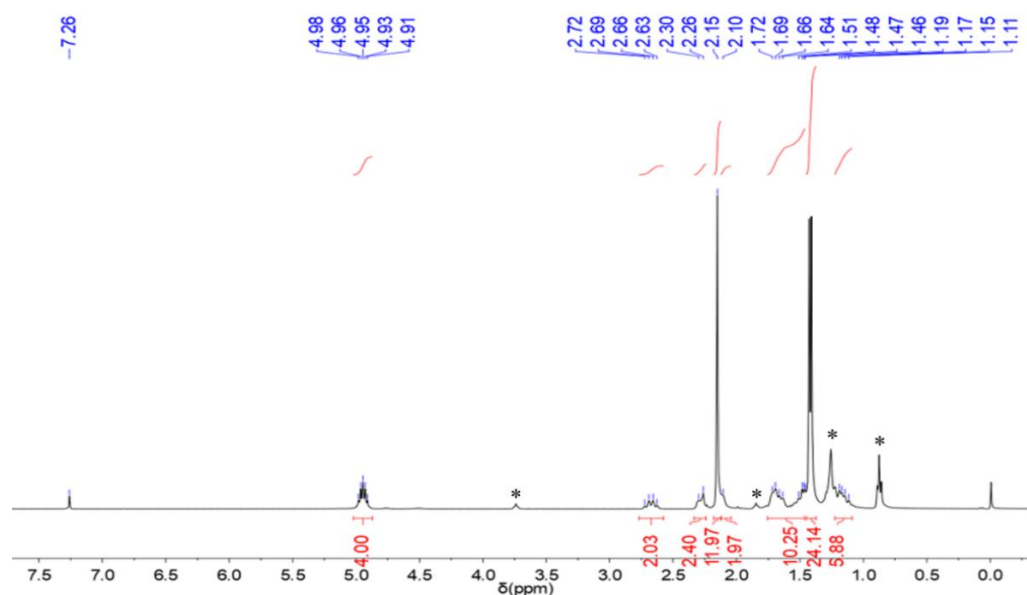


**Figure S24:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P2-CS<sub>2</sub>** in  $\text{CDCl}_3$ . \* denote THF.

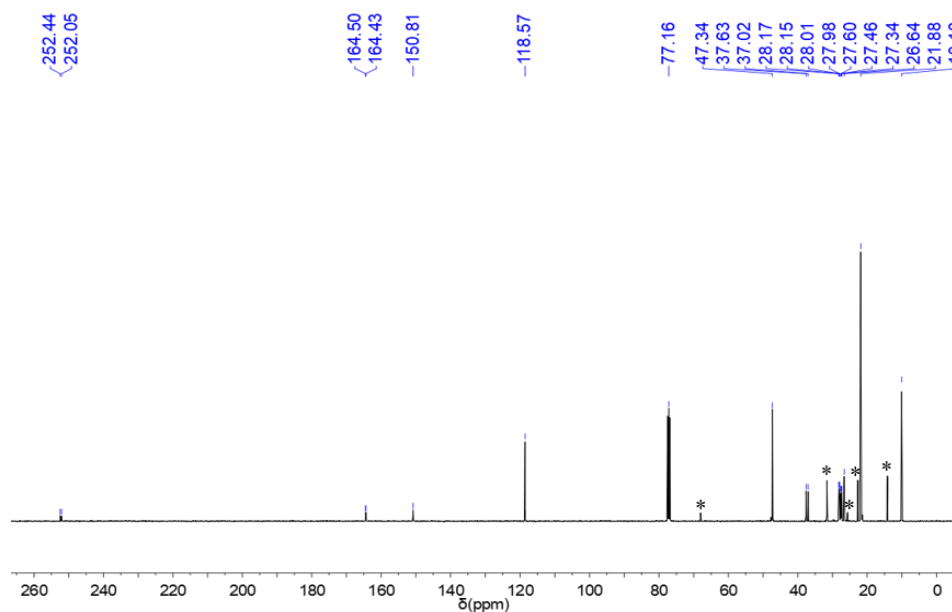


**Figure S25:**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P2-CS<sub>2</sub>** in  $\text{CDCl}_3$ .

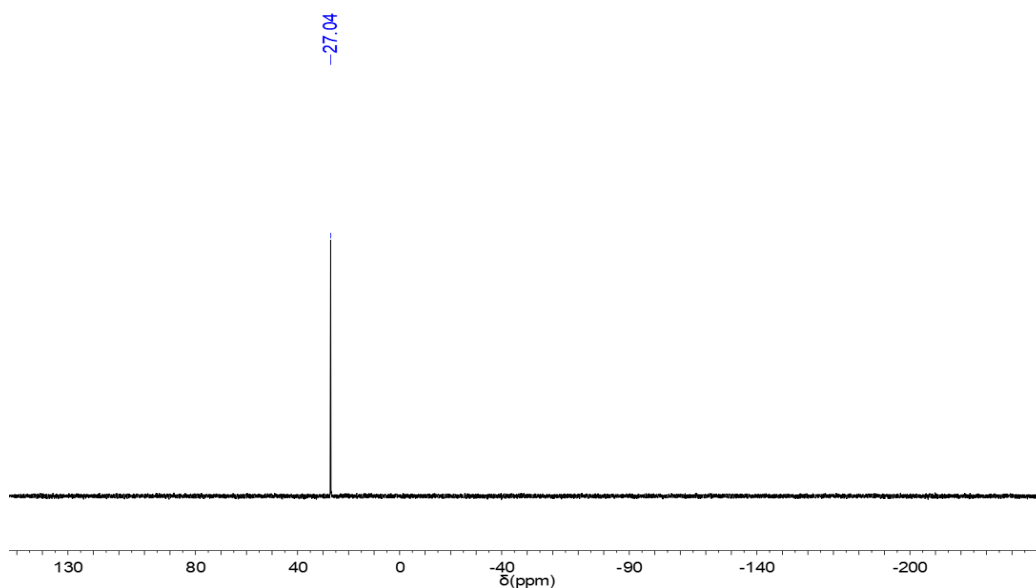
**BIG-P3-CS<sub>2</sub>** (61 mg, 89% yield). **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 4.95 (dt, 7.0 Hz, 4H), 2.67 (dd, *J* = 26.1, 12.5 Hz, 2H), 2.28 (d, *J* = 14.3 Hz, 2H), 2.15 (s, 12H), 2.10 (s, 2H), 1.58 (ddd, *J* = 21.5, 15.9, 6.6 Hz, 10H), 1.42 (d, *J* = 7.1 Hz, 24H), 1.15 (dd, *J* = 19.4, 10.3 Hz, 6H). **<sup>13</sup>C{<sup>1</sup>H} NMR** (101 MHz, CDCl<sub>3</sub>) δ 252.2 (d, *J* = 39.9 Hz), 164.5 (d, *J* = 7.1 Hz), 150.8 (s), 118.6 (s), 47.3 (s), 37.3 (d, *J* = 61.1 Hz), 28.1 (dd, *J* = 16.7, 2.6 Hz), 27.5 (dd, *J* = 26.1, 11.9 Hz), 26.6 (s), 21.9 (s), 10.1 (s). **<sup>31</sup>P{<sup>1</sup>H} NMR** (162 MHz, CDCl<sub>3</sub>) δ 27.0 (s). **HRMS** (ESI): [C<sub>35</sub>H<sub>63</sub>N<sub>7</sub>P]<sup>+</sup>[M-CS<sub>2</sub>+H]<sup>+</sup>: calcd. 612.4877, found 612.4875 m/z. **IR** (Film): 2973, 2928, 2850, 2057, 1549, 1497, 1417, 1268, 1215, 1106, 1028, 941, 847, 730, 560 cm<sup>-1</sup>.



**Figure S26:** <sup>1</sup>H NMR spectrum of **BIG-P3-CS<sub>2</sub>** in CDCl<sub>3</sub>. \* denote THF and *n*-hexane.

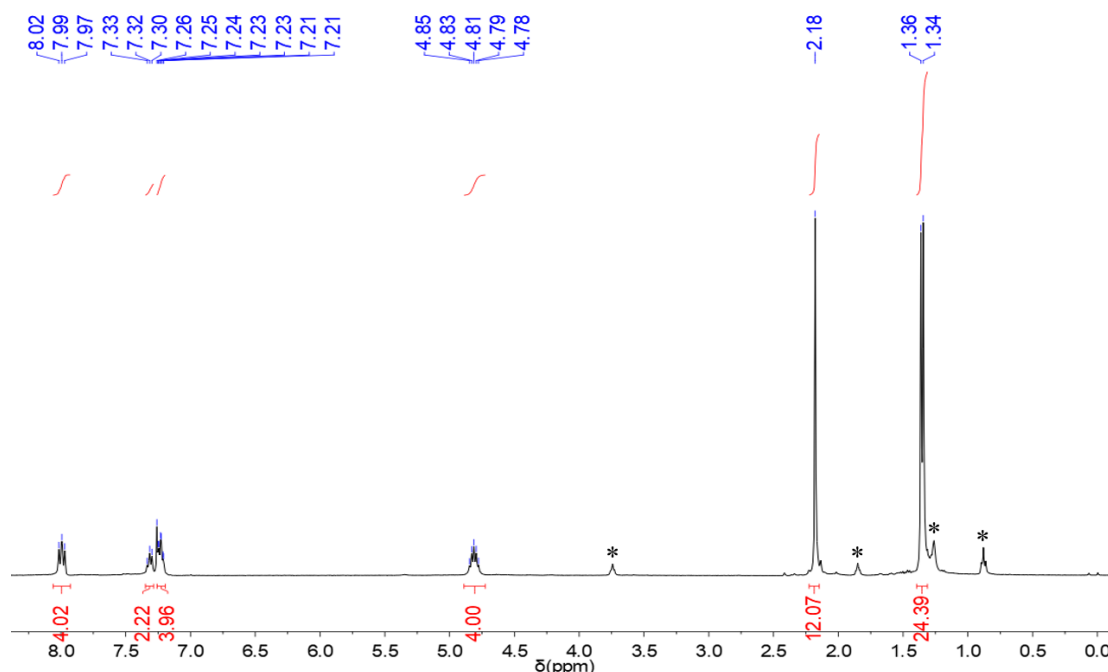


**Figure S27:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **BIG-P3-CS<sub>2</sub>** in CDCl<sub>3</sub>. \* denote THF and *n*-hexane.



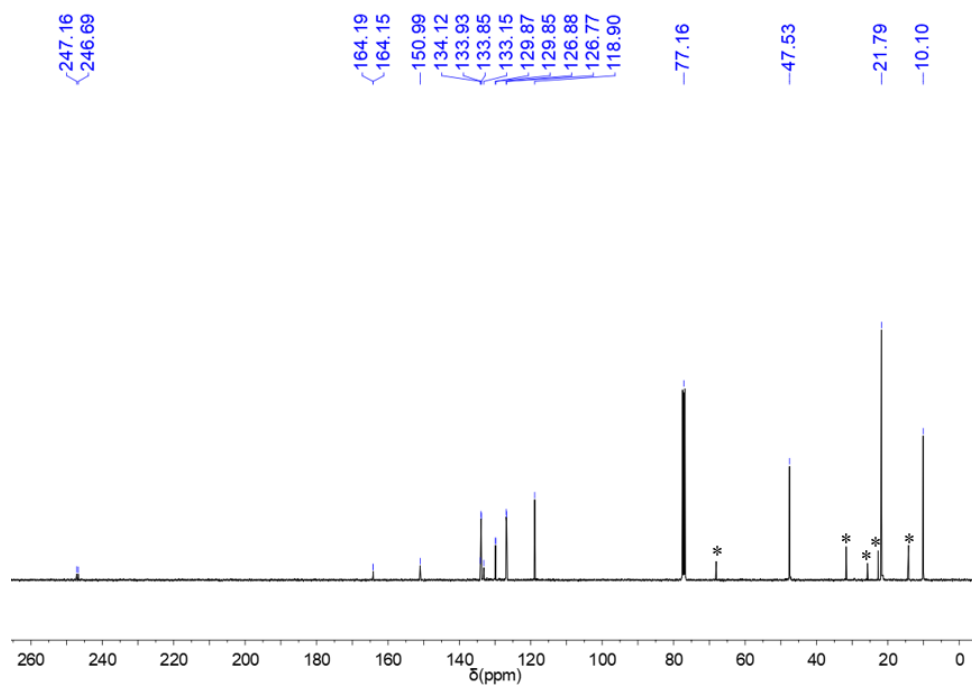
**Figure S28:**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P3-CS<sub>2</sub>** in  $\text{CDCl}_3$ .

**BIG-P4-CS<sub>2</sub>** (61 mg, 90% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02–7.97 (m, 4H), 7.32 (t,  $J = 7.1$  Hz, 2H), 7.23 (td,  $J = 7.5, 2.3$  Hz, 4H), 4.81 (dt,  $J = 13.9, 6.9$  Hz, 4H), 2.18 (s, 12H), 1.35 (d,  $J = 7.1$  Hz, 24H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  246.9 (d,  $J = 47.7$  Hz), 164.2 (d,  $J = 4.7$  Hz), 151.0 (s), 134.1 (s), 133.9 (d,  $J = 7.8$  Hz), 133.2 (s), 129.9 (d,  $J = 2.2$  Hz), 126.8 (d,  $J = 11.1$  Hz), 47.5 (s), 21.8 (s), 10.1 (s).  $^{31}\text{P}\{^1\text{H}\}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  3.5 (s). **HRMS** (ESI):  $[\text{C}_{35}\text{H}_{63}\text{N}_7\text{P}]^+[\text{M-CS}_2+\text{H}]^+$ : calcd. 600.3938, found 600.3944 m/z. **IR** (Film): 2964, 2925, 2853, 2056, 1547, 1498, 1430, 1216, 1107, 1040, 998, 944, 914, 729, 695, 544  $\text{cm}^{-1}$ .

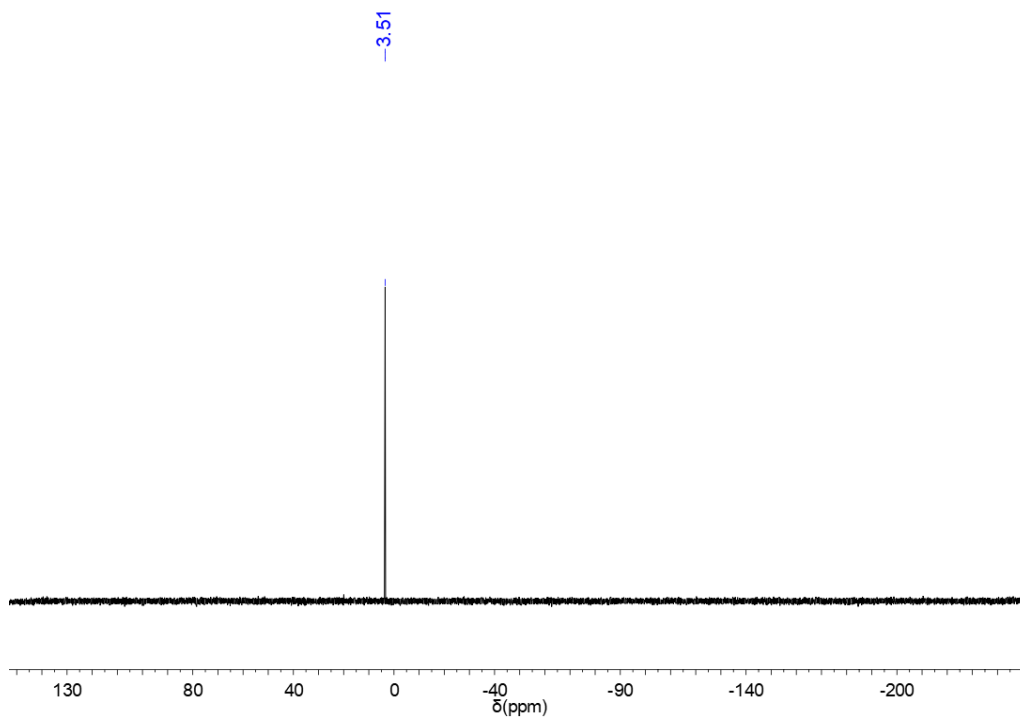


**Figure S29:**  $^1\text{H}$  NMR spectrum of **BIG-P4-CS<sub>2</sub>** in  $\text{CDCl}_3$ . \* denote THF and *n*-hexane.





