Electronic Supplementary Information

A rational approach towards selective ethylene oligomerization *via* PNP-ligand design with an *N*-triptycene functionality

Samir Barman,*[a] E. A. Jaseer,*[a] Nestor Garcia,[a] Mohamed Elanany,[b] Motaz Khawaji,[b] Wei Xu,[b] Sibo Lin,[c] Hassan Alasiri,[a,d] Muhammad Naseem Akhtar[a] and Rajesh Theravalappil[a]

a. Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia
E-mail:. samir.barman@kfupm.edu.sa, jaseer@kfupm.edu.sa.
b. Saudi Aramco, Chemicals R&D, Research and Development Center, Dhahran 34464, Saudi Arabia.
c. Aramco Services Company: Aramco Research Center – Boston, 400 Technology Sq., Cambridge, MA 02139, United States.
d. Chemical Engineering Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

Section S1 *General Comments*

All manipulations were performed under an inert atmosphere of dry argon using standard Schlenk techniques. Solvents, Ph_2PCl, Et_3N and other starting materials were purchased from Sigma Aldrich. MMAO-3A (7 wt% solution in heptane) was purchased from Nouryon. $Cr(acac)_3$ (97% purity) was purchased from Strem chemicals. The ethylene gas (99.995% purity) was procured from Abdulla Hashim Gas Co., Saudi Arabia. Solvents and amine were dried using the appropriate reagents (sodium metal, calcium hydride and molecular sieve) and distilled under an argon atmosphere prior to use. Nuclear magnetic resonance (NMR) spectra were obtained at RT with a Bruker 400 MHz instrument using $SiMe_4$ for ^1H and ^{13}C and 85% H_3PO_4 for ^{31}P as external standards. Gas chromatography-mass spectrometric (GC-MS) data were obtained using a GC system 7890A armed with 5975C inert MSD with Triple-Axis Detector (Column: DB1,30 m x 320 μm x 1 μm). GC/FID analyses Agilent Technologies 7890A. Column: PoraBOND, 60 m × 320μm × 0.5 μm.

Section S2 *Computational details*

Energy of PNP-to-PPN isomerization (ΔG_{PPN}) was calculated using the same procedure as in our prior study.[1] For percent buried volume calculations, geometries of catalytic intermediate metallocycloheptanes (cationic charge and quartet spin state) were optimized using the PBE functional and the DNP basis as implemented in DMol3 (Materials Studio, Biovia). Then the ligand atoms were isolated by deleting the Cr and metallocycloheptane atoms. Then percent buried volume about the nitrogen center was calculated with SambVca 2.1 using the default parameters: atomic radii = 1.17 * Bondi radii, evaluation radius around N = 3.5 Å, 0.10 mesh spacing or numerical integration, and ignoring hydrogen atoms.[2]

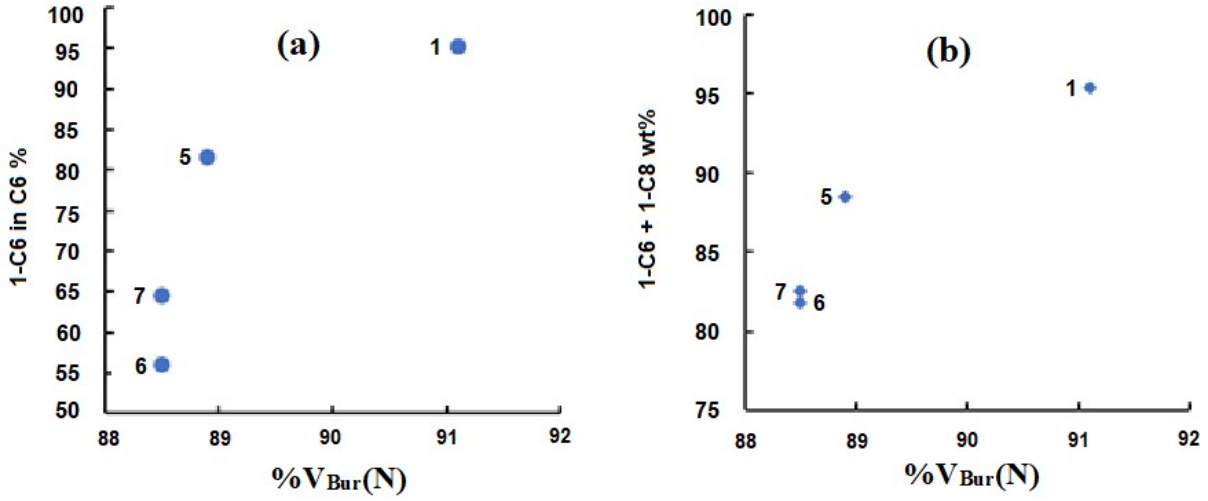
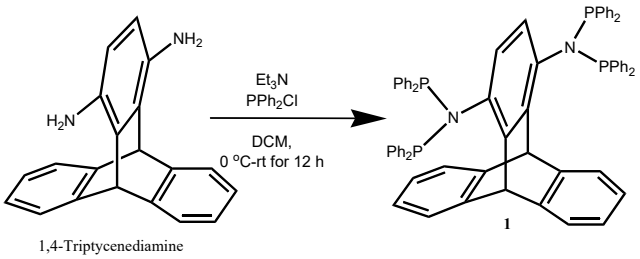


Fig S1. Correlations between %V_{Bur}(N) of ligands **1, 5-7** and catalytic outputs of $Cr(acac)_3$/ligand/MMAO-3A: (a) 1-C_6 in total C_6 % and (b) 1-C_6 + 1-C_8 wt%. Reaction conditions: $Cr(acac)_3$ 1 μmol, PNP/Cr = 1, MMAO-3A 2 mmol, total solution volume 100 mL, 45 ºC, 45 bar, 10 min.

Section S3 *Synthesis and Characterization*



Scheme S1. Synthetic scheme for the preparation of ditopic PNP ligand **1**.

Preparation of ditopic PNP ligand 1: To a solution of 1,4-Triptycenediamine[3,4] (0.161 g, 0.567 mmol) and triethylamine (0.34 g, 3.4 mmol) in 8 mL dichloromethane, Ph_2PCl (0.5 g, 2.26 mmol) dissolved in 2 mL dichloromethane was slowly added at 0 °C. The reaction mixture was stirred at this temperature for 1h then allowed to warm up to rt followed by additional stirring for 12 h. After this time, the solvent was removed under reduced pressure and the residue was extracted with anhydrous THF (3 × 5 mL). After removal of the THF solvent the remaining solid residue was triturated with dry CH_3CN (3 × 4 mL) followed by vacuum drying at 40 °C for 6 h to yield ligand **1**. Yield: 0.27 g, 47%. ^{1}H NMR ($CDCl_3$): δ 7.44–6.80 (m, aromatic H), 5.81 (s, 2H, aromatic), 5.55 (s, 2 tertiary H) ppm; ^{13}C NMR ($CDCl_3$): 49.31, 123.81, 124.64, 125.88, 128.02, 128.43, 129.50, 132.51, 132.71, 133.77, 134.01, 139.52, 142.15, 143.76, 144.98 ppm; ^{31}P NMR

($CDCl_3$): δ 59.34 (s) ppm. Anal. Calc. for $C_{68}H_{52}N_2P_4$: H 5.13, C 79.99, N 2.74%. Found H 4.6, C 79.14, N 3.52%.

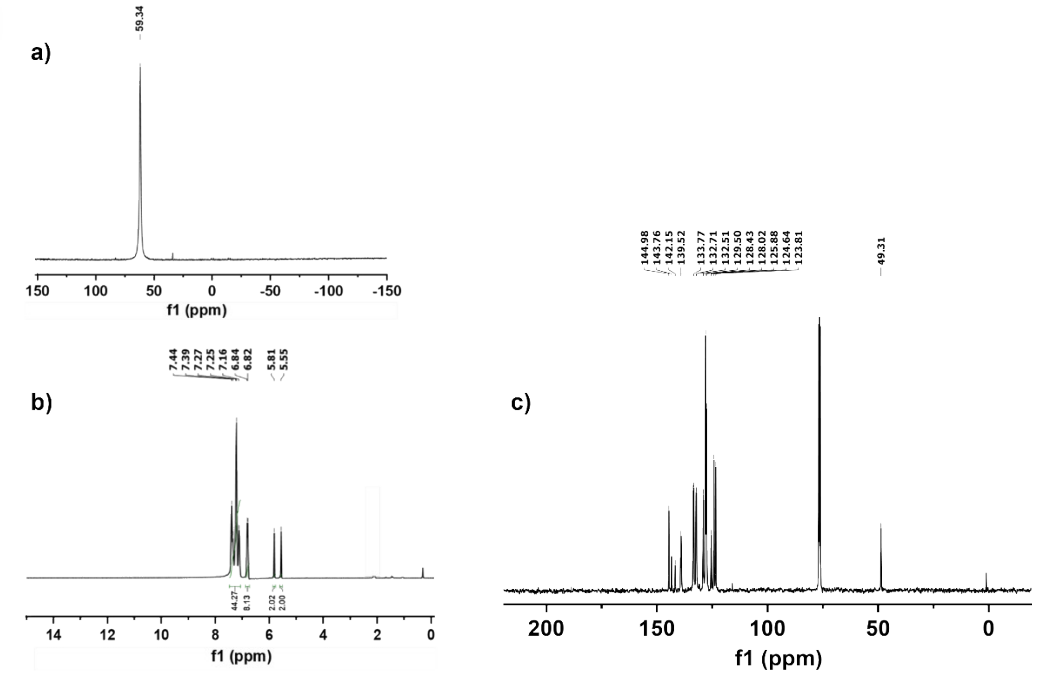
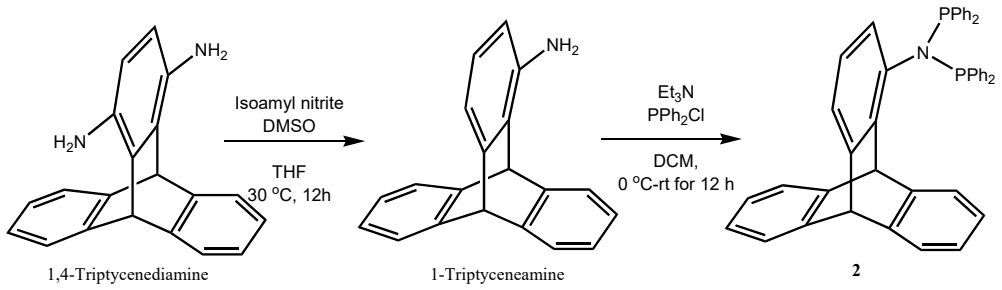


Fig S2. The liquid state ^{31}P (a) ^{1}H (b) and ^{13}C (c) NMR spectra of **1**.



Scheme S2. Synthetic scheme for the preparation of 1-PNP substituted triptycene ligand **2**.

Preparation of 1-Triptyceneamine. To a solution of 1,4-Triptycenediamine (0.50 g, 1.75 mmol) in THF (2 mL) was added dropwise over 20 min a solution of isoamyl nitrite (2.63 mmol) and DMSO (0.175 mmol) in THF (2 mL) at 30 °C. The mixture was stirred for additional 12 h. The solvent was evaporated, and the residue was purified by column chromatography on silica gel (hexane/ethyl acetate) to yield the desired 1-Triptyceneamine precursor in 15% yield. ^{1}H NMR ($CDCl_3$): δ 7.45 (m, 4H), 7.15 (m, 4H), 6.97 (d, 1H), 6.87 (t, 1H) 6.44 (d, 1H) 5.53 (s, 1H), 5.45 (s, 1H), 3.72 (br, 2H) ppm; ^{13}C NMR ($CDCl_3$): 48.01, 54.52, 113.8, 115.09, 123.46, 123.69, 125.08, 125.22, 125.89, 129.97, 140.81, 144.93, 145.72, 146.64 ppm. Anal. Calc. for $C_{20}H_{15}N$: H 5.61, C 89.19, N 5.20%. Found H 5.46, C 89.33, N 5.02%.

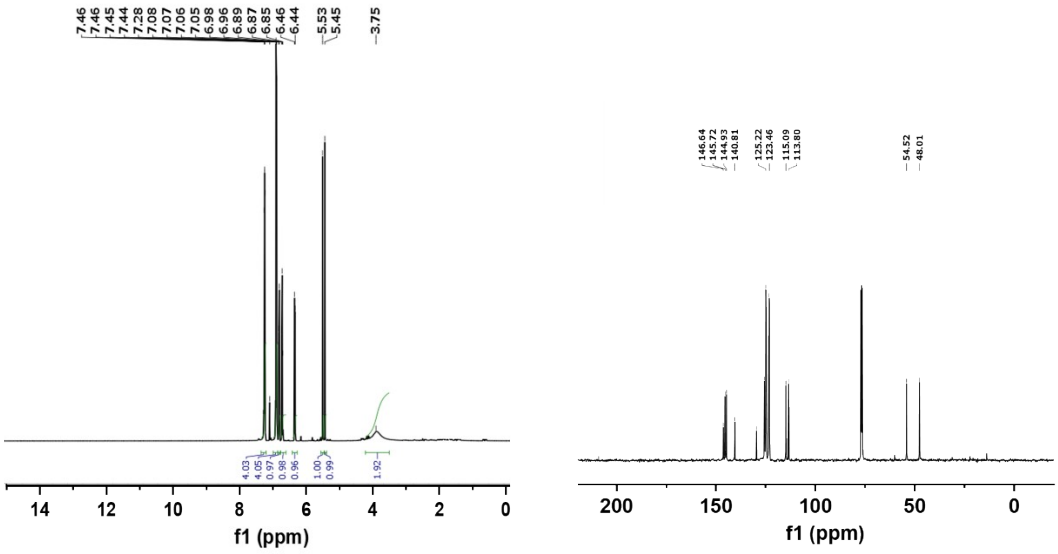


Fig S3. The liquid state ^{1}H (left) and ^{13}C (right) NMR spectra of 1-Triptyceneamine.

***Preparation of 2*:** To a solution of 1-Triptyceneamine (0.07 g, 0.26 mmol) and triethylamine (0.079 g, 0.78 mmol) in 1.5 mL dichloromethane, Ph_2PCl (0.115 g, 0.52 mmol) was slowly added at 0 °C. The mixture was stirred for 1 h and allowed to warm up to r.t. followed by additional stirring for 14 h. The volatiles were removed under reduced pressure and the residue was extracted with anhydrous THF (2 × 2 mL). After removing THF the remaining solid was degassed under vacuum at 50 °C for 3 h to yield desired ligand **2** in 62% yield. ^{1}H NMR (CD_2Cl_2): δ 6.14-7.49 (aromatic, 31H) 5.75 (s, 1H, bridge), 5.43 (s, 1H, bridge) ppm; ^{13}C NMR (CD_2Cl_2): 48.02, 54.36, 115.48, 116.31, 123.12, 123.42, 123.55, 123.92, 125.83, 128.41, 128.66, 130.95, 131.15, 140.76, 144.59, 144.8, 145.45, 145.65, 146.62 ppm; ^{31}P NMR (CD_2Cl_2): δ 60.09 (s) ppm. Elemental microanalysis: Calculated (%) for $C_{44}H_{33}NP_2$: H 5.22, C 82.87, N 2.20; Found (%) H 5.11, C 82.43, N 2.09.