**Figure S30:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **BIG-P4-CS<sub>2</sub>** in  $\text{CDCl}_3$ . \* denote THF and *n*-hexane.



**Figure S31:**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **BIG-P4-CS<sub>2</sub>** in  $\text{CDCl}_3$ .

## 8. TGA curves of BIG-Ps-CS<sub>2</sub>

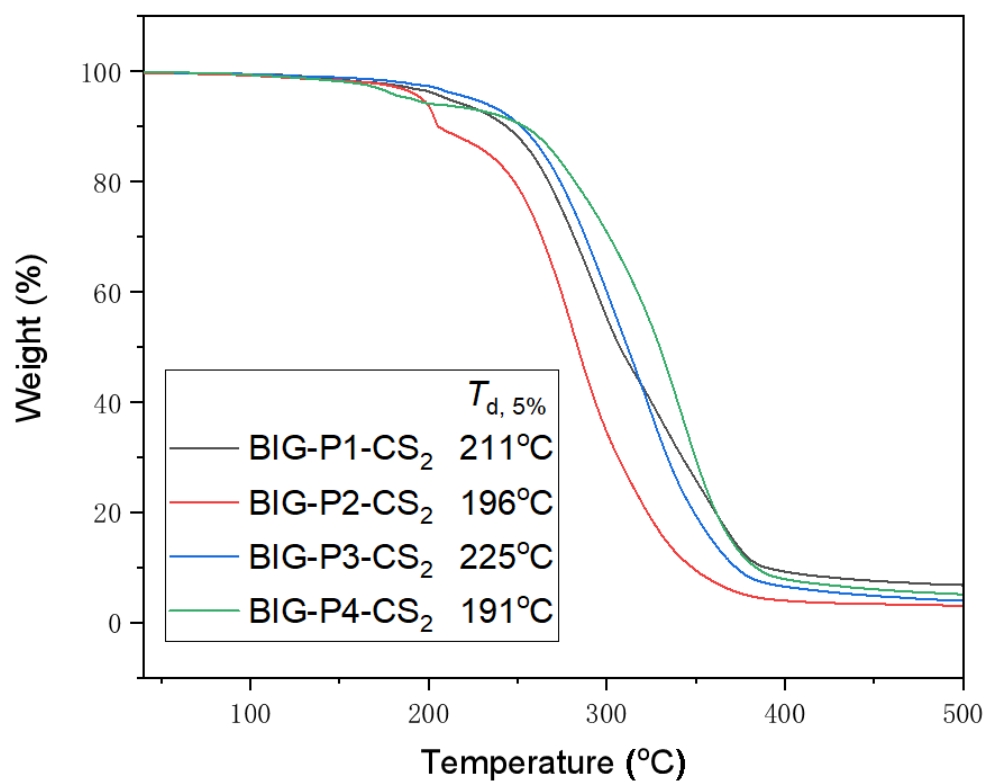


Figure S32. TGA curves of BIG-Ps-CS<sub>2</sub>.

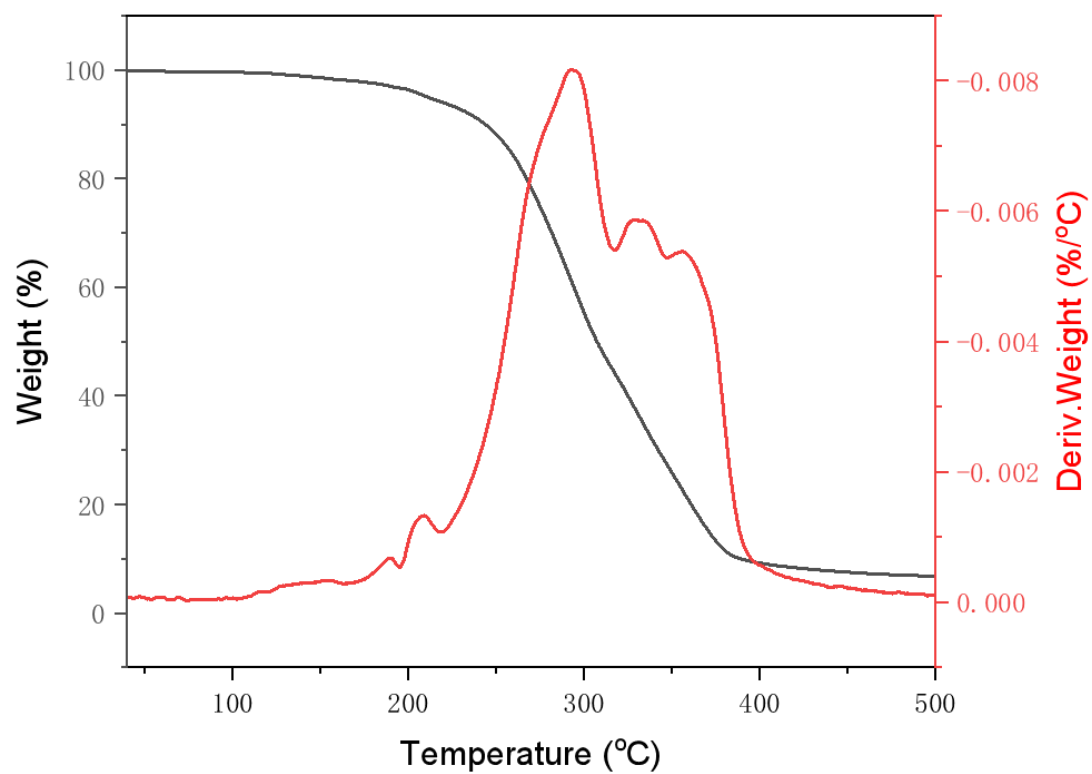
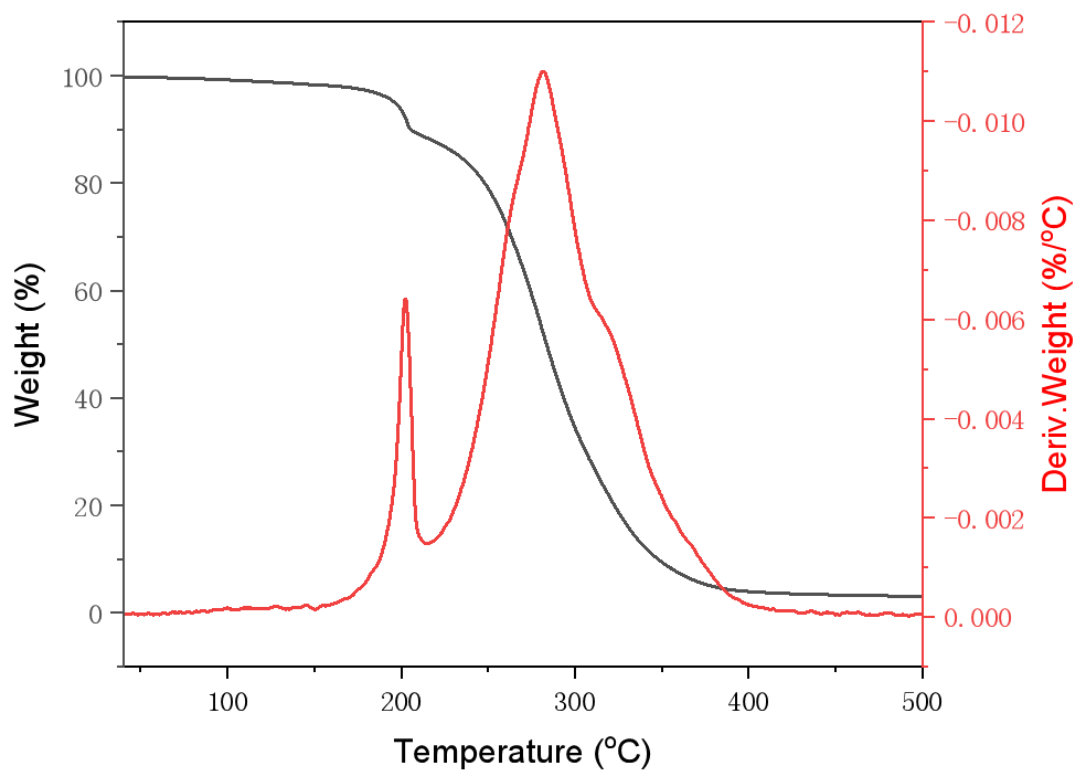
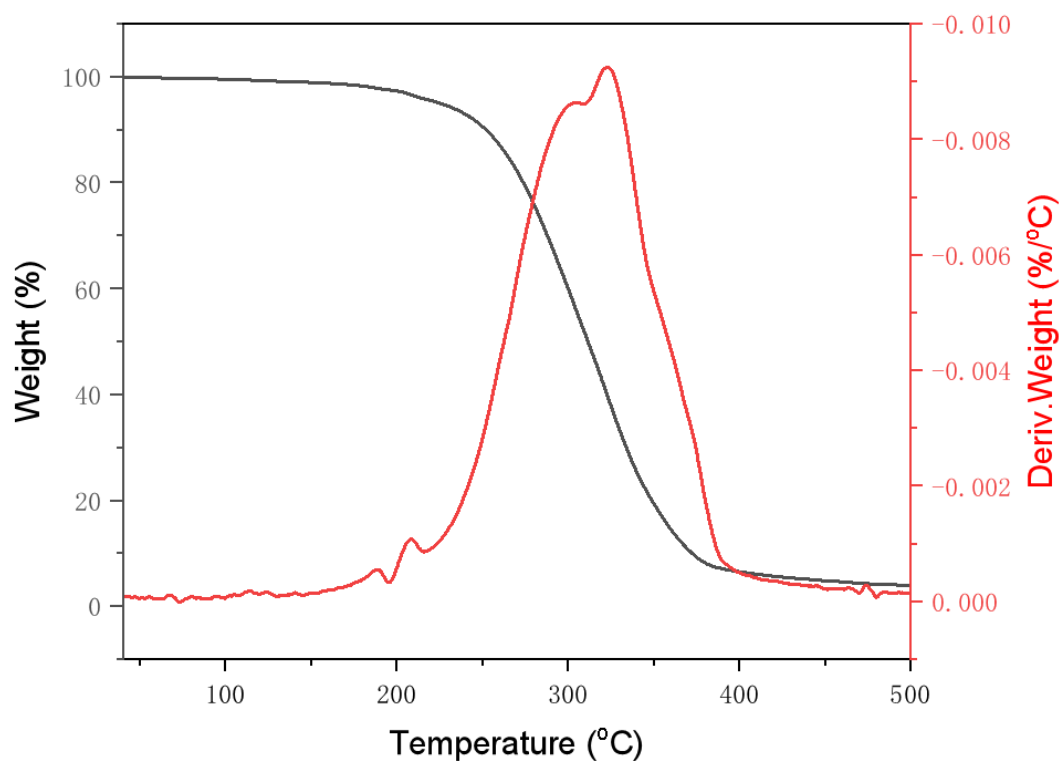


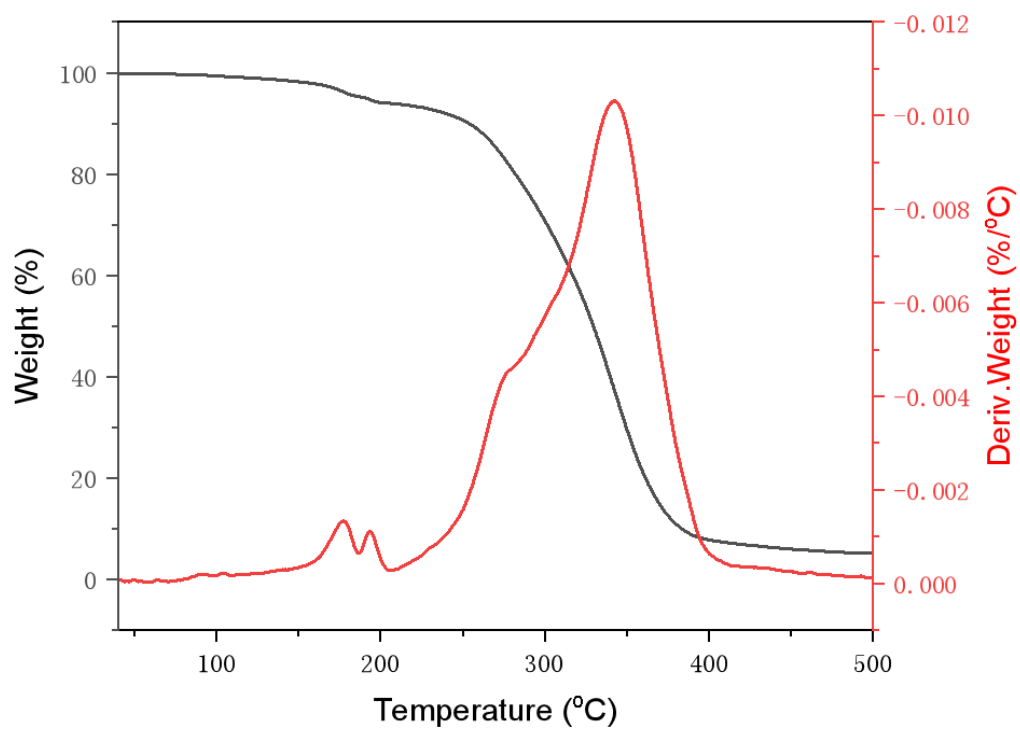
Figure S33. TGA and DTG curves of BIG-P1-CS<sub>2</sub>.



**Figure S34.** TGA and DTG curves of **BIG-P2-CS<sub>2</sub>**.



**Figure S35.** TGA and DTG curves of **BIG-P3-CS<sub>2</sub>**.



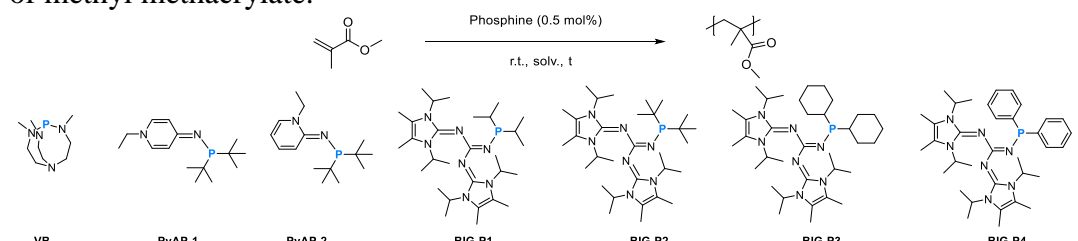
**Figure S36.** TGA and DTG curves of **BIG-P4-CS<sub>2</sub>**.

## 9. Phosphine-initiated polymerization of Michael-type monomers

Polymerizations were performed in 20 mL glass reactors inside the glovebox filled with argon for room temperature (25 °C). In a typical polymerization procedure, a predetermined amount of phosphine was first dissolved in corresponding solvents (toluene, THF or DMF), and started by rapid addition of the monomer via a gastight syringe to the above solution under vigorously stirring. After the measured time interval, a 0.1 mL aliquot was taken from the reaction mixture via pipet and quickly quenched into a 4-mL vial containing 0.5 mL of undried “wet” CDCl<sub>3</sub>, the quenched aliquots were later analyzed by <sup>1</sup>H NMR spectroscopy for monomer conversion. After the polymerization was stirred for the stated reaction time, the reactor was taken out of the glovebox. The reaction was quenched by addition of 1 ml of 5% HCl-acidified methanol. Then add a amount of methanol or diethyl ether to precipitate the polymer, filter and wash with methanol, and dried in a vacuum oven at 60 °C to a constant weight.