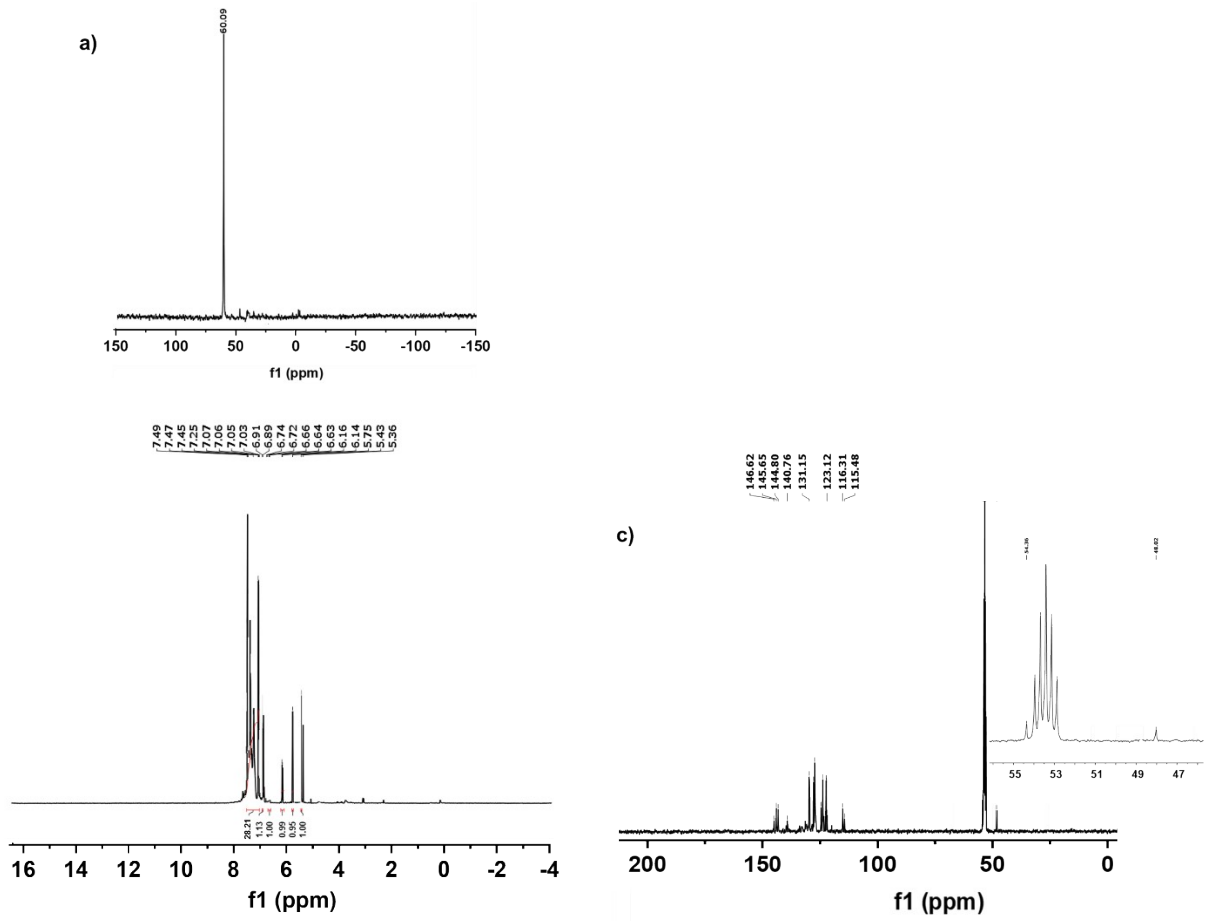
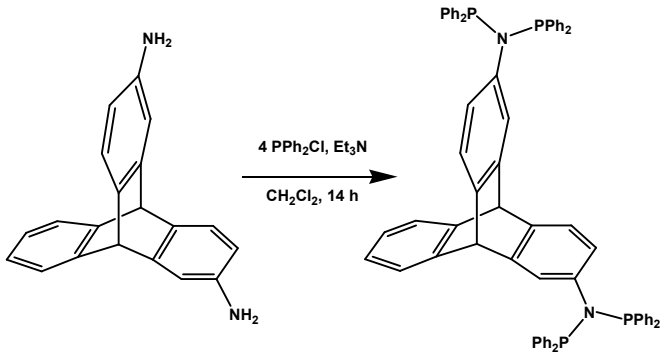


Fig S4. The liquid state ^{31}P (a) ^{1}H (b) and ^{13}C (c) NMR spectra of **2**.

***Preparation of 3*:** To a solution of 2,6-diaminotriptycene[5] (0.059 g, 0.21 mmol) and triethylamine (0.125 g, 1.24 mmol) in 2 mL dichloromethane, Ph_2PCl (0.18 g, 0.825 mmol) was slowly added at 0 °C. The mixture was stirred for 1 h and allowed to warm up to r.t. followed by additional stirring for 14 h. The volatiles were removed under reduced pressure and the residue was extracted with anhydrous THF (2 × 2 mL). After removing THF the remaining solid was triturated with anhydrous CH_3CN (1 × 3 mL) followed by degassing at 50 °C to yield desired ligand **3** as white solid in 63% yield. ^{1}H NMR (CD_2Cl_2): δ 6.30–7.31 (aromatic, 50H), 4.83 (bridge, 2H) ppm; ^{13}C NMR (CD_2Cl_2): Bridge carbon peak is merged with reference peak, 124.17, 127.15, 127.94, 128.20, 128.75, 129, 129.82, 132.33, 133.12, 133.23, 133.97, 139.35, 140.20, 142.13, 143.91, 144.85, 145.13; ^{31}P NMR (CD_2Cl_2): δ 65.95 (s) ppm. Anal. Calc. for $C_{68}H_{52}N_2P_4$: H 5.13, C 79.99, N 2.74%. Found H 4.93, C 79.08, N 2.52%.



Scheme S3. Synthetic scheme for the preparation of ligand **3**.

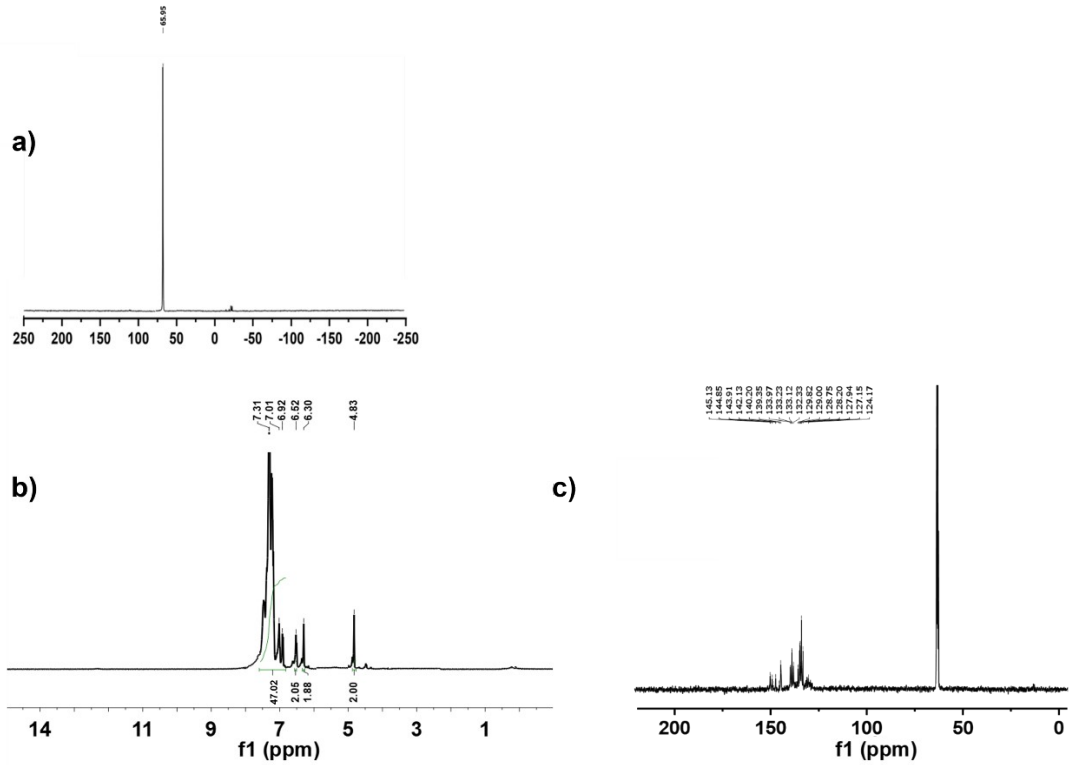
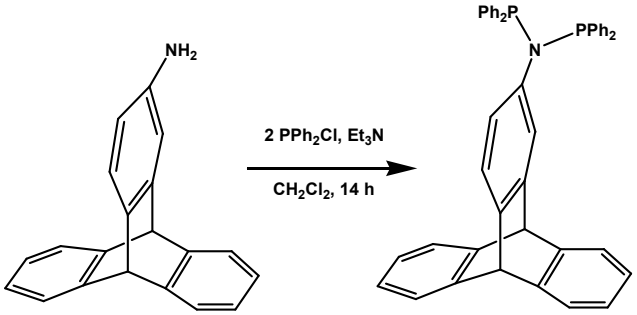


Fig S5. The liquid state ^{31}P (a) ^{1}H (b) and ^{13}C (c) NMR spectra of **3**.

***Preparation of 4*:** To a solution of 2-aminotriptycene[6] (0.11 g, 0.41 mmol) and triethylamine (0.125 g, 1.24 mmol) in 3 mL dichloromethane, Ph_2PCl (0.18 g, 0.825 mmol) was slowly added at 0 °C. The mixture was stirred for 1 h and allowed to warm up to r.t. followed by additional stirring for 14 h. The volatiles were removed under reduced pressure and the residue was extracted with anhydrous THF (2 × 2 mL). After removing THF the remaining solid was triturated with cold hexane (2 × 2 mL) followed by degassing at 50 °C to yield desired ligand **4** as white solid in 63% yield. ^{1}H NMR (CD_2Cl_2): δ 6.37-7.50 (aromatic, 31H), 5.33 (s, 1H, bridge), 4.98 (s, 1H, bridge) ppm; ^{13}C NMR (CD_2Cl_2): 106.97, 111.82, 112.14, 123.55, 124.95, 125.14, 127.92, 128.48, 128.99, 130.91, 131.12, 131.50, 133.18, 135.12, 135.37, 139.30, 144.23, 145.19, 145.86 ppm; ^{31}P NMR (CD_2Cl_2): δ 65.71 (s) ppm. Elemental microanalysis: Calculated (%) for $C_{44}H_{33}NP_2$: H 5.22, C 82.87, N 2.2; Found (%) H 4.89, C 82.13, N 2.33.



Scheme S4. Synthetic scheme for the preparation of ligand **4**.

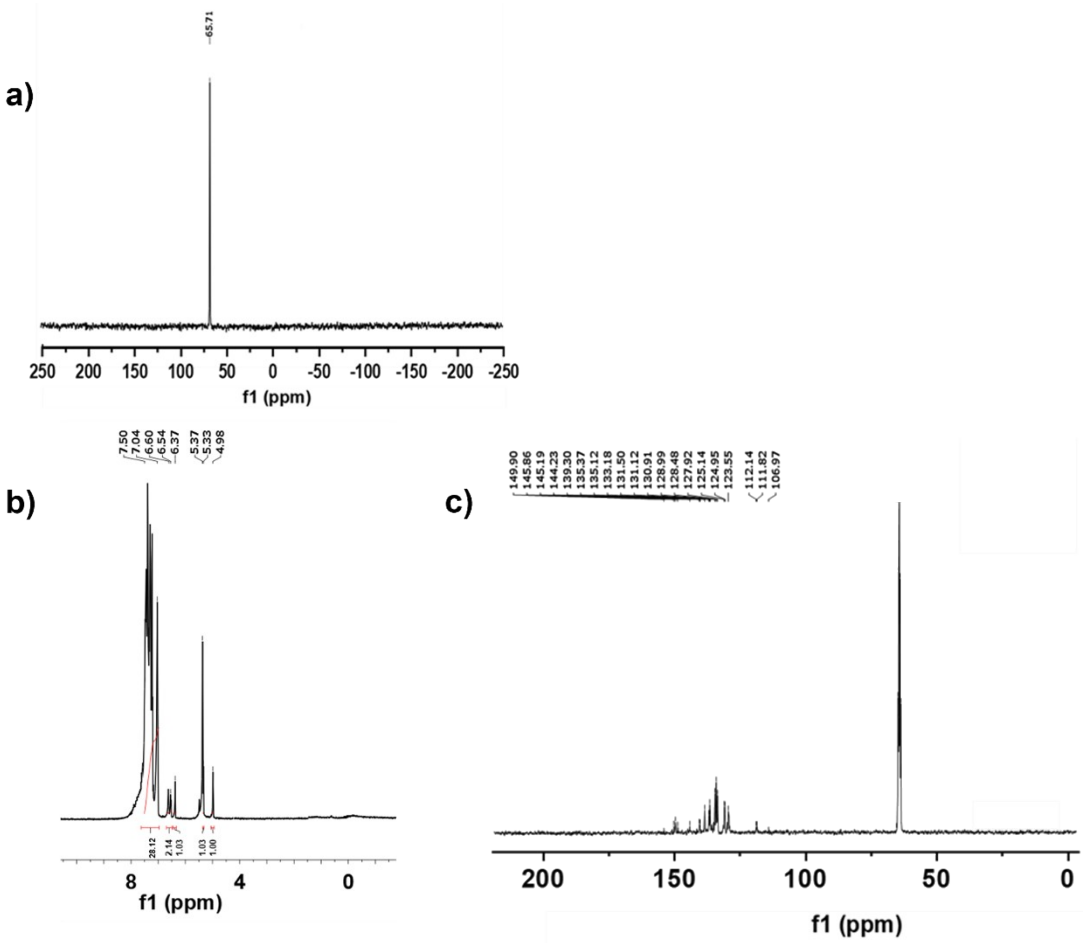
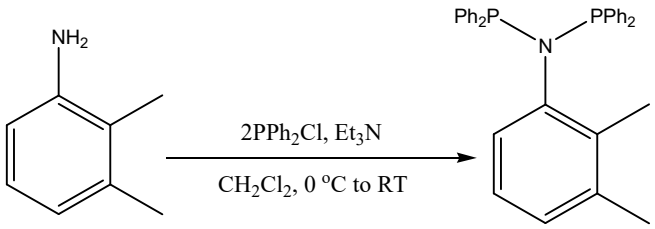


Fig S6. The liquid state ^{31}P (top) ^{1}H (bottom left) and ^{13}C (bottom right) NMR spectra of **4**.

***Preparation of 8*:** To a solution of 2,3-dimethylbenzenamine (0.10 g, 0.82 mmol) and triethylamine (2.47 mmol) in 3 mL dichloromethane, Ph_2PCl (1.65 mmol) was slowly added at 0 °C. The mixture was stirred for 1 h and allowed to warm up to r.t. followed by additional stirring for 14 h. The volatiles were removed under reduced pressure and the residue was extracted with anhydrous THF (2 × 2 mL). After removing THF the remaining solid was triturated with cold CH_3CN (3 × 2 mL) followed by degassing at 50 °C to yield desired ligand **8** as white solid in 43%

yield. ^{1}H NMR (CD_2Cl_2): δ 6.55-7.51 (aromatic, 23H), 2.15 (s, 3H, -C$\underline{H}_3$), 1.53 (s, 3H, -C$\underline{H}_3$) ppm; ^{13}C NMR (CD_2Cl_2):14.89, 20.53, 125.06, 127.75, 128.26, 128.51, 129.98, 130.93, 132.40, 132.62, 134.61, 134.88, 136.19, 137.94, 139.12, 139.26, 139.83, 139.91, 146.85 ppm; ^{31}P NMR (CD_2Cl_2): δ 59.67 (s) ppm. Elemental microanalysis: Calculated (%) for $C_{32}H_{29}NP_2$: H 5.97, C 78.51, N 2.86; Found (%) H 5.81, C 78.13, N 2.39.



Scheme S5. Synthetic scheme for the preparation of ligand **8**.

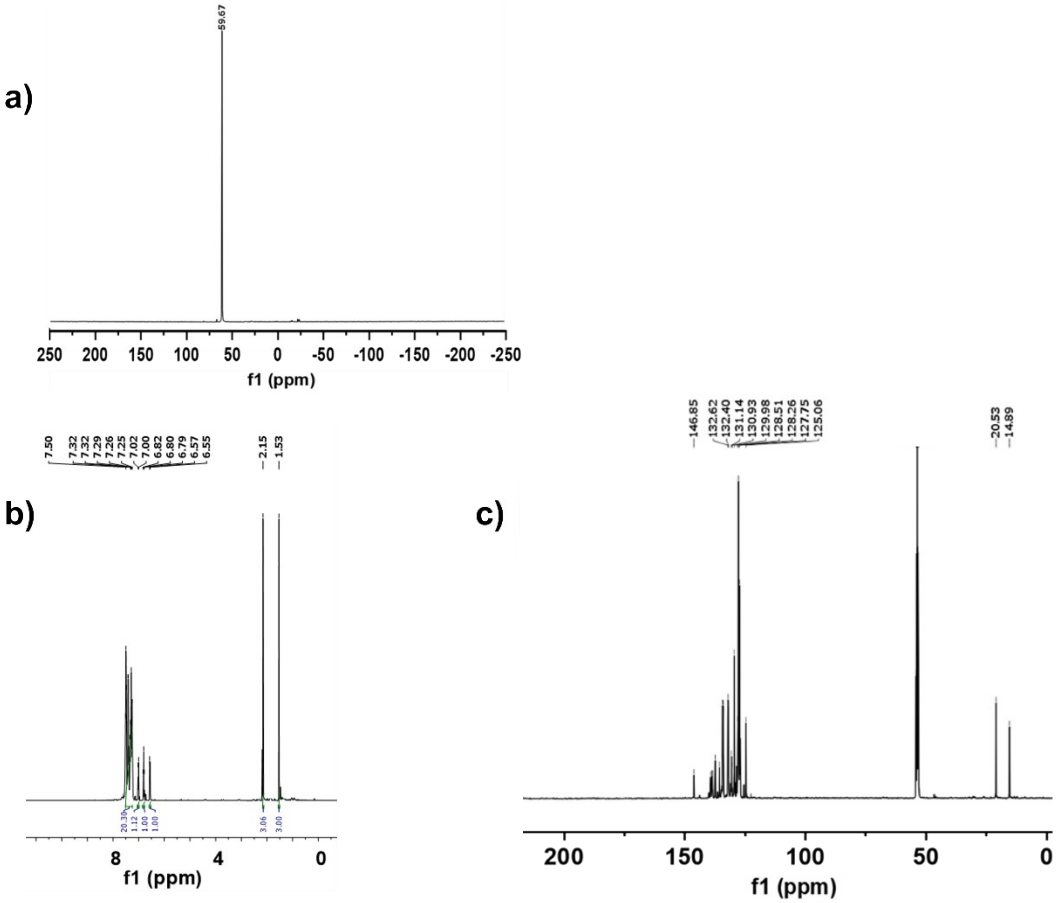


Fig S7. The liquid state ^{31}P (a) ^{1}H (b) and ^{13}C (c) NMR spectra of **8**.