### 9.1 Optimization of phosphine-initiated polymerization of MMA

**Table S3.** Optimization of phosphine-initiated conjugated addition polymerization of methyl methacrylate. <sup>[a]</sup>



Entry	Ini. [I]	Solv.	t [min]	Conv. <sup>[b]</sup> [%]	$M_n$ <sup>[c]</sup> (10 <sup>3</sup> g mol <sup>-1</sup> )	$\mathcal{D}$ <sup>[c]</sup> ( $M_w/M_n$ )
1	<b>PPh<sub>3</sub></b>	DMF	2880	0	-	-
2	<b>PEt<sub>3</sub></b>	DMF	2880	0	-	-
3	<b>PCy<sub>3</sub></b>	DMF	2880	0	-	-
4	<b>P<sup>n</sup>Bu<sub>3</sub></b>	DMF	2880	0	-	-
5	<b>VB</b>	DMF	2880	0	-	-
6	<b>PyAP1</b>	DMF	3	7	-	-
7	<b>PyAP2</b>	DMF	3	2	-	-
8	<b>BIG-P2</b>	Toluene	3	5	-	-
9	<b>BIG-P2</b>	THF	3	33	17.1	1.54

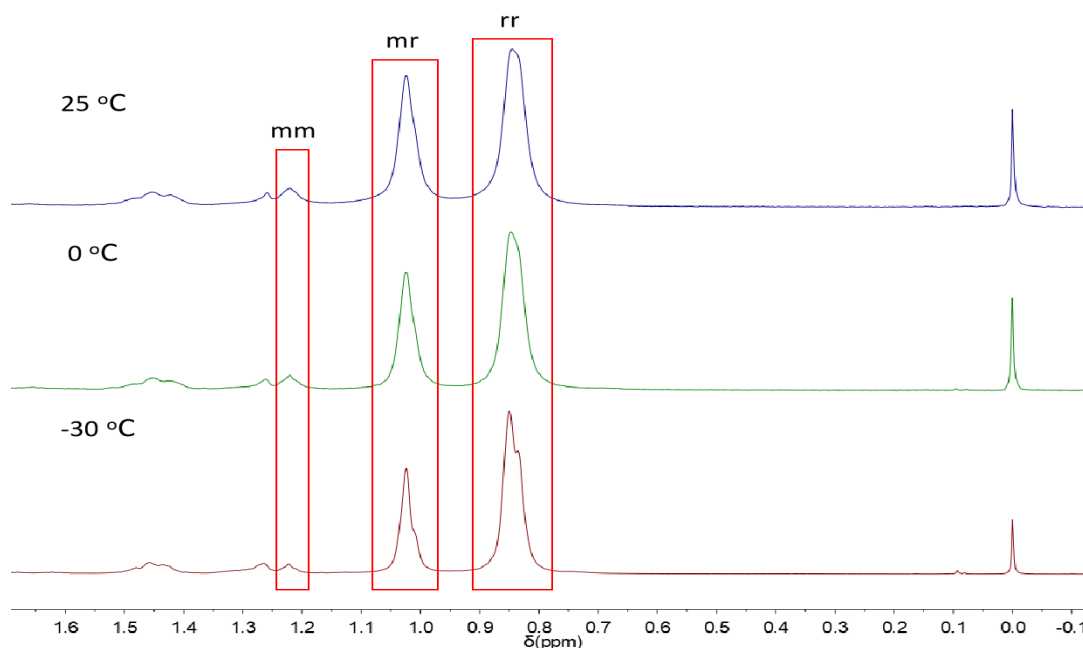
<sup>[a]</sup> General reaction conditions: The polymerization reactions were carried at room temperature;  $[M]_0 = 1.0$  mol/L. <sup>[b]</sup> Conv. = % monomer conversion measured by <sup>1</sup>H-NMR spectroscopy. <sup>[c]</sup> Number-average molecular weight ( $M_n$ ) and polydispersity index ( $\mathcal{D} = M_w/M_n$ ) determined by GPC in THF using polystyrene standards.

## 9.2 The tacticity of PMMA influenced by different temperature

**Table S4** MMA polymerization by BIG-P2-initiated at different temperature. <sup>[a]</sup>

Entry	T (°C)	Conv. <sup>[b]</sup> (%)	mm : mr : rr <sup>[b]</sup>	$M_n$ <sup>[c]</sup> ( $10^3 \text{ g mol}^{-1}$ )	$\mathcal{D}$ <sup>[c]</sup> ( $M_w/M_n$ )
1	25	>99	5.0 : 37.6 : 57.4	81.2	1.80
2	0	>99	4.2 : 34.2 : 61.6	83.0	1.52
3	-30	>99	3.1 : 30.1 : 66.8	110.1	1.48

<sup>[a]</sup> General reaction conditions: The polymerization reactions were carried by **BIG-P2** in DMF for 3 mins;  $[M]/[I]=800:1$ ;  $[M]_0 = 1.0 \text{ mol/L}$ . <sup>[b]</sup> Conv. = % monomer conversion and tacticity ratios measured by  $^1\text{H-NMR}$  spectroscopy. <sup>[c]</sup> Number-average molecular weight ( $M_n$ ) and polydispersity index ( $\mathcal{D} = M_w/M_n$ ) determined by GPC in THF using polystyrene standards.



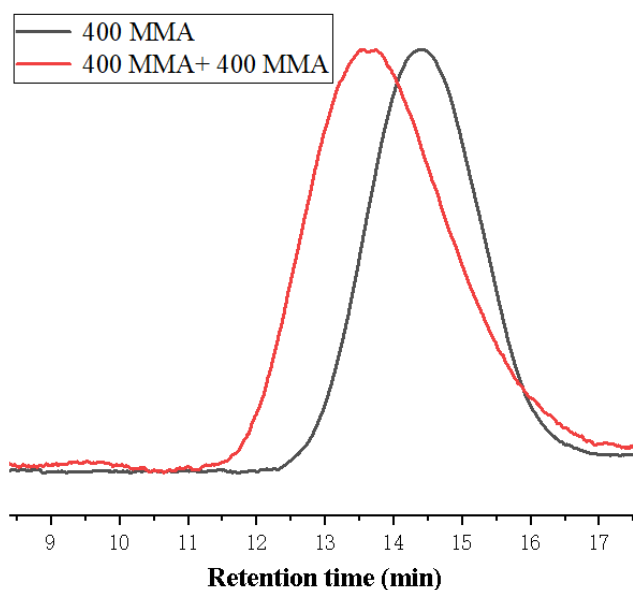
**Figure S37:**  $^1\text{H}$  NMR spectrum of the tacticity of PMMA at different temperature.

## 9.3 Chain extension experiments for MMA polymerization

**Table S5.** chain-extension polymerization by **BIG-P2**. <sup>[a]</sup>

Entry	M1/M2	Time (min)	Conv. <sup>[b]</sup> (%)	$M_{n(\text{SEC})}$ <sup>[c]</sup> ( $10^3 \text{ g mol}^{-1}$ )	$\mathcal{D}$ <sup>[c]</sup> ( $M_w/M_n$ )
1	400MMA	3	>99	58.7	1.90
2	400MMA+400MMA	3	>99	90.4	2.62

<sup>[a]</sup> General reaction conditions: The polymerization reactions were carried at RT in DMF;  $[I]$ : **BIG-P2**;  $[M]_0 = 1.0 \text{ mol/L}$ . <sup>[b]</sup> Conv. = % monomer conversion measured by  $^1\text{H-NMR}$  spectroscopy. <sup>[c]</sup> Number-average molecular weight ( $M_n$ ) and polydispersity index ( $\mathcal{D} = M_w/M_n$ ) determined by GPC in THF using polystyrene standards.

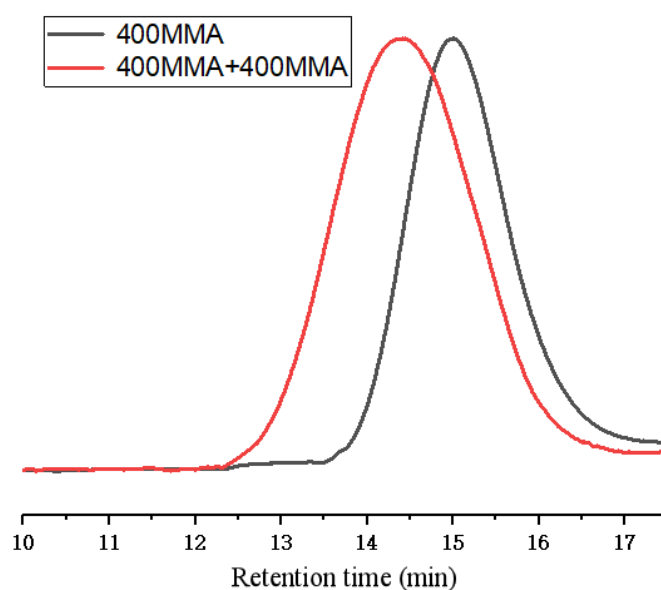


**Figure S38.** GPC curves of PMMA obtained by sequential addition of two batches of MMA.

**Table S6.** chain-extension polymerization by **BIG-P2**.<sup>[a]</sup>

Entry	M1/M2	Time (min)	Conv. <sup>[b]</sup> (%)	$M_{n(\text{SEC})}$ <sup>[c]</sup> ( $10^3 \text{ g mol}^{-1}$ )	$\mathcal{D}$ <sup>[c]</sup> ( $M_w/M_n$ )
1	400MMA	0.5	>99	57.6	1.82
2	400MMA+400MMA	0.5	>99	89.1	2.19

<sup>[a]</sup> General reaction conditions: The polymerization reactions were carried at RT in DMF; [I]: BIG-P2;  $[M]_0 = 1.0 \text{ mol/L}$ . <sup>[b]</sup> Conv. = % monomer conversion measured by  $^1\text{H-NMR}$  spectroscopy. <sup>[c]</sup> Number-average molecular weight ( $M_n$ ) and polydispersity index ( $\mathcal{D} = M_w/M_n$ ) determined by GPC in DMF using PMMA standards.



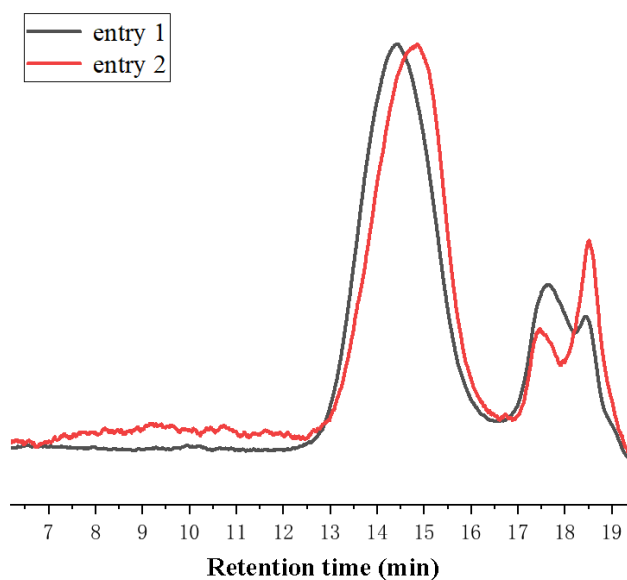
**Figure S39.** GPC curves of PMMA obtained by sequential addition of two batches of MMA.

## 9.4 BIG-P2-based FLPs catalyzed MMA polymerization

**Table S7.** BIG-P2-based FLPs catalyzed MMA polymerization.<sup>[a]</sup>

Entry	LA	[M]:LB:LA	Conv. <sup>[b]</sup> (%)	$M_n(\text{Calc.})$ <sup>[c]</sup> ( $10^3 \text{ g mol}^{-1}$ )	$M_n(\text{SEC})$ <sup>[c]</sup> ( $10^3 \text{ g mol}^{-1}$ )	$\mathcal{D}$ <sup>[c]</sup> ( $M_w/M_n$ )
1	$\text{Al}(\text{C}_6\text{F}_5)_3$	200:1:2	>99	20.4	25.7	1.63
					1.6	1.38
2	$\text{AlMe}(\text{BHT})_2$	200:1:2	>99	20.4	21.9	1.52
					1.2	1.31

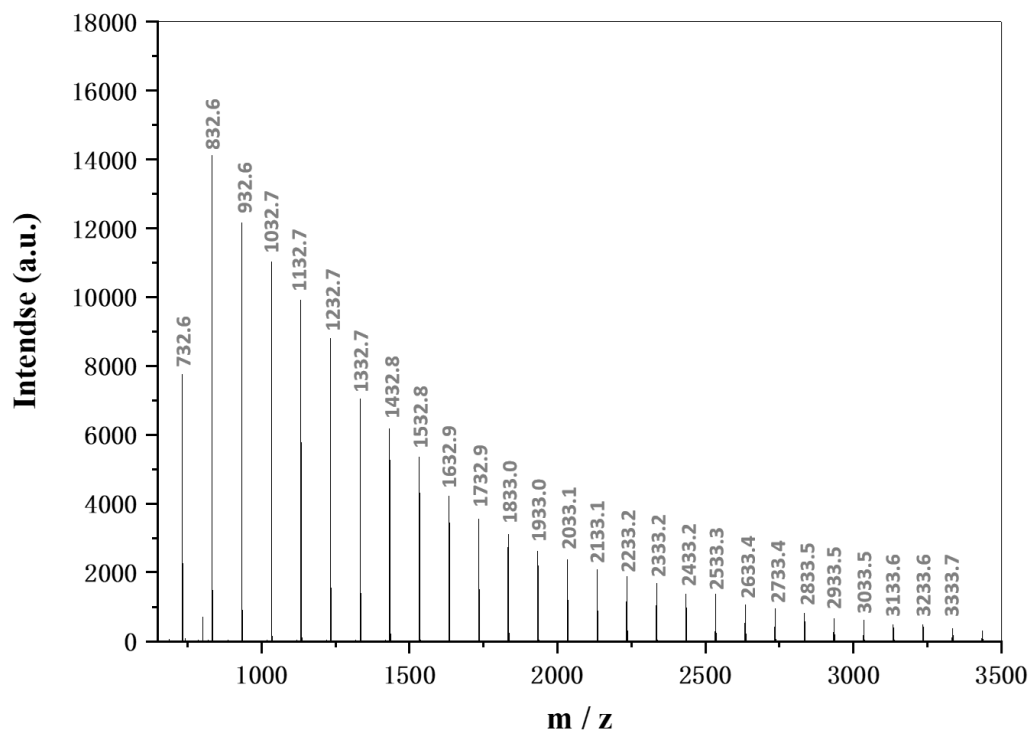
<sup>[a]</sup> General reaction conditions: The polymerization reactions were carried at RT in toluene for 3 mins; LB: BIG-P2;  $[\text{M}]_0 = 1.0 \text{ mol/L}$ . <sup>[b]</sup> Conv. = % monomer conversion measured by  $^1\text{H-NMR}$  spectroscopy. <sup>[c]</sup> Number-average molecular weight ( $M_n$ ) and polydispersity index ( $\mathcal{D} = M_w/M_n$ ) determined by GPC in THF using polystyrene standards.



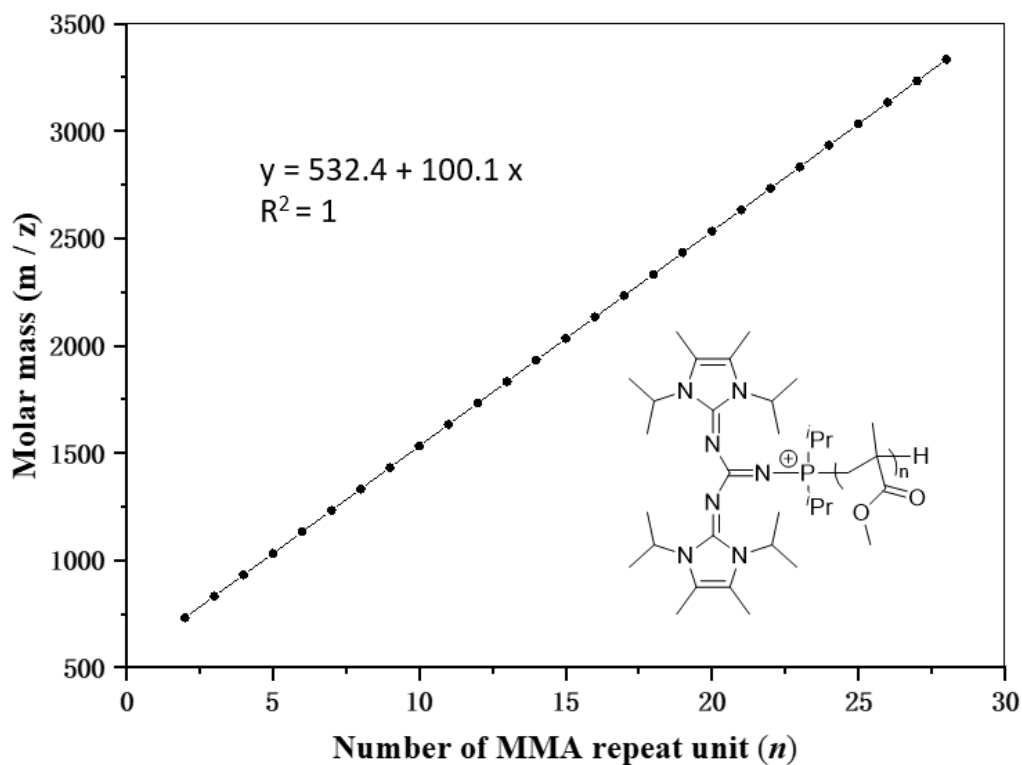
**Figure S40.** The GPC traces of PMMA samples obtained from BIG-P2-based FLPs.