Section S4 *General Oligomerization Procedure*

All runs for ethylene oligomerization were carried out in a 250 mL stainless steel (vessel) Buchi reactor system equipped with a propeller-like stirrer (1000 rpm) and injection barrel. Co-catalyst diluted in 95 mL of desired solvent and pre-catalyst mixture (containing $Cr(acac)_3$ and ligand dissolved in 5 mL of chlorobenzene or toluene) was charged to the reactor and pressurized with ethylene at 45 bar at the required temperature. The reaction temperature was maintained constant during the reaction by circulating hot oil in the jacket and by allowing the cool liquid to flow from the chiller through the cooling coil present inside the reactor vessel. The SCADA software controlled the reaction temperature and pressure of the reactor precisely using an electronic controller. Ethylene was fed on demand to keep the reactor pressure constant, and the uptake was monitored using a mass flow controller (MFC). After the desired reaction time, 2 mL methanol was injected to quench the reaction which was then cooled and depressurized slowly to atmospheric pressure. The small portion of the crude products was filtered and analyzed by GC-FID using nonane as internal standard. The remaining mixture was added to 50 mL of acidic methanol (5% HCl) and the polymeric products were recovered by filtration and washed with distilled water (3 × 50 mL) followed by drying at 60 °C under vacuum.

Section S5 *Cartesian coordinates (.xyz) of optimized molecules*

126
Ligand 1 (PNP-PNP isomer)
C -1.51097191 -3.01946919 0.60646490
C -2.32400274 -4.00692208 0.05937560
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126
Ligand 1 (PNP-PPN isomer)
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C -0.75446810 -3.48094959 -0.74384289
C 0.22222091 -2.72849720 0.15717029
C -0.25263550 -2.97833911 1.58359567
C 0.47547303 -3.55681389 2.61771934
C -0.12944272 -3.72833475 3.87423221
C -1.45169501 -3.32826662 4.07823202
C -2.18848401 -2.75389405 3.03040256
C -1.58719883 -2.57775689 1.79004024
C -2.24012738 -2.01042983 0.53206746
C -1.35665040 -0.85598352 0.05036797
C -1.76192296 0.45410427 -0.23769666
C -0.77667474 1.34998438 -0.69721593
C 0.54802198 0.96708561 -0.85288892
C 0.97736269 -0.35372619 -0.56363457
C -0.02152978 -1.24801592 -0.12769618
N 2.26681770 -0.82786095 -0.68690347
P 3.66313460 -0.10620229 -0.88053773
C 3.87141940 0.75288400 -2.49109756
C 2.85462085 0.57372046 -3.44293577
C 2.92629157 1.23055215 -4.67420513
C 4.01240838 2.06077548 -4.96693806
C 5.02944221 2.24053069 -4.02255670
C 4.95801884 1.59501313 -2.78537528
H 5.74051640 1.76520735 -2.04173891
H 5.87716813 2.89306806 -4.24622178
H 4.06520335 2.57414675 -5.93042799
H 2.12381179 1.09658534 -5.40334668
H 2.00175475 -0.06701105 -3.20901561
C 4.93316192 -1.41004522 -0.73217843
C 4.67341727 -2.46819284 0.15539365
C 5.63846668 -3.45399271 0.36801378
C 6.86460720 -3.39519285 -0.30305434
C 7.12376777 -2.34630400 -1.19020444
C 6.16347656 -1.35284538 -1.40324372
H 6.37570751 -0.54570878 -2.10621064
H 8.07662596 -2.30078354 -1.72350094
H 7.61832123 -4.16909329 -0.13622118
H 5.43122235 -4.27166419 1.06283588
H 3.71431180 -2.50479510 0.67390972
P 4.44862943 1.40114603 0.67376694
C 4.13494284 0.31277159 2.13121224
C 2.88440064 -0.24818537 2.46069284
C 2.76202371 -1.10645610 3.55588934
C 3.88477247 -1.43402492 4.32444637
C 5.13277675 -0.89616098 3.99860998
C 5.25490346 -0.02616984 2.91107349
H 6.23322471 0.39110887 2.65777850
H 6.01466632 -1.15102674 4.59191698
H 3.78451168 -2.11188591 5.17634528
H 1.78540349 -1.53071275 3.79529393
H 2.00077565 -0.02945901 1.86085413
C 3.08494840 2.64832720 0.66869440
C 3.00719271 3.50269135 -0.44937990
C 1.99466073 4.45859457 -0.54717041
C 1.06041999 4.60261206 0.48267791
C 1.16497366 3.80046309 1.62201236
C 2.16836522 2.83381273 1.71822393
H 2.22305981 2.21528922 2.61428347
H 0.44306729 3.91731046 2.43299499
H 0.25441489 5.33290575 0.40571477
H 1.93460895 5.09185682 -1.43612270
H 3.72626464 3.40546374 -1.26527743
H 1.26922914 1.70338789 -1.20386535
H -1.06387286 2.37377411 -0.93308555
N -3.12150910 0.89117510 -0.09513279
P -3.67757710 1.81085849 1.29117201
C -2.68570157 1.11521402 2.68966367
C -1.27963623 1.16033354 2.76556331
C -0.61419174 0.64452702 3.87848024
C -1.33865615 0.08846164 4.93890589
C -2.73304944 0.05024033 4.88275690
C -3.40056480 0.55590315 3.76176549
H -4.49328417 0.52430524 3.72031551