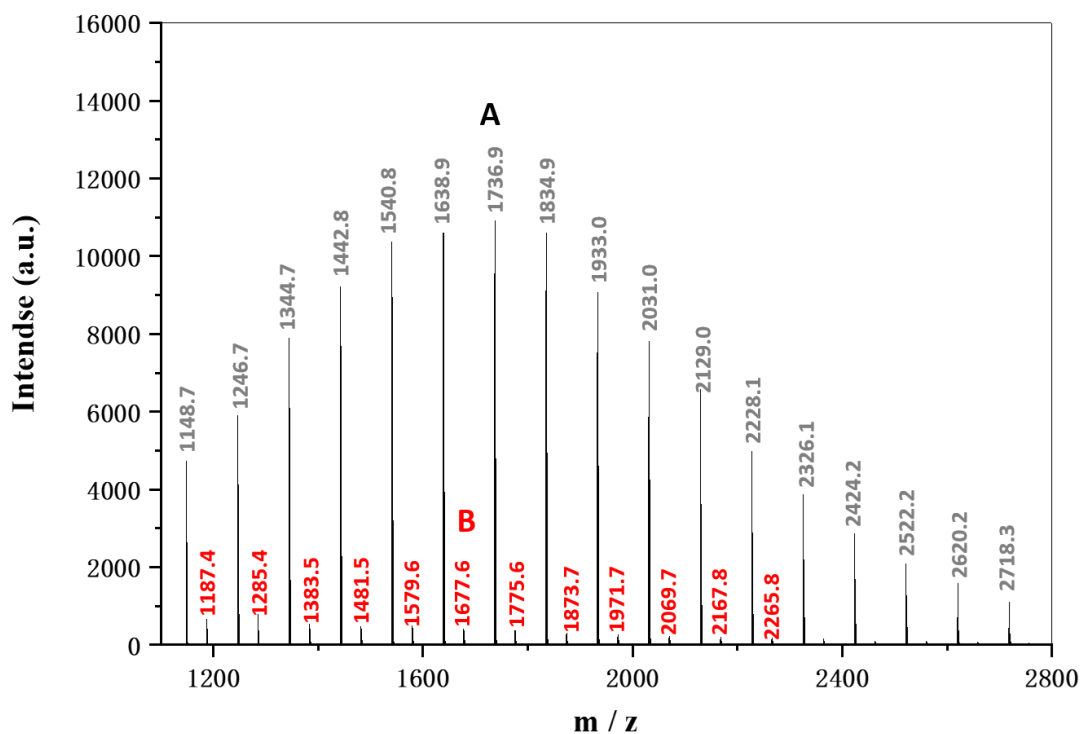
## 9.5 MALDI-TOF MS spectra



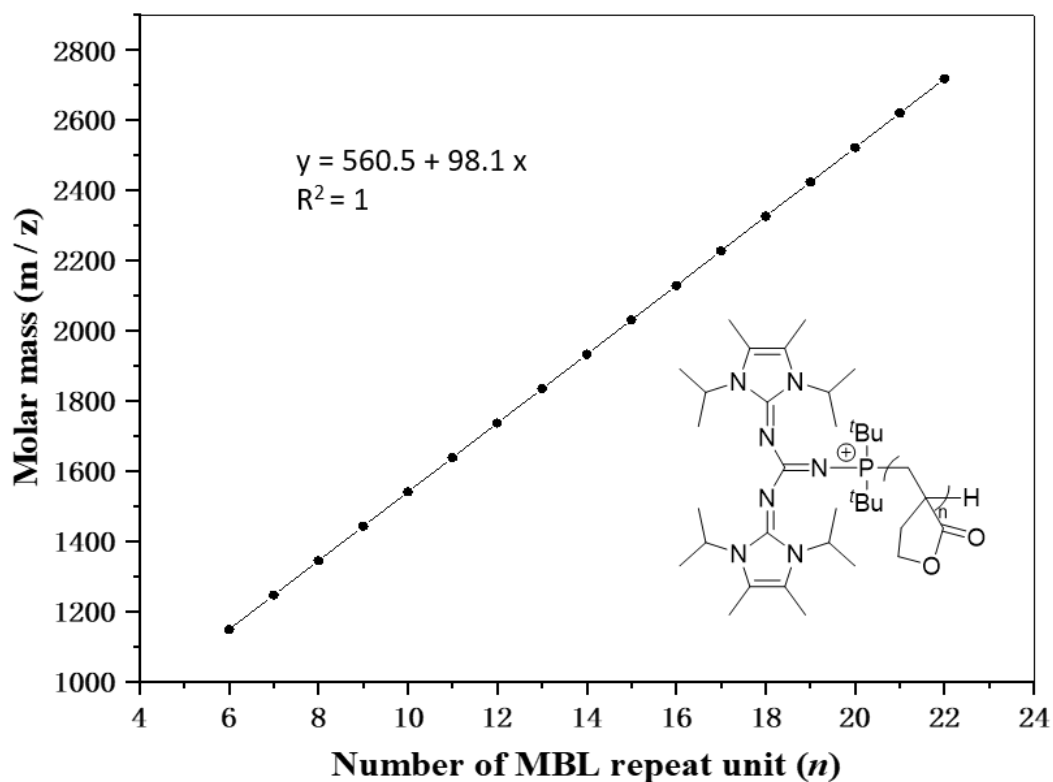
**Figure S41:** MALDI-TOF MS spectrum of the low-M<sub>w</sub> PMMA sample produced by **BIG-P1** in DMF at RT.



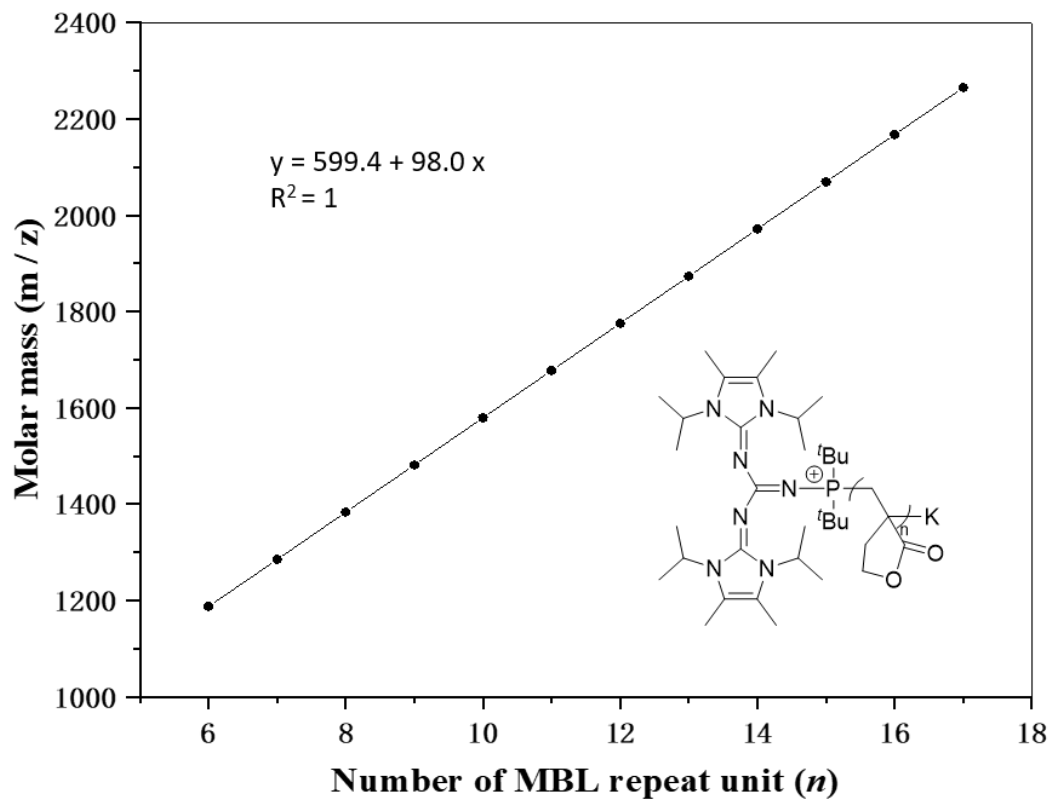
**Figure S42:** Plot of m/z values taken from Figure S33 vs the number of MMA repeat units ( $n$ ).



**Figure S43:** MALDI-TOF MS spectrum of the low-M<sub>w</sub> PMBL sample produced by **BIG-P2** in DMF at RT.

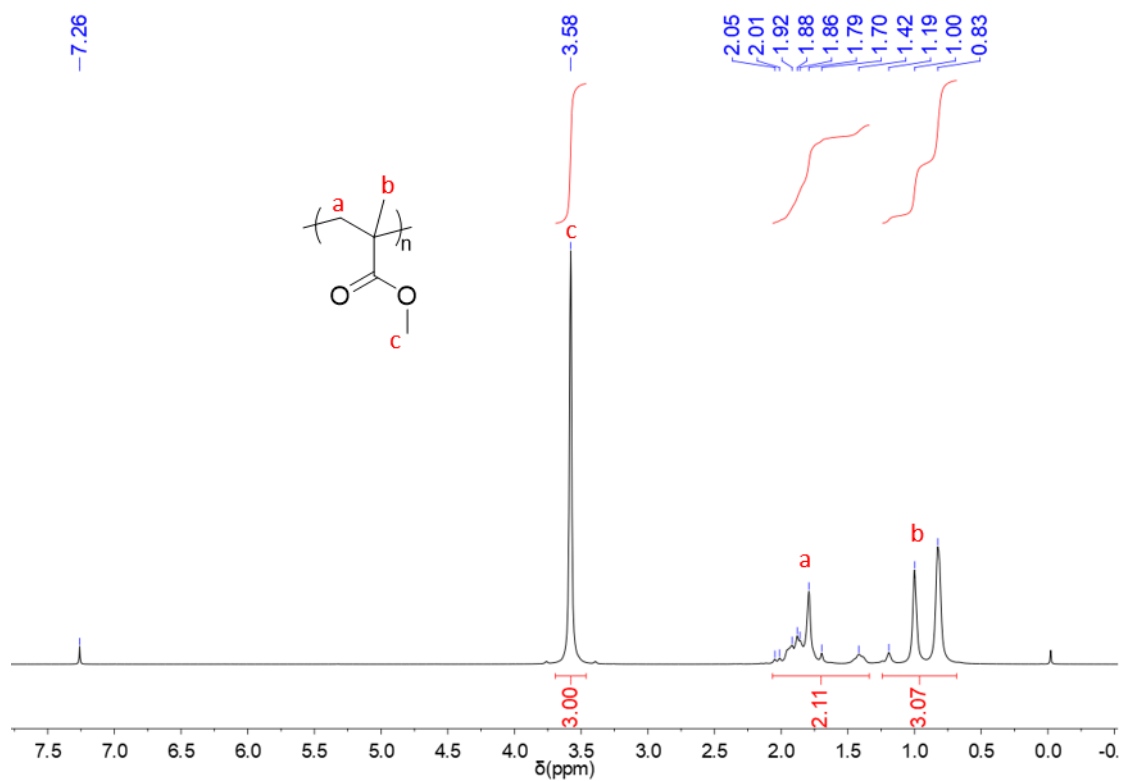


**Figure S44:** Plot of m/z values taken from Figure S35 vs the number of MBL repeat units ( $n$ ), major peaks (A).



**Figure S45:** Plot of  $m/z$  values taken from Figure S35 vs the number of MBL repeat units ( $n$ ), minor peaks (B).

### 9.6 NMR data of polymers



**Figure S46.**  $^1\text{H}$  NMR spectrum of PMMA in  $\text{CDCl}_3$ .

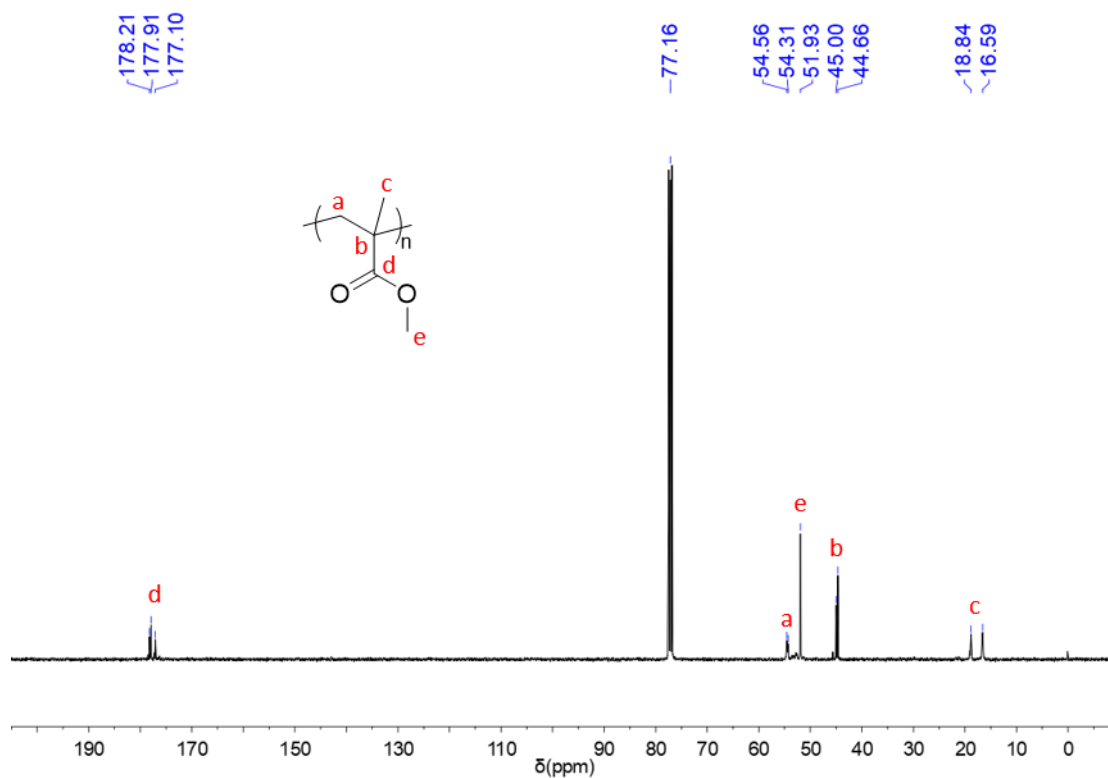


Figure S47. <sup>13</sup>C NMR spectrum of PMMA in CDCl<sub>3</sub>.

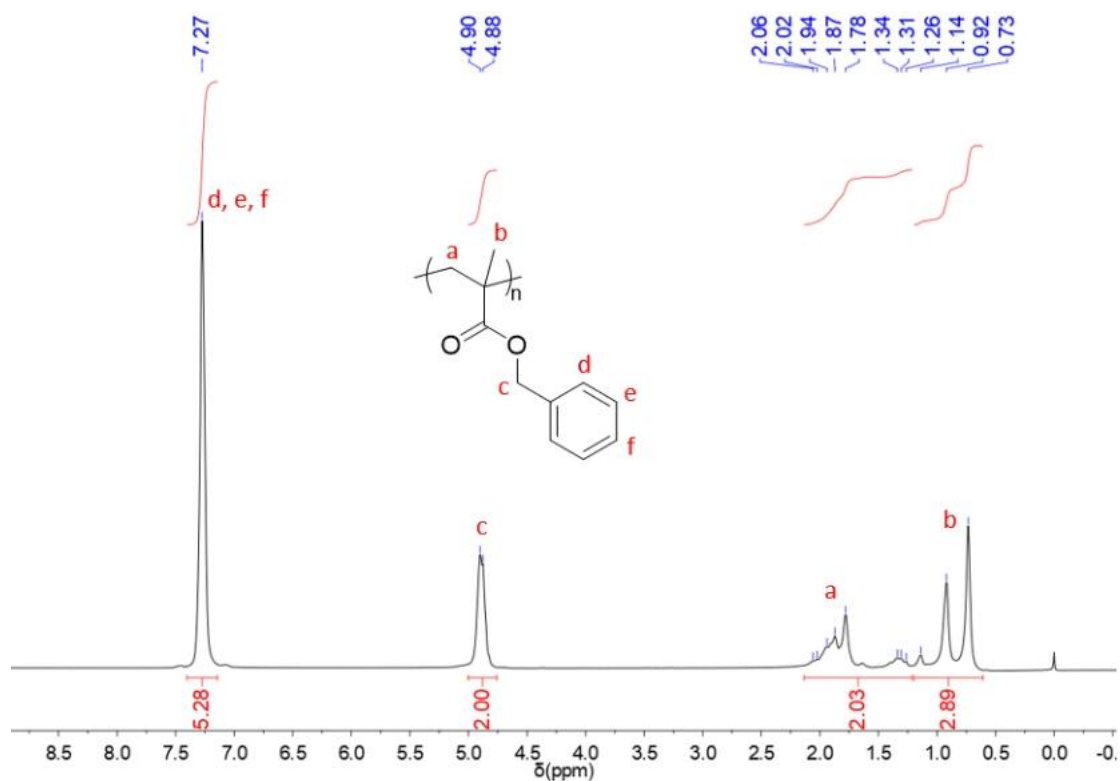


Figure S48. <sup>1</sup>H NMR spectrum of PBnMA in CDCl<sub>3</sub>.

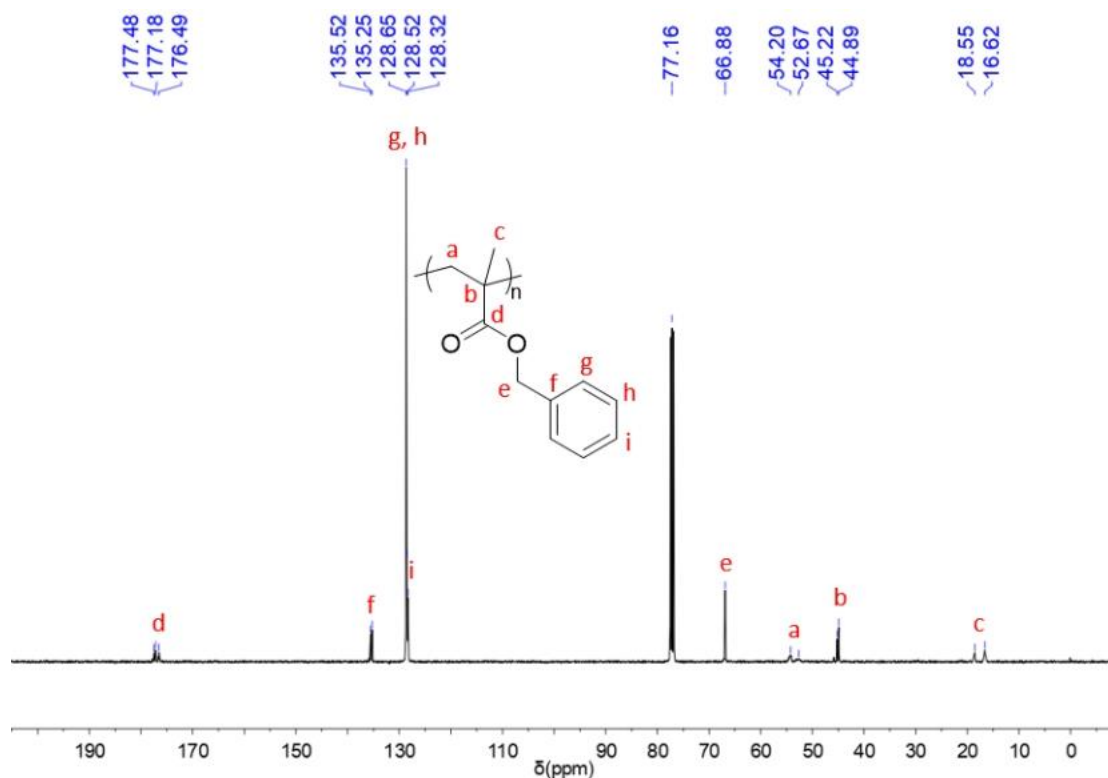


Figure S49. <sup>13</sup>C NMR spectrum of PBnMA in CDCl<sub>3</sub>.

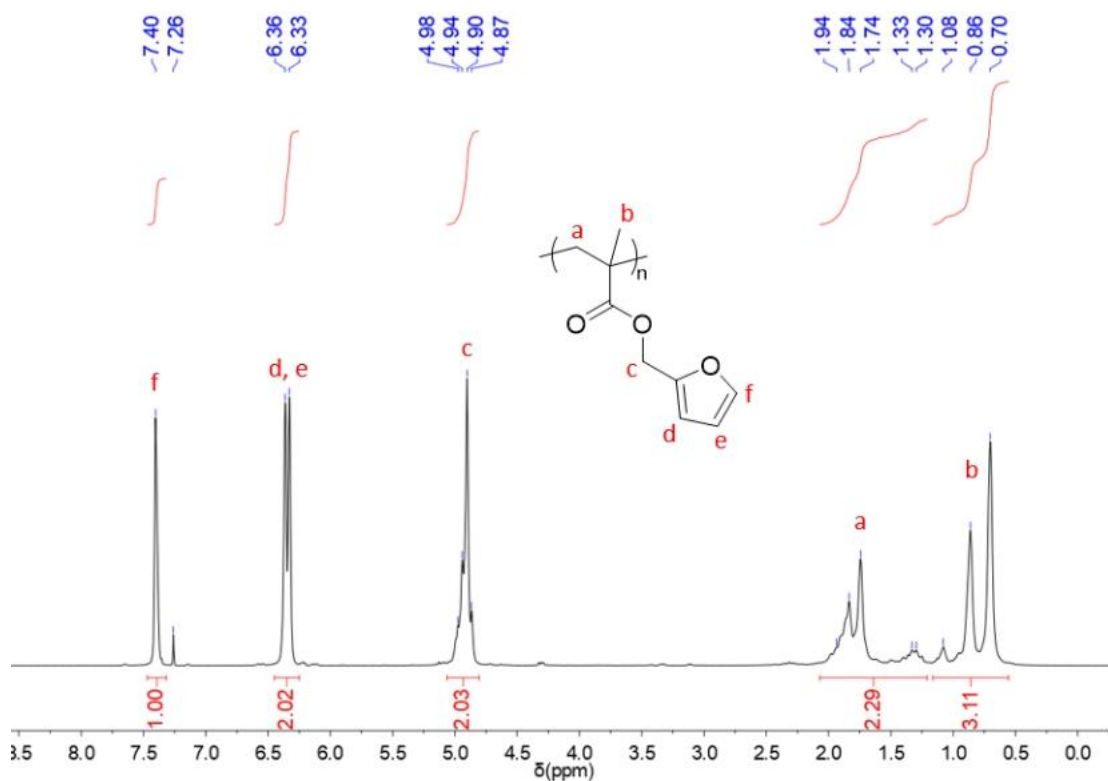


Figure S50. <sup>1</sup>H NMR spectrum of PFMA in CDCl<sub>3</sub>.

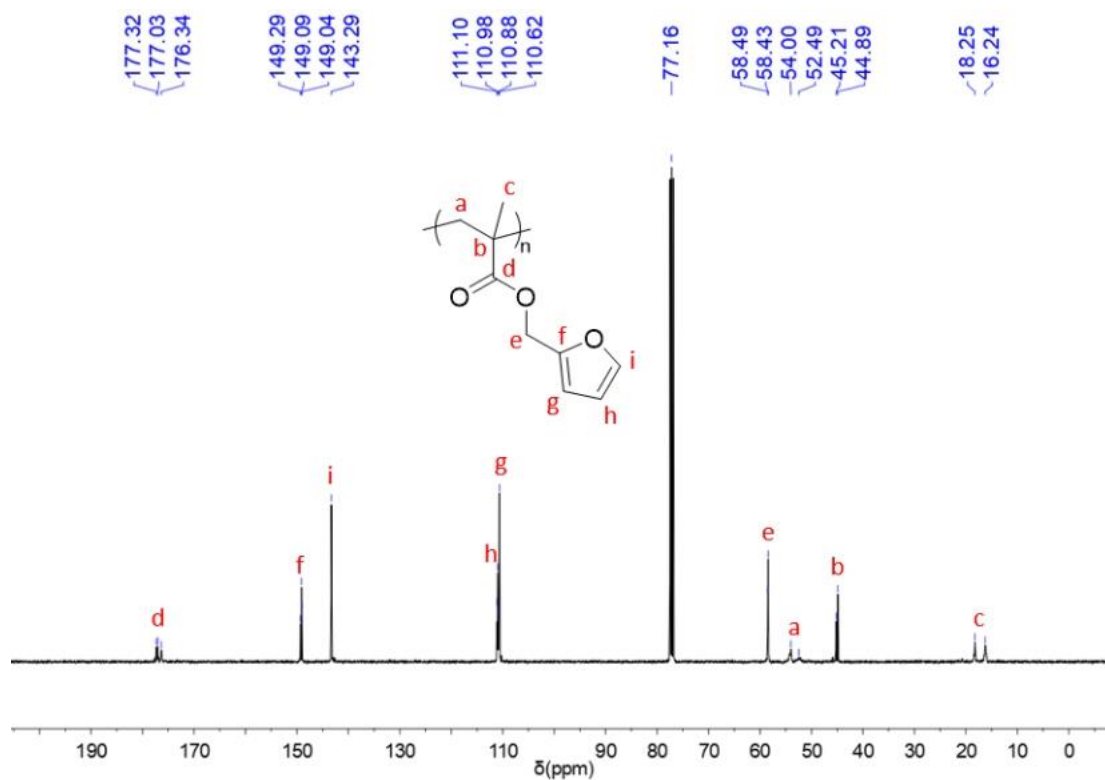


Figure S51.  $^{13}\text{C}$  NMR spectrum of PFMA in  $\text{CDCl}_3$ .

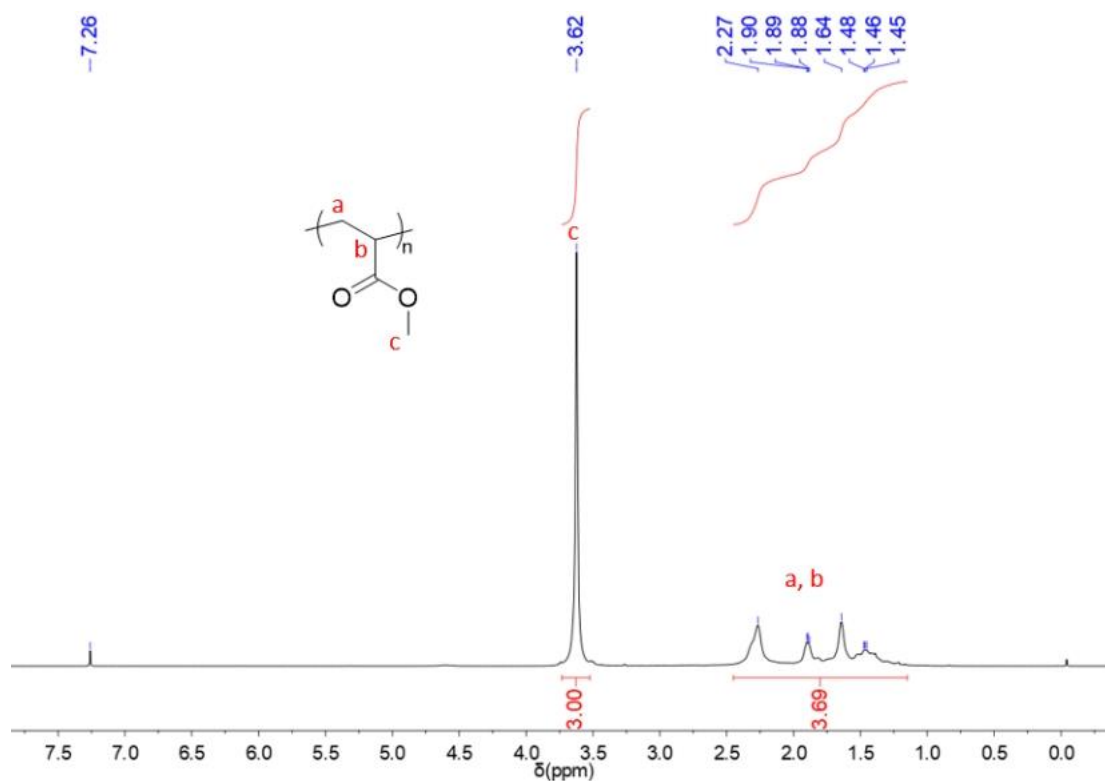


Figure S52.  $^1\text{H}$  NMR spectrum of PMA in  $\text{CDCl}_3$ .

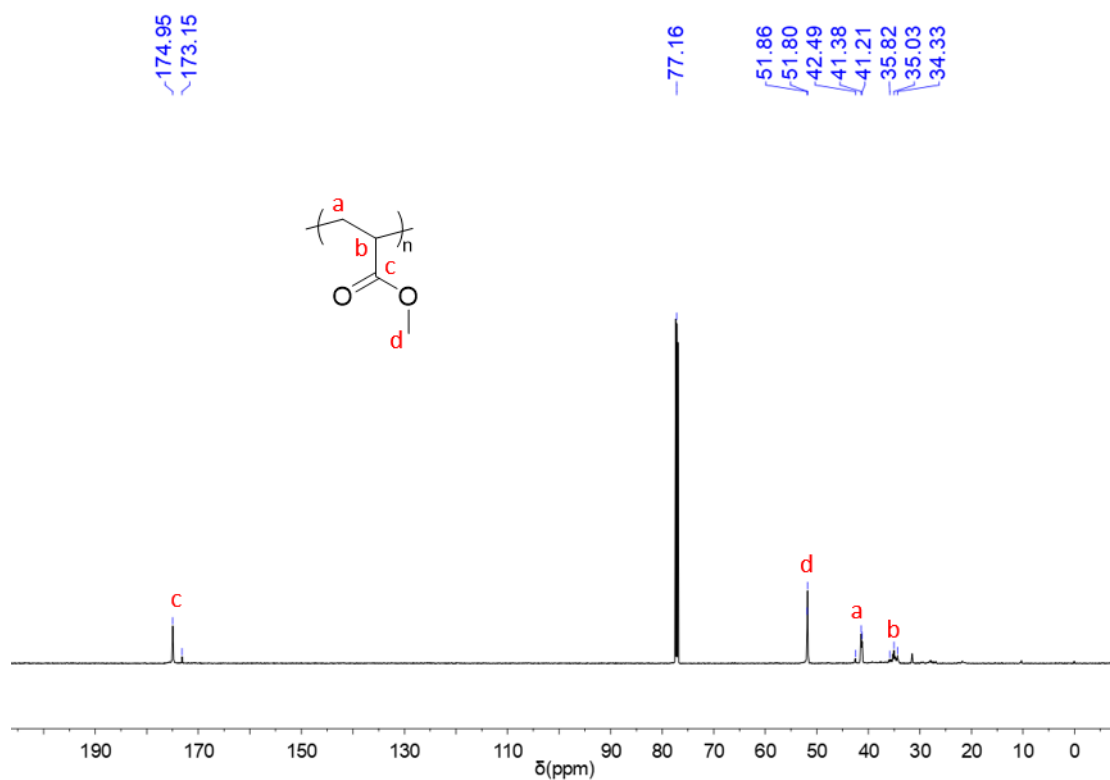


Figure S53.  $^{13}\text{C}$  NMR spectrum of PMA in  $\text{CDCl}_3$ .