H -3.30465929 -0.38208001 5.70812869
H -0.81260091 -0.31941607 5.80552674
H 0.47699657 0.67500779 3.91787945
H -0.70160238 1.60555375 1.95555512
C -2.90806515 3.49657303 1.11823625
C -2.51975578 4.23641756 2.24982593
C -2.15530536 5.58203764 2.13760728
C -2.17473040 6.21656155 0.89176731
C -2.55364336 5.49042937 -0.24275252
C -2.92048489 4.14761281 -0.12902213
H -3.23197205 3.60145480 -1.02210592
H -2.56822516 5.97386514 -1.22332497
H -1.89257435 7.26894176 0.80474520
H -1.85328895 6.13679770 3.03011188
H -2.50187567 3.75908321 3.23274734
P -4.24914613 0.92241294 -1.46668985
C -3.06732560 0.67964730 -2.86656854
C -2.74417247 1.80771590 -3.63805883
C -1.75889827 1.73767721 -4.62866071
C -1.08925022 0.53307045 -4.86113658
C -1.41240902 -0.60205109 -4.10843523
C -2.39634612 -0.53007467 -3.12128307
H -2.62710301 -1.41993981 -2.53621504
H -0.89312341 -1.54842298 -4.27919313
H -0.31934614 0.47540458 -5.63562522
H -1.51465147 2.62521325 -5.21819651
H -3.26306288 2.75340398 -3.45582676
C -5.14263926 -0.69865012 -1.39329473
C -5.53189225 -1.37584400 -2.56263766
C -6.37094108 -2.49232113 -2.49665768
C -6.84164607 -2.94920412 -1.26167053
C -6.47353767 -2.27444077 -0.09233752
C -5.63954372 -1.15561481 -0.15889788
H -5.37544873 -0.62589326 0.75986588
H -6.83860559 -2.62087567 0.87811166
H -7.49222142 -3.82577963 -1.20990496
H -6.65090807 -3.01293219 -3.41632356
H -5.16857916 -1.03735300 -3.53590495
H -3.27674743 -1.70627245 0.69009687
H -3.22096453 -2.43588527 3.18895378
H -1.91728098 -3.46027749 5.05832720
H 0.43713346 -4.18071945 4.69274114
H 1.50930085 -3.87088118 2.45146417
H 1.26745519 -3.00756306 -0.01020439
H 0.60486635 -4.71745738 -1.87536560
H -1.22864445 -5.77715547 -3.21135430
H -3.60159682 -5.13963532 -2.79821916
H -4.15688906 -3.42639743 -1.07379903
61
Ligand 6 (PNP isomer)
C 2.51080279 2.30216630 -1.95023400
C 1.22917598 2.01337438 -1.48132021
C 0.88805364 0.71216530 -1.06547541
C 1.86335638 -0.28974893 -1.15549212
C 3.15905550 0.01685283 -1.57983795
C 3.49491094 1.31006561 -1.98589031
H 4.50820045 1.53414945 -2.32139651
C 4.19785355 -1.07016290 -1.50522666
F 5.32601612 -0.75449456 -2.16223889
F 3.74731825 -2.23540331 -2.00532527
F 4.54572630 -1.31547326 -0.21816711
H 1.62072777 -1.31074633 -0.86792231
N -0.40357535 0.43634461 -0.52243549
P -0.61971745 -0.17243390 1.13105467
C 0.80203771 0.61002024 2.02239330
C 0.50785057 1.76261625 2.77329543
C 1.52089889 2.46700272 3.43078183
C 2.84439276 2.02329816 3.35242587
C 3.14741706 0.86682471 2.62596747
C 2.13491793 0.16225831 1.97144141
H 2.39423130 -0.74066258 1.41958899
H 4.17821268 0.50995009 2.55755373
H 3.63879036 2.57419026 3.86283220
H 1.27442613 3.36112079 4.00944319
H -0.52665140 2.10961970 2.84277711
C -0.11677708 -1.94932985 1.03462100
C -0.38169093 -2.71558933 -0.11373014
C -0.14327017 -4.09191408 -0.12378250
C 0.35523219 -4.73026180 1.01607942
C 0.60876202 -3.98071338 2.16899519
C 0.37014167 -2.60365289 2.18101815
H 0.57639903 -2.03340589 3.09063634
H 0.99962586 -4.46903497 3.06564842
H 0.54587241 -5.80637437 1.00631727
H -0.34914430 -4.66651176 -1.03058583
H -0.77044192 -2.23195966 -1.01056998
P -1.78620929 0.92716862 -1.50026746
C -2.67677413 2.12233849 -0.40983816
C -1.95577106 2.99460445 0.42461046
C -2.60911653 3.99412697 1.14995560
C -3.99540067 4.14651742 1.04782079
C -4.72156115 3.29434545 0.20986365
C -4.06882218 2.29380564 -0.51574183
H -4.65314557 1.63351771 -1.16191611
H -5.80561360 3.40538365 0.12211049
H -4.50758668 4.92601145 1.61747356
H -2.02997071 4.65519800 1.80040736
H -0.87372895 2.88534018 0.52070863
C -2.86972143 -0.57192414 -1.42756162
C -3.61825922 -0.97114318 -0.30543142
C -4.31245968 -2.18293790 -0.31445704
C -4.27553870 -3.00873474 -1.44367649
C -3.55073381 -2.61390009 -2.57172400
C -2.85594030 -1.40046184 -2.56346075
H -2.28503135 -1.09458419 -3.44508484
H -3.52657541 -3.25008294 -3.46025243

H -4.81586018 -3.95896216 -1.44445312
H -4.88015888 -2.48832298 0.56825792
H -3.64557889 -0.33745479 0.58270074
H 0.48115920 2.80662519 -1.42447835
H 2.75177550 3.31914858 -2.26885898
61
Ligand 6 (PPN isomer)
C 2.33659589 1.73514358 3.16758249
C 1.11982590 1.14001999 2.83732842
C 0.98424450 0.31540769 1.69412009
C 2.14494408 0.11379463 0.90618363
C 3.35785051 0.70677547 1.25117885
C 3.47221035 1.52712973 2.38153009
H 4.42768242 1.98876937 2.63703234
C 4.58943306 0.46334621 0.41980298
F 5.56194019 -0.13751969 1.13652757
F 4.35585325 -0.31599881 -0.65386380
F 5.12269006 1.61839738 -0.04117952
H 2.09508940 -0.49791183 0.00783170
N -0.25017398 -0.25096331 1.45144562
P -0.90525034 -0.89648025 0.15611694
C 0.02519123 -2.29583909 -0.59352173
C -0.09475655 -2.68338298 -1.93782942
C 0.64562991 -3.76572305 -2.42309487
C 1.50916161 -4.46313749 -1.57303425
C 1.63157086 -4.07984465 -0.23301870
C 0.89340823 -3.00101607 0.25708961
H 0.99533516 -2.68904087 1.29924148
H 2.30997810 -4.61937205 0.43239279
H 2.09190547 -5.30453170 -1.95638559
H 0.55032417 -4.06093002 -3.47104702
H -0.75886667 -2.13708147 -2.61171839
C -2.52776426 -1.55945318 0.65619131
C -3.01903884 -1.28988446 1.94100944
C -4.28504345 -1.75166545 2.30968826
C -5.06254146 -2.47672390 1.40106179
C -4.57158461 -2.74665312 0.11898312
C -3.30619434 -2.28969897 -0.25535802
H -2.92642576 -2.50895661 -1.25621727
H -5.17532561 -3.31650374 -0.59164615
H -6.05350474 -2.83448045 1.69226109
H -4.66688185 -1.54231943 3.31217982
H -2.39530590 -0.72110030 2.63290131
P -1.43680497 0.45573516 -1.60786392
C -2.64754303 1.55434423 -0.74774944
C -2.52861960 2.02750671 0.57435589
C -3.52879295 2.83004102 1.12810222
C -4.65817039 3.17369735 0.37774693
C -4.78911525 2.70601107 -0.93247957
C -3.79289138 1.89829293 -1.48840008
H -3.90535040 1.52673169 -2.51071644
H -5.67073054 2.96599173 -1.52395676
H -5.43764825 3.80234542 0.81616141
H -3.42525231 3.18591347 2.15650241
H -1.66432366 1.74860276 1.17917561
C 0.16226566 1.38052516 -1.64815111
C 0.41369185 2.58242933 -0.96725793
C 1.67630318 3.17631901 -1.02973694
C 2.70257747 2.58223925 -1.76877943
C 2.45586490 1.39671638 -2.46705296
C 1.19294459 0.80553747 -2.41636182
H 1.01268402 -0.12420709 -2.96286180
H 3.25564372 0.92131302 -3.03884904
H 3.69751676 3.03035122 -1.78662291
H 1.86373780 4.10153081 -0.47933483
H -0.36947351 3.05496694 -0.37397468
H 0.23597697 1.29892606 3.45936667
H 2.40068131 2.37076933 4.05497414
145
1-chromacycloheptane (cationic, quartet)
Cr -3.42938 12.22645 -4.96529
P -3.04008 10.31846 -6.50322
P -4.15004 10.07846 -4.02498
N -3.83994 9.17740 -5.47257
C -3.88947 7.74275 -5.55327
C -1.65760 13.88208 -6.35836
C -3.12785 13.50017 -6.51738
C -3.69727 13.11921 -3.15313
C -1.12627 13.65954 -4.91990
C -1.69682 14.59441 -3.82474
C -2.42317 13.84107 -2.69816
H -10.33582 8.26860 -5.07132
C -9.53441 7.61444 -5.41615
C -9.66895 6.22772 -5.30464
C -8.64402 5.37308 -5.74017
C -7.49025 5.93017 -6.28256
C -7.35611 7.32278 -6.39158
C -8.36953 8.17183 -5.95857
H -10.58258 5.80293 -4.88378
H -8.75583 4.29019 -5.66163
C -6.03972 7.74169 -7.03252
H -8.25255 9.25482 -6.03254
C -6.29632 5.17573 -6.85902
C -4.94103 7.09413 -6.20585
C -5.06656 5.69706 -6.12692
C -4.12120 4.92966 -5.43269
C -3.04683 5.59115 -4.80800
C -2.92862 6.97522 -4.86883
H -2.10087 7.47325 -4.36616
H -5.70488 7.30094 -11.76990
C -5.83782 6.83907 -10.78995
C -6.04578 5.46188 -10.69130
C -6.20320 4.85907 -9.43484
C -6.16153 5.65529 -8.29649
C -5.99003 7.04468 -8.39428
C -5.81129 7.64156 -9.63967