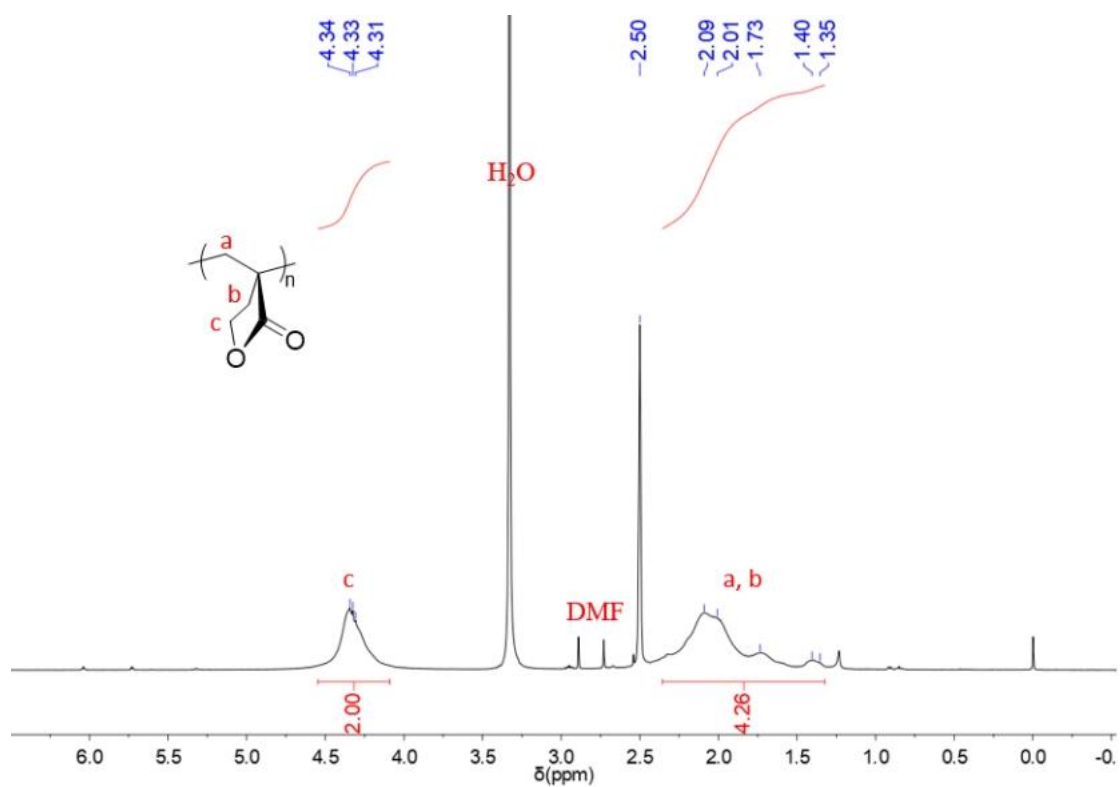


Figure S54.  $^1\text{H}$  NMR spectrum of PMBL in  $\text{DMSO-d}_6$ .

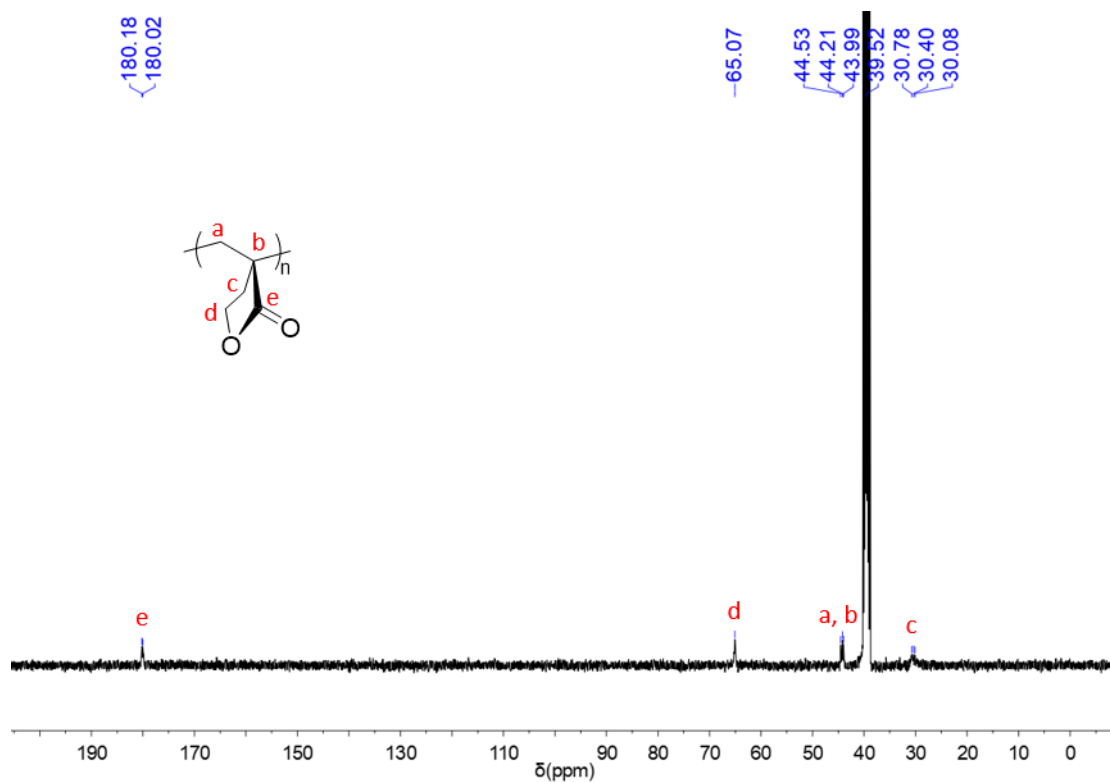


Figure S55.  $^{13}\text{C}$  NMR spectrum of PMBL in  $\text{DMSO-d}_6$ .

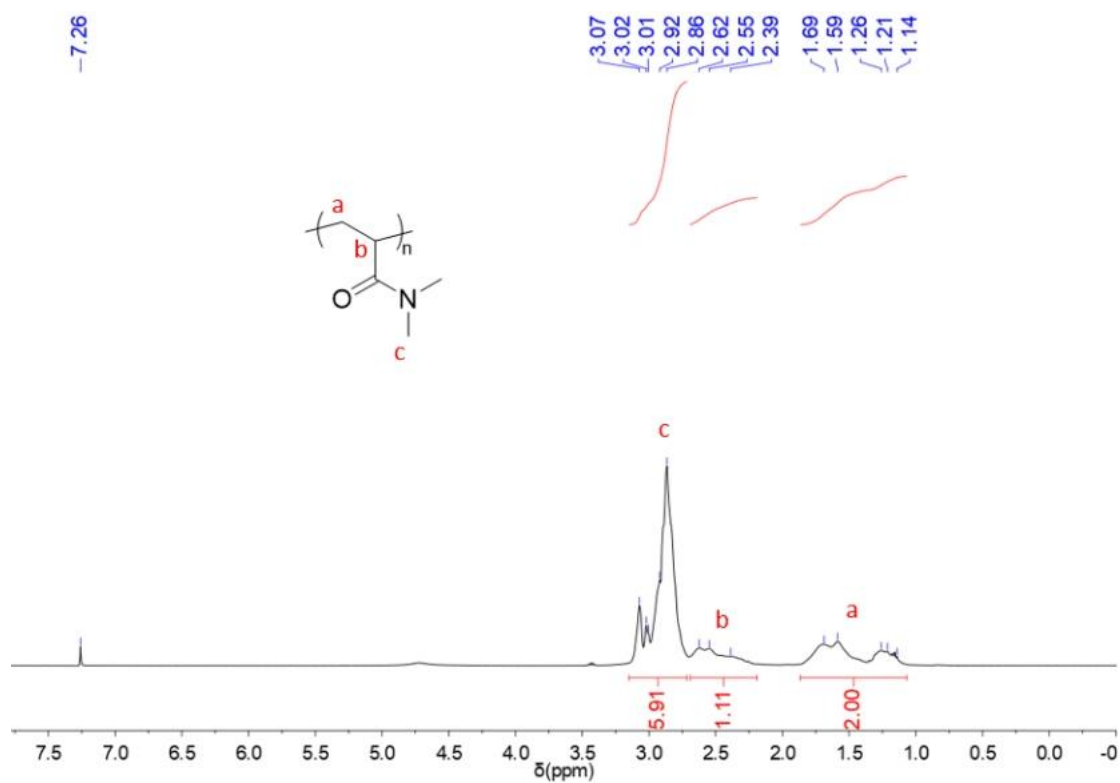
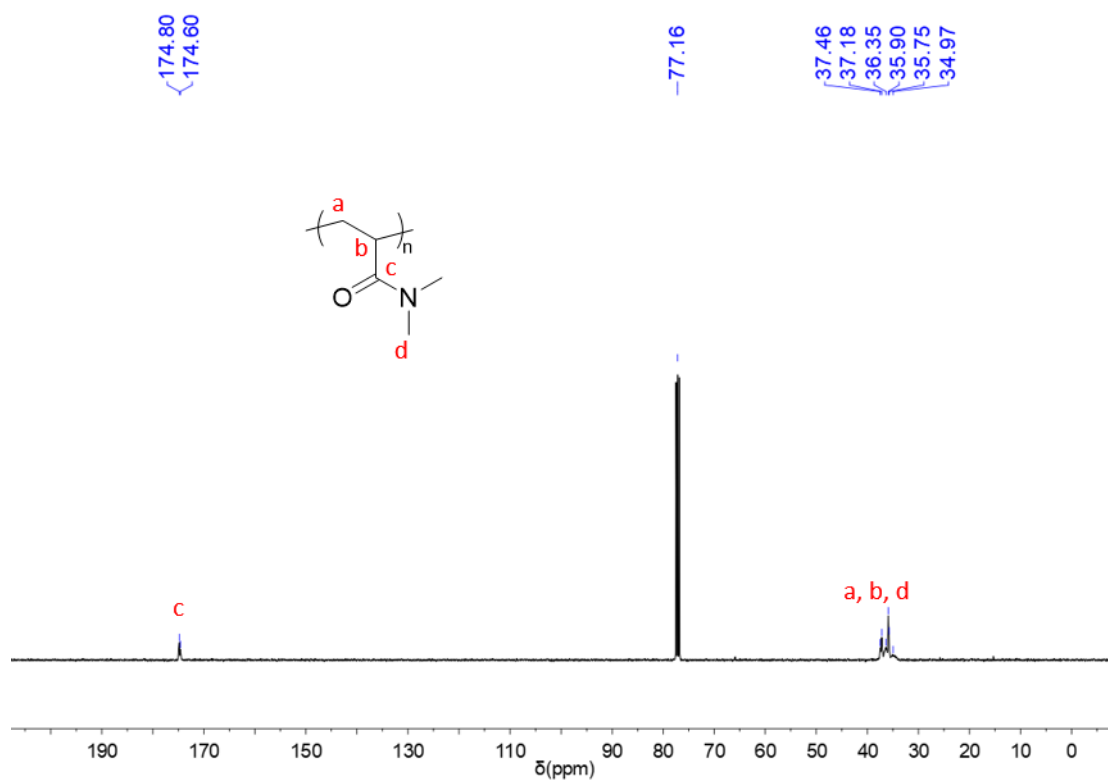
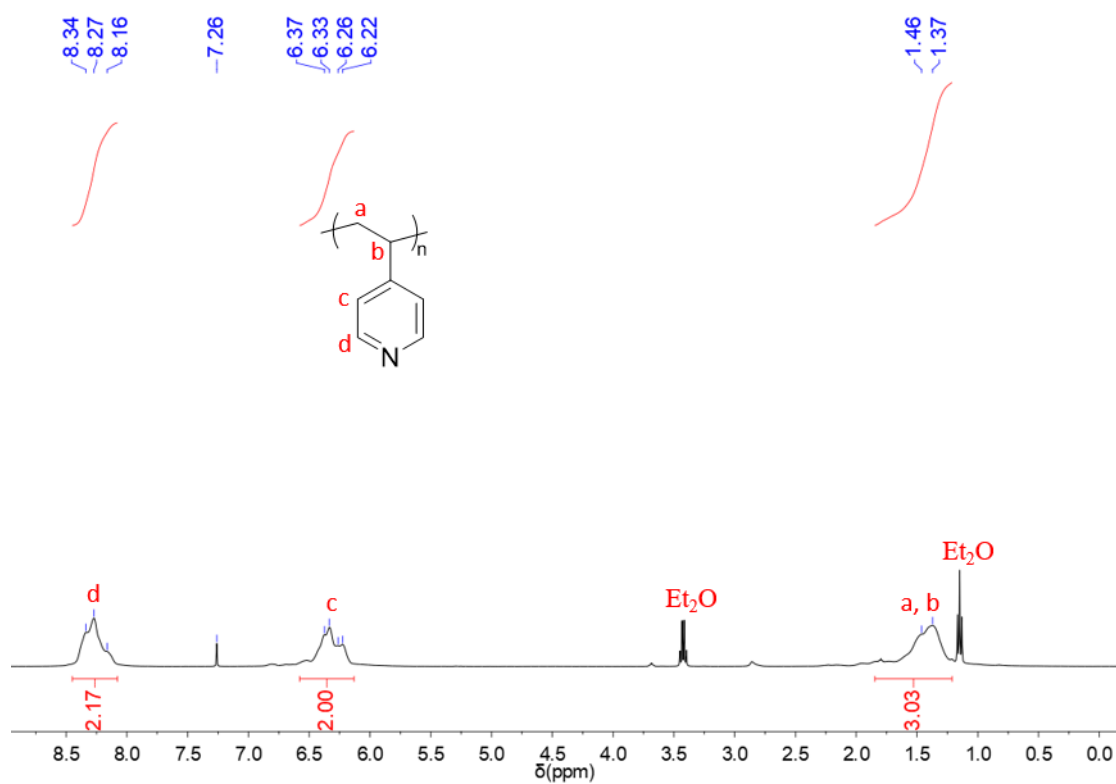


Figure S56.  $^1\text{H}$  NMR spectrum of PDMAA in  $\text{CDCl}_3$ .