H -6.07148 4.84706 -11.59246
H -6.33788 3.77993 -9.34965
H -5.67253 8.71728 -9.73010
H -5.93458 8.82436 -7.10636
H -6.41140 4.09404 -6.79238
C -1.44945 2.88257 -5.67448
C -1.17473 2.43859 -4.36651
C 0.08046 2.63980 -3.79075
C 1.09549 3.26918 -4.52173
C 0.84392 3.68658 -5.83100
C -0.41712 3.49307 -6.40542
H -1.95004 1.93241 -3.79182
H 1.63306 4.16237 -6.41576
H -0.59023 3.82083 -7.42977
H 2.08192 3.41544 -4.07942
H 0.26978 2.28998 -2.77492
C -3.08189 3.27066 -8.01170
C -2.80169 4.62390 -8.29347
C -2.74274 5.07616 -9.61079
C -2.94665 4.19061 -10.67378
C -3.22402 2.84635 -10.41306
C -3.29800 2.39543 -9.09143
H -2.61993 5.32562 -7.48212
H -3.38226 2.14804 -11.23609
H -3.51142 1.34221 -8.89363
H -2.90376 4.55288 -11.70140
H -2.55582 6.13174 -9.81589
P -3.12971 2.47806 -6.34010
C -6.66534 1.95826 -5.30505
C -7.83682 1.56618 -4.62850
C -8.87068 0.91798 -5.30749
C -8.76462 0.67412 -6.68188
C -7.60921 1.06709 -7.36523
C -6.56438 1.69447 -6.67918
H -7.94263 1.77723 -3.56105
H -7.51451 0.88161 -8.43676
H -5.66635 1.98312 -7.22485
H -9.57662 0.18202 -7.21903
H -9.76641 0.61340 -4.76468
C -4.61378 1.54901 -3.38355
C -4.53823 0.22330 -3.84116
C -3.85535 -0.74128 -3.09516
C -3.24762 -0.39233 -1.88389
C -3.33259 0.92124 -1.41096
C -4.01796 1.88675 -2.15528
H -5.01324 -0.05345 -4.78373
H -2.87299 1.19013 -0.45783
H -4.09289 2.91107 -1.78458
H -2.72152 -1.15019 -1.30058
H -3.79687 -1.76686 -3.46167
P -5.45227 2.91337 -4.29377
N -4.21757 3.49974 -5.39063
C -2.97555 9.53000 -2.72542
C -3.35968 8.86614 -1.55090
C -2.39644 8.50695 -0.60395
C -1.04894 8.81112 -0.81377
C -0.66066 9.49288 -1.97231
C -1.61890 9.85279 -2.91595
H -4.40620 8.62069 -1.37126
H 0.38691 9.74643 -2.14001
H -1.30458 10.37864 -3.81788
H -0.30137 8.52709 -0.07179
H -2.70179 7.98531 0.30305
C -5.79319 9.57763 -3.43243
C -6.12170 8.22349 -3.20949
C -7.37895 7.88598 -2.71280
C -8.30870 8.88793 -2.41676
C -7.98849 10.23167 -2.63371
C -6.73550 10.57868 -3.14638
H -5.40723 7.43036 -3.42566
H -8.71164 11.01184 -2.39558
H -6.48501 11.62851 -3.30825
H -9.29045 8.62142 -2.02616
H -7.63044 6.83514 -2.56607
C -3.93565 10.53103 -8.07545
C -3.28570 10.48474 -9.31932
C -3.96121 10.88147 -10.47791
C -5.28295 11.33001 -10.40604
C -5.93480 11.38381 -9.16628
C -5.26103 11.00190 -8.00810
H -2.25015 10.15067 -9.38934
H -6.96547 11.73489 -9.10277
H -5.76504 11.08058 -7.04186
H -5.80459 11.64045 -11.31245
H -3.44943 10.84351 -11.44042
C -1.46522 9.51501 -6.91925
C -0.26628 10.04625 -6.42382
C 0.93505 9.35633 -6.60445
C 0.94407 8.13213 -7.27811
C -0.24699 7.59846 -7.78037
C -1.44897 8.28553 -7.60597
H -0.26332 11.00033 -5.89663
H -0.24210 6.64454 -8.30858
H -2.37512 7.86153 -7.99800
H 1.88205 7.59426 -7.41767
H 1.86354 9.77981 -6.21817
H -2.30245 5.00456 -4.27242
H -1.05973 13.27616 -7.05654
H -1.47815 14.93848 -6.63142
H -3.42941 13.30299 -7.55228
H -3.82661 14.25273 -6.08566
H -4.45627 13.83649 -3.54877
H -4.16915 12.57264 -2.32616
H -1.29549 12.59745 -4.60919
H -0.02780 13.71724 -4.93581

H -0.88178 15.19607 -3.39832
H -2.39563 15.31670 -4.27873
H -1.73773 13.10237 -2.24691
H -2.67322 14.55456 -1.89070
80
6-chromacycloheptane (cationic, quartet)
Cr 0.82567 7.49388 -0.78442
P 0.38676 5.91859 0.94116
P 0.85656 5.10956 -1.66195
N 0.28959 4.54201 -0.10256
C 0.25162 3.16091 0.31158
C -0.69045 8.51005 -2.60279
C -1.09361 7.85419 -1.28629
C 1.26474 9.06756 0.45030
C 0.68803 9.24333 -2.56305
C 0.79131 10.48179 -1.63651
C 1.70735 10.25538 -0.42291
C 0.16727 0.46742 1.08409
C 1.31022 1.22980 1.32354
C 1.36114 2.56885 0.93179
C -0.89185 2.39586 0.05646
C -0.92910 1.05524 0.44065
H 2.26379 3.15339 1.09758
H -1.74382 2.83759 -0.45130
C -2.15777 0.22104 0.16503
C 2.43605 4.26280 -1.97257
C 3.60109 5.04610 -1.95549
C 4.85617 4.45185 -2.11576
C 4.95127 3.06842 -2.28613
C 3.79510 2.28056 -2.30590
C 2.53797 2.87077 -2.15280
H 3.52953 6.12939 -1.83101
H 3.86971 1.20050 -2.44228
H 1.64325 2.24752 -2.18053
H 5.92970 2.60133 -2.41084
H 5.75491 5.06908 -2.11269
C -0.30614 4.46442 -2.90356
C -1.68807 4.52163 -2.65140
C -2.60118 4.15090 -3.63712
C -2.14740 3.74410 -4.89627
C -0.77426 3.70451 -5.16165
C 0.14532 4.06485 -4.17503
H -2.05220 4.85336 -1.67979
H -0.41485 3.38776 -6.14127
H 1.21306 4.02559 -4.39525
H -2.86195 3.45758 -5.66764
H -3.66991 4.18278 -3.42119
C 1.62306 5.56390 2.22572
C 2.97355 5.79962 1.91493
C 3.97349 5.42089 2.81088
C 3.62943 4.81646 4.02549
C 2.28619 4.59173 4.34392
C 1.28110 4.96302 3.44862
H 3.24987 6.26267 0.96594
H 2.01793 4.12490 5.29189
H 0.23563 4.77450 3.69388
H 4.41013 4.52240 4.72815
H 5.02029 5.60211 2.56527
C -1.19706 6.13761 1.79548
C -1.26669 7.13085 2.78965
C -2.48850 7.42043 3.39831
C -3.64557 6.73138 3.01502
C -3.57944 5.75373 2.01866
C -2.35962 5.46054 1.40270
H -0.37000 7.67523 3.09157
H -4.47768 5.21250 1.71898
H -2.31373 4.70057 0.62651
H -4.59856 6.95921 3.49323
H -2.53912 8.18568 4.17244
H 0.12839 -0.57838 1.39252
H 2.17396 0.77833 1.81119
F -3.14718 0.93606 -0.43950
F -2.68231 -0.29784 1.31401
F -1.87390 -0.83788 -0.64948
H -0.66289 7.75708 -3.40553
H -1.43117 9.27017 -2.91036
H -1.78416 7.01110 -1.40507
H -1.48475 8.54976 -0.52938
H 0.35660 9.31274 1.02924
H 2.04689 8.77902 1.17654
H 1.55537 8.54158 -2.35653
H 0.93221 9.51175 -3.60102
H 1.15691 11.34044 -2.21856
H -0.22018 10.75013 -1.29049
H 2.73752 10.08831 -0.78525
H 1.75011 11.18315 0.17582
76
7-chromacycloheptane (cationic, quartet)
Cr 3.09930 -1.72100 3.36810
P 4.72680 -0.47691 2.12300
P 4.53940 -3.17520 1.98680
N 5.50330 -1.85250 1.42470
C 6.75530 -1.76670 0.58970
C 0.35230 -2.31210 2.68300
C 0.25810 -2.49250 4.21110
C 1.56960 -3.01770 4.84710
C 1.44361 -1.33050 2.25280
C 2.78170 -0.73320 5.10330
C 2.32120 -2.03010 5.79530
C 6.69630 -2.67200 -0.64100
C 8.03760 -1.99300 1.39350
C 6.74190 1.51630 2.25950
C 7.79070 2.17260 2.90930
C 8.12470 1.83630 4.22640
C 7.40020 0.84950 4.90400