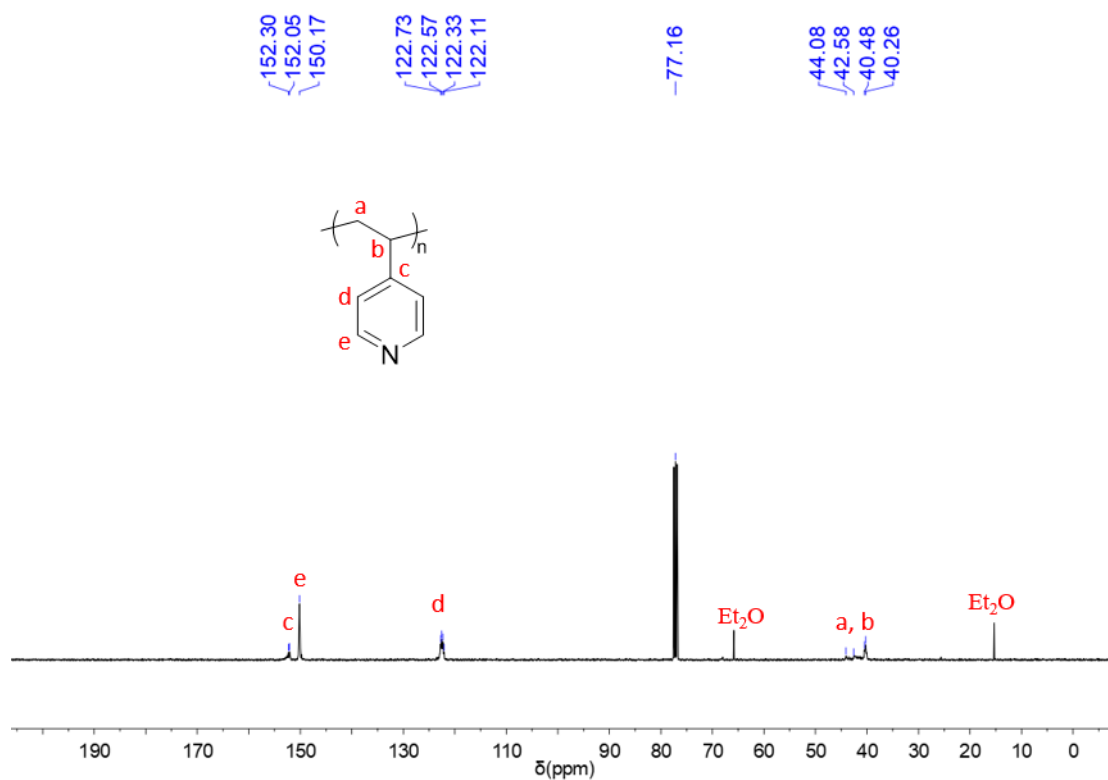




**Figure S57.**  $^{13}\text{C}$  NMR spectrum of PDMAA in  $\text{CDCl}_3$ .

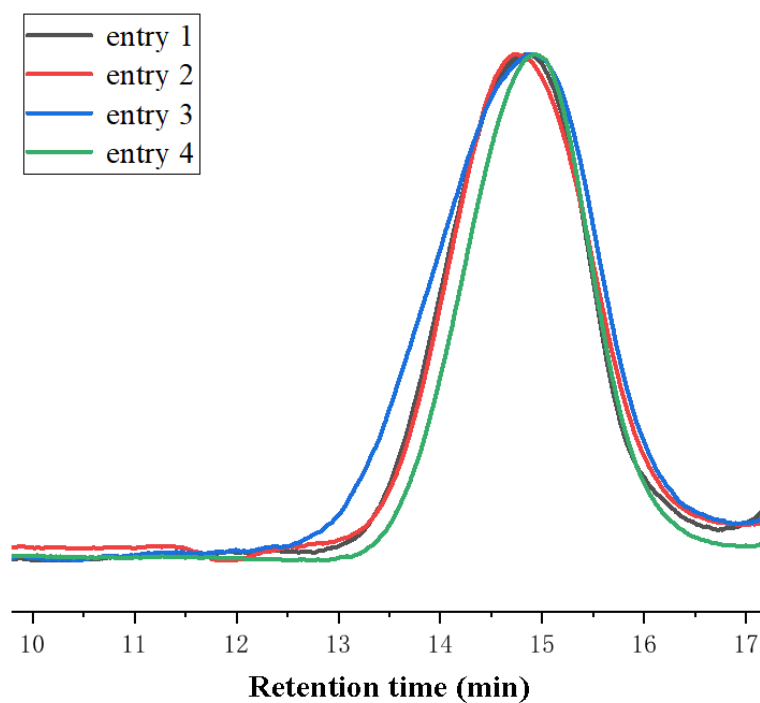


**Figure S58.**  $^1\text{H}$  NMR spectrum of P4-VP in  $\text{CDCl}_3$ .

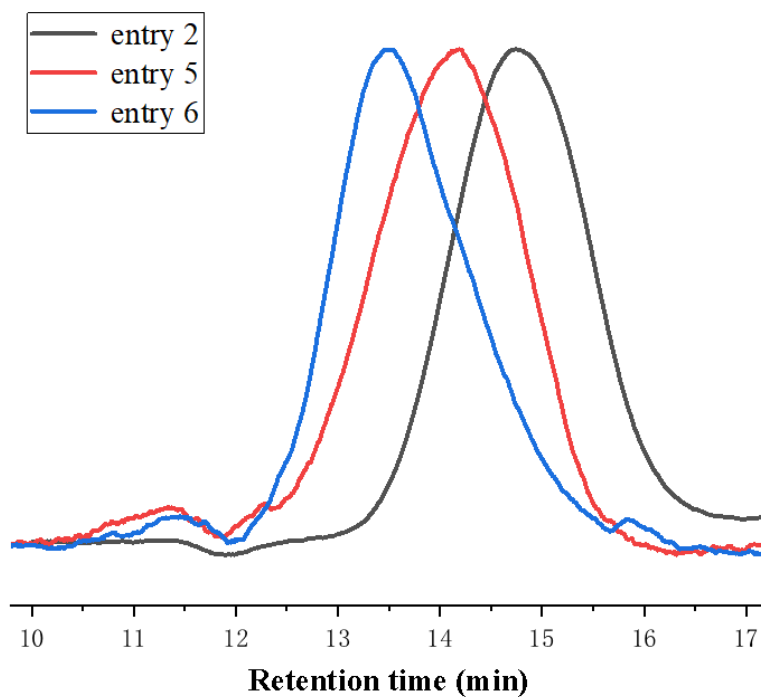


**Figure S59.** <sup>13</sup>C NMR spectrum of P4-VP in CDCl<sub>3</sub>.

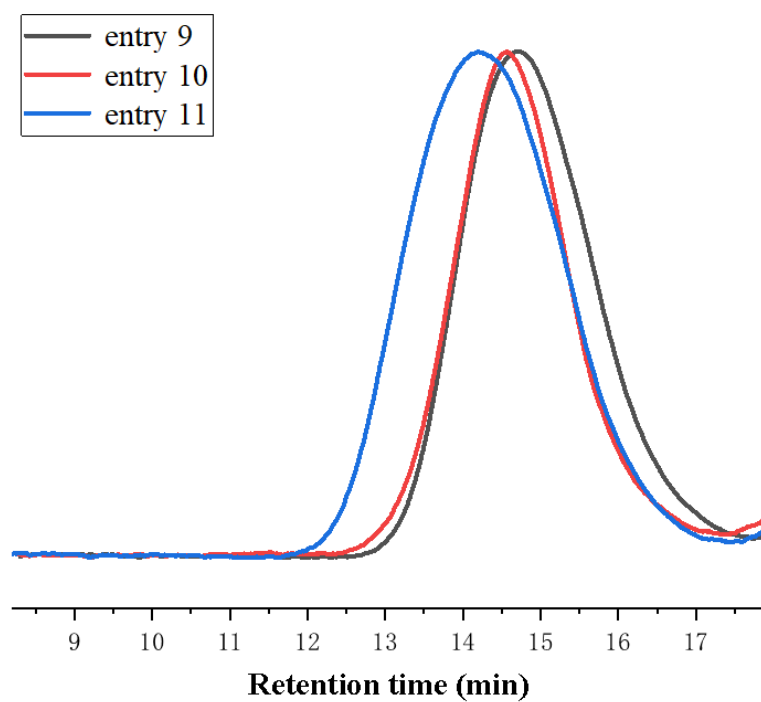
### 9.7 GPC data



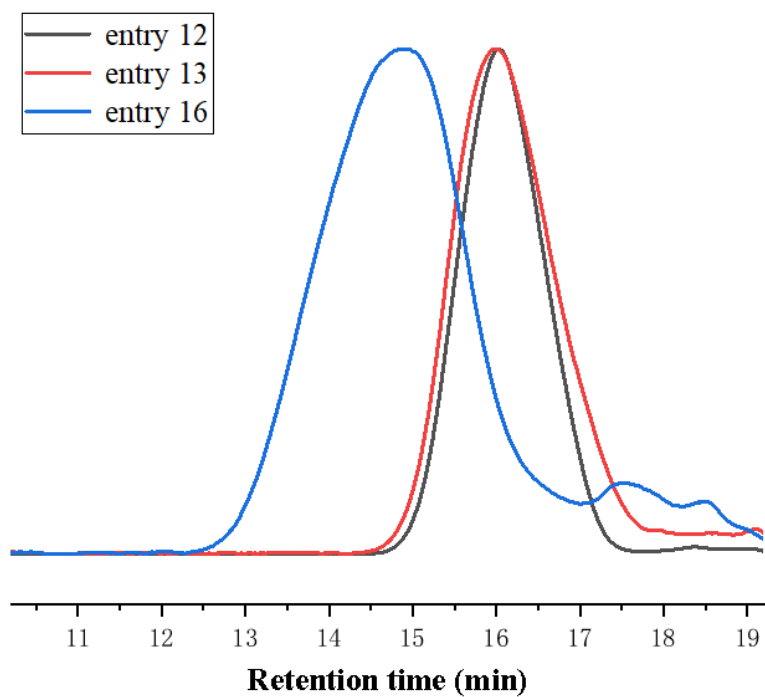
**Figure S60:** The GPC traces of PMMA in Table 2 (entry 1-4).



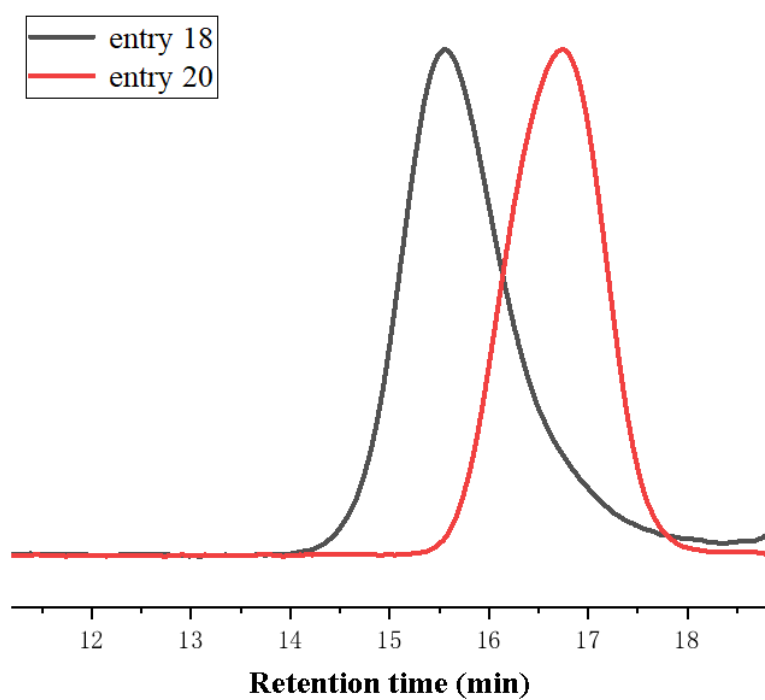
**Figure S61:** The GPC traces of PMMA in Table 2 (entry 2 and entry 5-6).



**Figure S62:** The GPC traces of PBnMA in Table 2 (entry 9-11).



**Figure S63:** The GPC traces of PFMA and PMA in Table 2 (entry 12-13 and entry 16).

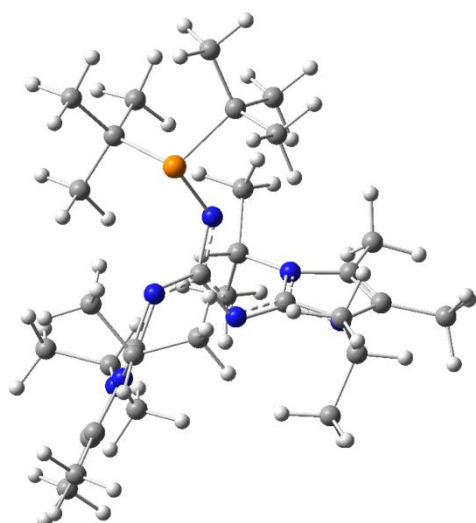


**Figure S64:** The GPC traces of PDMAA and P4-VP in Table 2 (entry 18 and entry 20).

## 10. DFT calculated phosphine-mediated conjugate-addition polymerization

To disclose the possible mechanism of **BIG-Ps**-mediated conjugate-addition polymerization of Michael-type monomer, a density functional theory (**DFT**) calculation of such a reaction was performed with Gaussian 16.<sup>[S6]</sup> **MA** and **BIG-P2** were selected as the model monomer and initiator, respectively. All geometries of the reactants, products, intermediates (**INT**), and transition states (**TS**) involved in this mechanistic study were fully optimized in DMF solvent using SMD solvent model at the M06-2X/6-31G (d, p) level of theory. Intrinsic reaction coordinate (**IRC**) scans were conducted when necessary to check that the transition state correctly connects the two relevant minima. To improve the accuracy of the energy, the single point energy of each optimized structure was calculated at the M06-2X (SMD, DMF)/6-311++G (d, p) level. The relative free energy ( $\Delta G_{\text{sol}}$ ) was obtained by combining the single-point energy with Gibbs free energy correction at the M06-2X/6-31G (d, p) level.

### Cartesian coordinates of INT and TS



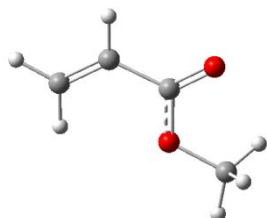
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C	1.15688	1.80862	-0.21522
C	-2.01689	2.2353	2.68223

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H	-2.9729	2.59477	3.06764
C	2.04391	1.23842	2.03091
H	1.2266	0.52639	1.90726
C	3.34835	4.29401	-1.80484
H	2.68932	5.14803	-1.99124
H	3.60711	3.85128	-2.77221
H	4.26697	4.67032	-1.35308
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C	2.70764	3.29886	-0.89889
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C	-2.08404	0.77888	2.23669
H	-1.07553	0.47362	1.95659
C	-0.05508	-0.21261	-0.14112
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H	3.6301	-0.17077	1.57382
H	3.05885	-0.19828	3.25393
H	4.11424	1.1067	2.71489
C	-3.44449	-2.61966	-1.78607
H	-3.54821	-3.19406	-2.71116
H	-4.2465	-2.9164	-1.1037
H	-2.48122	-2.86213	-1.32942
C	1.66294	2.26036	3.09889
H	2.48757	2.94694	3.31114
H	1.41217	1.73881	4.02776
H	0.79635	2.84765	2.78688
C	1.05065	-3.41147	1.31607
C	2.6157	-2.87736	-1.28767
C	4.38368	3.10198	1.0368
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C	3.1218	2.80451	0.29697
C	0.59292	1.61271	-3.2473
H	1.57786	1.1895	-3.46498
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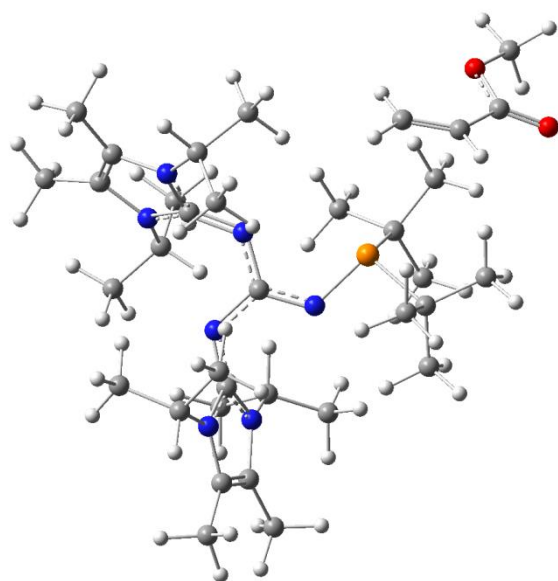
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H	-6.68285	0.85846	-0.39498
H	-6.33403	-0.70456	-1.14271
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H	-1.25346	2.91452	-1.5736
H	-1.10263	3.81843	-3.0972
H	-0.4556	4.50287	-1.59414
C	0.73086	2.9017	-2.44441
H	1.33986	3.59757	-3.02508
C	-2.57607	-0.15348	3.34132
H	-3.5771	0.11709	3.68893
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C	2.36996	-3.22896	2.06431
H	2.26486	-3.58513	3.09867
H	3.18584	-3.7952	1.60577
H	2.66028	-2.17525	2.10277
C	0.72549	-4.90578	1.1976
H	1.49392	-5.45725	0.64894
H	0.65141	-5.35126	2.19853
H	-0.23178	-5.0649	0.68896
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H	3.80141	-4.52044	-2.05046
H	3.30634	-4.74302	-0.36954
H	2.1313	-4.97505	-1.67893
C	2.3544	-2.39162	-2.72321
H	1.57149	-2.98198	-3.21209
H	2.04041	-1.34177	-2.72957
H	3.2692	-2.47667	-3.32363
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H	0.11711	-1.6756	2.26118

H	-1.0413	-2.86858	1.65424
H	-0.1145	-3.20977	3.13165
C	3.79041	-2.06887	-0.73085
H	4.66066	-2.18132	-1.39189
H	3.53384	-1.00714	-0.68106
H	4.0917	-2.39769	0.26637



**MA**

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H	2.39513	-0.15601	0.89047
H	2.35627	-1.7079	0.00083
O	0.59212	1.53364	0.00005
C	-2.15759	-0.7642	0.00006
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H	-1.64154	-1.71914	0.0002



**INT0**

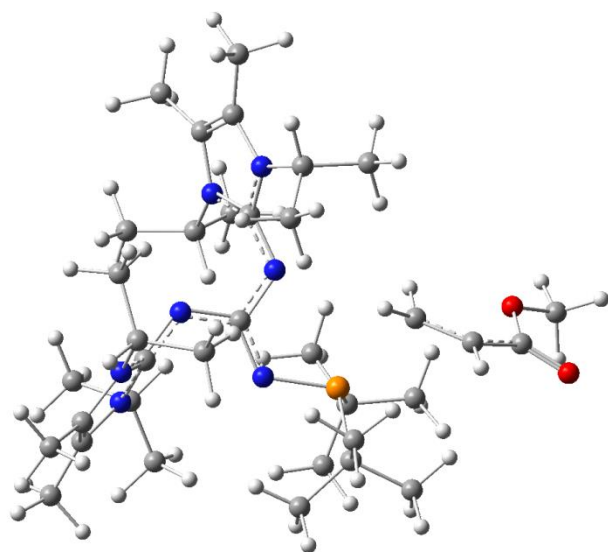
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H	3.74185	1.30689	3.18853
H	3.92495	2.99772	2.73662
C	2.37169	-2.07112	1.91124
H	1.63227	-1.27012	1.87364
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H	4.48288	-3.55352	-3.16107
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C	1.6643	-3.3366	2.38459
H	0.95041	-3.69068	1.63607
H	1.11652	-3.107	3.30304
H	2.36763	-4.13978	2.61414
C	-1.97042	3.39846	-1.25949
H	-2.68962	3.52894	-2.07367
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H	-2.12897	2.41744	-0.80292
C	3.50725	-1.66419	2.8465
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H	3.09922	-1.42279	3.83292
H	4.0311	-0.78524	2.46394
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H	-0.51885	-0.10731	2.50544
H	-1.80146	1.01888	2.0349
H	-1.9532	0.0849	3.53905
C	-1.16498	-3.80084	-0.46991
H	-1.36876	-4.67886	-1.0981
H	-0.115	-3.5249	-0.59612
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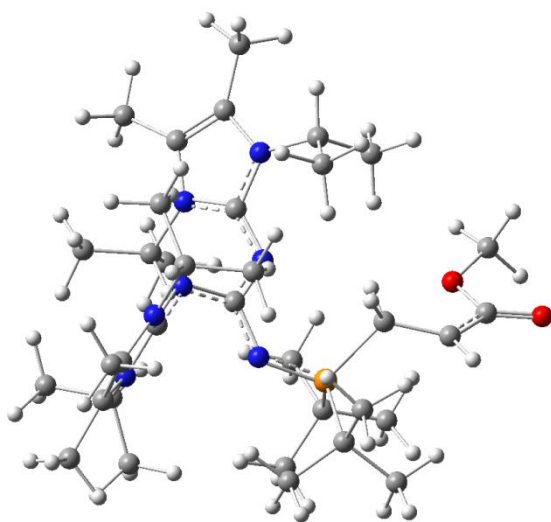
**TS1**

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H	5.77195	-2.15292	-2.66206
H	4.4638	-3.26682	-3.0912
H	5.61736	-3.70235	-1.82604
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H	-2.56739	3.49534	-2.87477
H	-2.28636	4.42594	-1.38863
H	-2.3837	2.65408	-1.32316
C	3.77758	-1.11341	2.90772
H	4.55526	-1.87487	3.00485
H	3.38676	-0.90887	3.90892
H	4.23304	-0.1994	2.52024
C	-2.16684	-1.58961	1.85018
C	-1.84482	-2.98705	-0.88695
C	4.57764	-3.75993	0.82945
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C	3.99937	-2.60101	0.08649
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H	1.65984	5.1277	2.83212
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C	-0.14073	2.20078	-3.0025
H	0.94673	2.13337	-3.09842
H	-0.56638	2.32391	-4.0026
H	-0.51477	1.27111	-2.57227
C	-0.53446	3.4028	-2.15385
H	-0.20558	4.29923	-2.68392
C	0.76181	5.90264	-1.09604
H	1.34836	5.82848	-2.01759
H	1.20539	6.68534	-0.47928
H	-0.25054	6.21939	-1.36651
C	3.62515	0.94106	-2.76957
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H	3.56118	1.35126	-3.78147
H	4.65835	1.04011	-2.42355
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H	3.91961	-1.05628	-3.44071
C	0.20298	2.66175	3.42595
H	0.43317	3.67252	3.77375
H	0.27256	1.98625	4.28409
H	-0.82701	2.64634	3.05986
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H	-2.28804	-3.76671	2.0843
H	-0.66971	-3.09656	2.35886
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H	-0.39963	-0.56469	2.61367
H	-1.72099	0.52998	2.17246
H	-1.83525	-0.44405	3.65623
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H	-0.86534	-4.8849	-1.18807
H	0.23547	-3.58931	-0.67493
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C	-5.63754	-0.35776	-0.78193
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O	-6.65843	-1.00053	-1.00405
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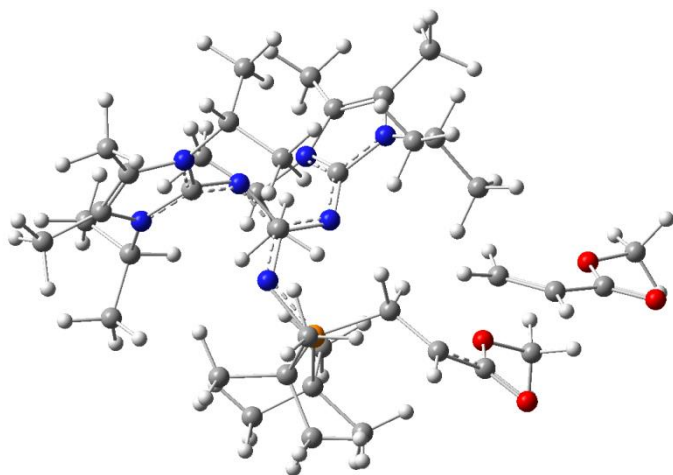
**IN1**

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H	5.76558	-0.32743	-3.17656
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C	-1.28411	4.44414	-0.38378
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C	0.4245	0.23148	-0.04652
C	3.15619	-1.78749	2.54932
H	2.56766	-2.49971	1.96604
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H	4.15595	-2.19735	2.70916
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H	-4.20481	1.86263	-2.26712
H	-4.08838	2.87464	-0.81457
H	-3.41628	1.23092	-0.81346
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H	5.20388	0.09408	2.54903
H	3.89158	0.68193	3.57471
H	4.23182	1.48426	2.02876
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C	-0.36618	-3.72494	-0.31779
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H	6.4323	-2.14804	-0.17811
H	5.18935	-2.90596	0.82
C	4.58448	-1.11194	-0.1968
C	1.52129	-0.33527	-3.36119
H	1.68772	-1.41522	-3.40933
H	1.16746	0.00288	-4.33959
H	0.74467	-0.13041	-2.62016
C	0.01656	5.63614	1.48143
H	-0.12199	5.52022	2.55881
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H	-0.54494	2.15782	-3.1767
H	-2.12013	1.60953	-3.779
H	-1.35285	0.76685	-2.41759
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C	-1.95219	5.56575	-1.10294
H	-1.5715	5.67655	-2.12338
H	-1.77335	6.50338	-0.57538
H	-3.03455	5.41382	-1.1617
C	2.71872	1.90221	-3.06532
H	1.97707	2.27194	-2.35656
H	2.42977	2.20458	-4.07578
H	3.68556	2.35823	-2.83307
C	2.82019	0.38215	-3.00995
H	3.58197	0.07272	-3.728
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H	-0.53277	3.77114	3.67374
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C	-0.57015	-2.80525	2.93681
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H	0.4432	-2.40776	2.82255
C	-2.96189	-2.70794	2.16379
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H	-3.22107	-2.71819	3.23028
H	-3.71153	-2.11891	1.63062



C	-1.33041	-4.85424	0.06791
H	-1.00216	-5.77266	-0.43328
H	-1.32777	-5.04867	1.14371
H	-2.35428	-4.64036	-0.24811
C	-0.27889	-3.64856	-1.85151
H	-1.26356	-3.55781	-2.31762
H	0.34162	-2.8063	-2.1735
H	0.18399	-4.57071	-2.22034
C	-1.66722	-0.62054	2.50816
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H	-2.36165	-0.03877	1.89572
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H	1.75806	-3.28725	-0.09396
H	1.06241	-4.13187	1.30361
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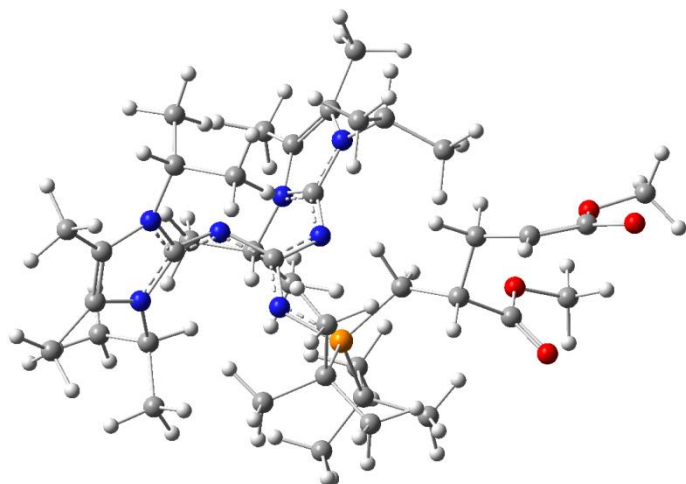
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C	-3.30699	3.24866	-1.91316
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C	-4.31314	-0.47994	-1.26173
H	-3.37267	0.00797	-1.52807
C	-5.28616	-1.55776	3.60529
H	-5.57622	-0.72004	4.24714
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C	-4.71613	-1.08306	2.31262
C	-0.64153	4.53274	-0.74985
C	-1.89143	2.70013	-2.04279
H	-1.93515	1.62526	-1.87201
C	-1.17722	0.2422	-0.03598
C	-4.38833	-1.81205	-1.99998
H	-3.65057	-2.51676	-1.60902
H	-4.17633	-1.63882	-3.05885
H	-5.38184	-2.26058	-1.931
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H	3.27033	3.12999	-0.19846
H	2.73818	1.4356	-0.13362
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C	-6.25149	-2.16968	0.56284

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H	-1.52107	-1.59688	3.43669
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H	-1.45362	5.65891	-2.40708
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H	1.1389	0.74334	1.86168
C	1.76349	2.74945	1.31152
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C	1.15283	5.64037	0.74121
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H	1.1476	-3.58269	1.57594
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H	-0.25447	-4.64513	1.76636
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O	3.86909	-0.48606	-1.33789
C	4.98288	0.042	-2.02683
H	5.89385	-0.04481	-1.43311
H	5.14085	-0.47293	-2.98289
H	4.75913	1.09401	-2.22211
O	5.17867	-2.28019	-0.85713
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H	1.33868	-1.27828	1.11828
H	1.84745	-0.38685	-0.2912
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H	5.6159	-2.30802	2.67897
C	6.27747	-0.54625	1.65454
O	5.77798	0.54402	1.00548
C	6.74671	1.48507	0.56848
H	7.26677	1.9367	1.419
H	7.48918	1.02037	-0.08529
H	6.19946	2.25434	0.0212
O	7.48192	-0.69069	1.80516
C	3.91641	-1.21119	1.97179
H	3.17675	-1.80569	2.50075
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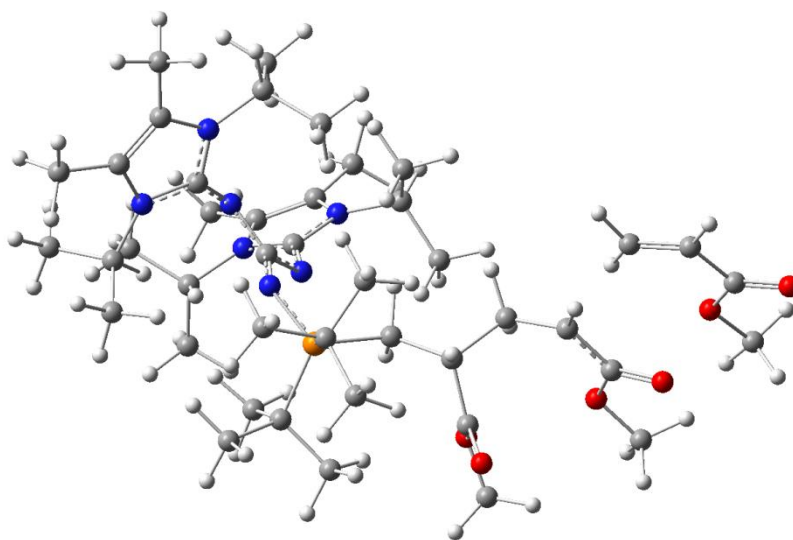
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H	-0.93084	-0.35104	4.311
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H	-3.34092	5.52607	-0.71082
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O	4.12389	0.30944	-1.17747
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H	5.04789	0.4206	-3.0381
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C	5.1995	-1.41261	1.97414

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C	6.37652	-0.74789	1.66815
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H	6.98399	2.13746	0.22278
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**TS3**

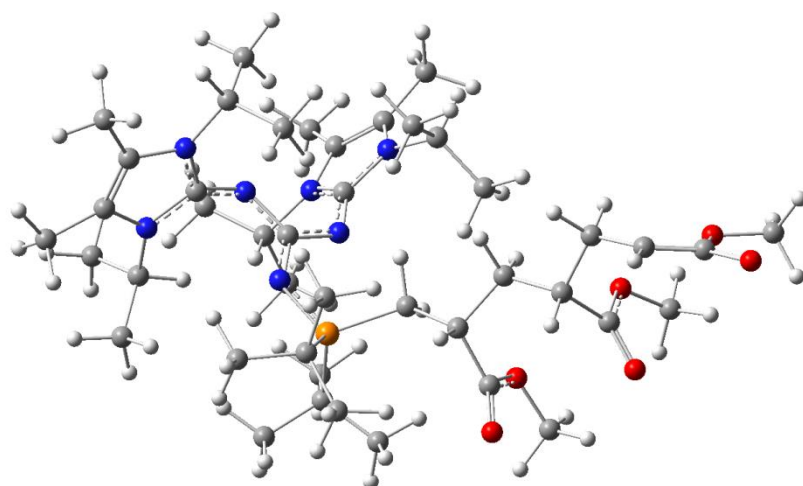
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C	-0.46245	-3.47613	0.45167
C	-7.0153	-2.06551	1.74
H	-7.87901	-1.4603	1.44923
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H	-6.8944	-2.86096	1.00306
C	-5.78068	-1.23842	1.88673
C	-1.80395	0.06419	3.54293
H	-1.83956	-0.99537	3.81257
H	-1.14526	0.57863	4.24874
H	-1.38211	0.15653	2.53976
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H	0.77775	-0.35353	0.42605
H	1.06159	-0.32729	-1.29057
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H	9.22216	2.97826	0.77784
H	9.4062	1.38905	0.00725
H	8.31126	2.6054	-0.71422
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**INT3**

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C	2.44993	-1.4692	-0.28591

H	2.39994	-2.45552	0.17411
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H	4.59674	-0.81382	2.93793
H	5.25199	0.63796	2.18533
C	4.73584	-0.93455	0.81291
H	4.8529	-2.02246	0.74934

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