C 6.34670 0.19590 4.26220
C 6.02110 0.51480 2.93180
C 3.88220 0.02740 -0.51500
C 3.24890 0.79651 -1.49450
C 2.78100 2.07630 -1.18660
C 2.94470 2.59280 0.10360
C 3.57970 1.83270 1.08630
C 4.06000 0.54890 0.77560
C 3.11230 -3.97330 -0.20760
C 2.76600 -4.78880 -1.28610
C 3.47350 -5.97230 -1.51920
C 4.52470 -6.34060 -0.67250
C 4.88400 -5.52270 0.40080
C 4.18130 -4.32970 0.63230
C 4.81880 -5.28680 3.79050
C 5.30020 -5.88220 4.95680
C 6.35110 -5.29290 5.67050
C 6.91510 -4.09900 5.21240
C 6.43620 -3.49690 4.04710
C 5.39730 -4.09280 3.31240
H -0.62950 -1.97090 2.30630
H 0.53160 -3.29390 2.21260
H -0.00750 -1.52890 4.67460
H -0.56510 -3.18140 4.44860
H 1.39510 -3.94310 5.41570
H 2.22870 -3.43710 4.03050
H 1.63980 -1.36230 1.17110
H 1.19980 -0.28990 2.52790
H 1.97810 0.01120 4.99870
H 3.63980 -0.25800 5.59830
H 1.64240 -1.82530 6.64200
H 3.19080 -2.55980 6.22060
H 6.75570 -0.72370 0.23541
H 7.54400 -2.42970 -1.29640
H 6.77790 -3.73180 -0.36951
H 5.76800 -2.53790 -1.21220
H 8.90550 -1.78990 0.75110
H 8.10190 -1.31900 2.25690
H 8.11820 -3.03260 1.74060
H 7.64610 0.59670 5.93600
H 8.94450 2.35200 4.72900
H 6.48410 1.78830 1.23540
H 8.34580 2.95380 2.38930
H 5.76940 -0.55730 4.79920
H 2.57500 3.58930 0.34860
H 2.28150 2.67220 -1.94970
H 4.22450 -0.97910 -0.75640
H 3.11900 0.39010 -2.49800
H 3.69500 2.23850 2.09320
H 5.07030 -7.26900 -0.84821
H 3.19750 -6.61400 -2.35660
H 2.55280 -3.05540 -0.01740
H 1.93820 -4.50380 -1.93590
H 5.71290 -5.81080 1.04820
H 7.73230 -3.62950 5.76150
H 6.72930 -5.76320 6.57830
H 3.99010 -5.75350 3.25380
H 4.85320 -6.81130 5.31030
H 6.88020 -2.56500 3.70740

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5-chromacycloheptane (cationic, quartet)

Cr -5.398800 -0.149300 -0.321300
P -3.291600 -1.599700 -0.268500
P -3.431700 1.168500 0.067900
N -2.341700 -0.169300 -0.012800
C -0.909000 -0.032900 0.017400
C -6.926000 -1.870500 0.857400
C -6.074700 -0.762900 1.473100
C -6.640700 1.407300 -0.801800
C -7.488700 -1.536900 -0.559100
C -8.495000 -0.362500 -0.642400
C -7.944200 0.850600 -1.404500
H -6.338500 -2.799300 0.789300
H -7.802300 -2.097300 1.491000
H -5.338400 -1.127500 2.201000
H -6.663000 0.061500 1.904400
H -6.833400 1.986000 0.119500
H -6.127000 2.083000 -1.508900
H -6.674400 -1.388800 -1.332900
H -7.934200 -2.462600 -0.950800
H -9.422200 -0.710300 -1.120200
H -8.773300 -0.058700 0.380100
H -7.765700 0.555000 -2.453200
H -8.721000 1.635800 -1.444300
C -0.230400 0.069800 1.239100
C 1.122200 0.403800 1.253400
C 1.817800 0.643000 0.058000
C 1.157300 0.428600 -1.161300
C -0.196800 0.106200 -1.180100
H -0.711100 -0.005900 -2.132400
C 4.543800 0.521800 -2.382400
C 3.850000 1.556100 -3.029600
C 4.075700 1.835600 -4.380400
C 4.983100 1.069400 -5.116200
C 5.687800 0.038200 -4.481300
C 5.483100 -0.221700 -3.124500
H 3.152900 2.176100 -2.469700
H 6.405900 -0.559500 -5.045500
H 6.060300 -1.010100 -2.636600
H 5.160800 1.289300 -6.170100
H 3.543700 2.663900 -4.853500
C 3.841000 -1.472600 -0.408000
C 3.332200 -2.234200 -1.469700
C 2.837400 -3.522600 -1.245100
C 2.811400 -4.052100 0.047700

C	3.307300	-3.297800	-1.115600
C	3.833500	-2.025800	0.884400
H	3.332600	-1.823400	-2.479800
H	3.311000	-3.711000	2.126500
H	4.240800	-1.452600	1.718100
H	2.423900	-5.055700	0.223900
H	2.468800	-4.116000	-2.083100
P	4.525000	0.234700	-0.558400
C	4.727200	2.598300	2.019800
C	5.447500	3.768400	2.326900
C	6.440200	3.756900	3.307900
C	6.729000	2.580500	4.006400
C	6.006000	1.417200	3.722800
C	5.007000	1.430100	2.747600
H	5.236500	4.698500	1.795100
H	6.214700	0.494700	4.268100
H	4.438000	0.520800	2.549900
H	7.508300	2.573100	4.770100
H	6.993600	4.674300	3.519000
C	3.941600	3.759000	-0.486500
C	5.264400	3.736100	-0.960700
C	5.611900	4.451200	-2.109000
C	4.646000	5.196400	-2.794700
C	3.330200	5.234700	-2.324700
C	2.982000	4.521900	-1.172600
H	6.017900	3.135000	-0.450500
H	2.572800	5.812500	-2.856700
H	1.949100	4.535100	-0.813800
H	4.917100	5.741100	-3.700700
H	6.635600	4.402700	-2.485000
P	3.287900	2.711300	0.884400
N	3.160800	1.132600	0.113900
C	-3.048800	2.287300	-1.316800
C	-3.047000	3.681300	-1.157100
C	-2.849100	4.512100	-2.261900
C	-2.670500	3.959500	-3.534300
C	-2.697800	2.570800	-3.701900
C	-2.894300	1.736600	-2.602500
H	-3.195000	4.124300	-0.172700
H	-2.566500	2.133600	-4.692300
H	-2.917600	0.655300	-2.749800
H	-2.511000	4.608800	-4.395600
H	-2.836500	5.593600	-2.123400
C	-3.060000	2.075300	1.597800
C	-1.830600	2.740700	1.773300
C	-1.526300	3.320600	3.004600
C	-2.443700	3.253400	4.058400
C	-3.672400	2.609900	3.882400
C	-3.979000	2.013200	2.657800
H	-1.106300	2.799000	0.960200
H	-4.393300	2.572700	4.699700
H	-4.933000	1.505300	2.520800
H	-2.203000	3.711800	5.018000
H	-0.568000	3.822000	3.142300
C	-2.947900	-2.721400	1.125400
C	-2.971900	-4.115000	0.945600
C	-2.859300	-4.966900	2.046500
C	-2.723100	-4.438000	3.333700
C	-2.710700	-3.052200	3.519000
C	-2.829300	-2.195300	2.424000
H	-3.072600	-4.540000	-0.054100
H	-2.608900	-2.634300	4.521200
H	-2.826900	-1.116300	2.582300
H	-2.632600	-5.105100	4.191500
H	-2.870900	-6.046300	1.893800
C	-2.598900	-2.411000	-1.743600
C	-3.376800	-2.398400	-2.914500
C	-2.864800	-2.915200	-4.108800
C	-1.570000	-3.439400	-4.138500
C	-0.791500	-3.458600	-2.974400
C	-1.300100	-2.952200	-1.776500
H	-4.388800	-1.985300	-2.895100
H	0.218400	-3.869700	-2.996800
H	-0.683100	-2.974000	-0.877500
H	-1.164800	-3.839700	-5.068900
H	-3.476900	-2.907100	-5.010900
H	1.687500	0.567100	-2.100900
H	-0.768800	-0.072600	2.174900
H	1.642400	0.527200	2.203000

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