Electronic Supplementary Material (ESI) for ChemComm.

# [($^{Cl}$Im$^{Dipp}$)P=P(Dipp)][GaCl$_4$]: A Polarized, Cationic Diphosphene

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## Supporting Information

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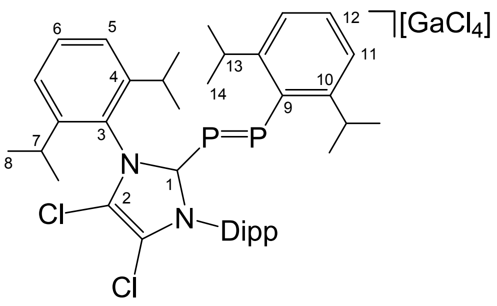
## 1. Materials and Methods

### *General Remarks.*

All manipulations were performed in a Glovebox MB Unilab produced by MBraun or using standard Schlenk technique[S1] under an inert atmosphere of purified Argon (purchased from Westfalen AG). Dry, oxygen-free solvents (drying agents in brackets; [$CaH_2$]: $CH_2Cl_2$, $C_6H_5F$, 1,2-$C_6H_4F_2$, [sodium]: pentane, *n*-hexane, [sodium/benzophenone]: $Et_2O$) were employed. Deuterated benzene ($C_6D_6$) was purchased from Sigma-Aldrich and distilled from sodium prior to use. Deuterated dichloromethane ($CD_2Cl_2$, ampoule) was purchased from Sigma-Aldrich and stored over molecular sieves for at least 2 d prior to use. Reagents such as MeOTf and $GaCl_3$ were purchased from Sigma Aldrich and sublimed or distilled prior to use. Compound **6** was prepared according to literature known procedures.[S2] All glassware was oven-dried at temperatures above 180°C prior to use. NMR spectra of compounds **7**[$GaCl_4$] and **8**[OTf] were measured on a Bruker AVANCE 400 ($^1H$ (400.03 MHz), $^{13}C$ (100.59 MHz), $^{31}P$ (161.94 MHz; 81.01 MHz)) at 300 K. NMR spectra of compound **9**[$GaCl_4$] were measured on a Bruker AVANCE III HD Nanobay ($^1H$ (400.13 MHz), $^{13}C$ (100.61 MHz), $^{31}P$ (161.98 MHz) $^{71}Ga$ (122.02 MHz)) at 300 K. All $^{13}C$ NMR spectra were exclusively recorded with composite pulse decoupling. Assignments of the carbon atoms in the $^{13}C$ spectra were performed via indirect deduction from the cross-peaks in 2D correlation experiments (HMBC; HSQC). Chemical shifts were referenced to $\delta_{TMS} = 0.00$ ppm ($^1H$, $^{13}C$) and $\delta_{H3PO4(85\%)} = 0.00$ ppm ($^{31}P$, externally). Chemical shifts ($\delta$) are reported in ppm. Coupling constants ($J$) are reported in Hz. Absolute values are reported except for coupling constants derived by means of line shape iteration (*vide infra*). Assignments of individual resonances were done using 2D techniques (HMBC, HSQC, HH-COSY, PP-COSY) when necessary. The designation of spin systems in $^{31}P$ NMR spectra was performed by convention. The spin system is considered to be higher order and consecutive letters are assigned if $\Delta\delta(P_iP_{ii})/^nJ(P_iP_{ii}) < 10$. For $\Delta\delta(P_iP_{ii})/^nJ(P_iP_{ii}) > 10$, the spin system is considered to be *pseudo* first order and the assigned letters are separated. Melting points of compounds 7[$GaCl_4$] and **8**[OTf] were recorded on an electrothermal melting point apparatus (Barnstead Electrothermal IA9100) in sealed capillaries under Argon atmosphere and are uncorrected. The melting point of compound **9**[$GaCl_4$] was recorded on an electrothermal melting point apparatus (Büchi Switzerland, Melting point M-560) in a sealed capillary under Argon atmosphere and is uncorrected. Infrared (IR) and Raman spectra were recorded at ambient temperatures using a Bruker Vertex 70 instrument equipped with a RAM II module (Nd:YAG laser, 1064 nm). The Raman intensities are reported in percent relative to the most intense peak and are given in parenthesis. An ATR unit (diamond) was used for recording IR spectra. The intensities are reported relative to the most intense peak and are given in parenthesis using the following abbreviations: vw = very weak, w = weak, m = medium, s = strong and vs = very strong. UV/Vis spectra were recorded on a Varian Cary 50 Conc UV/Visible spectrophotometer. Mass spectra where recorded on a Thermo Scientific Orbitrap LTQ XL at the Organisch Chemisches Institut, University of Münster, Germany. Parent cations were separated and fragmented using appropriate potentials in order to obtain exact masses of the fragment-cations. Elemental analyses of compounds **7**[$GaCl_4$] and **8**[OTf] were performed on a Vario EL III CHNS elemental analyzer at the IAAC, University of Münster, Germany. Elemental analysis of **9**[$GaCl_4$] was performed on a vario MICRO cube Elemental Analyzer by Elementar Analysatorsysteme GmbH.

## S2. Syntheses and Spectroscopic Data

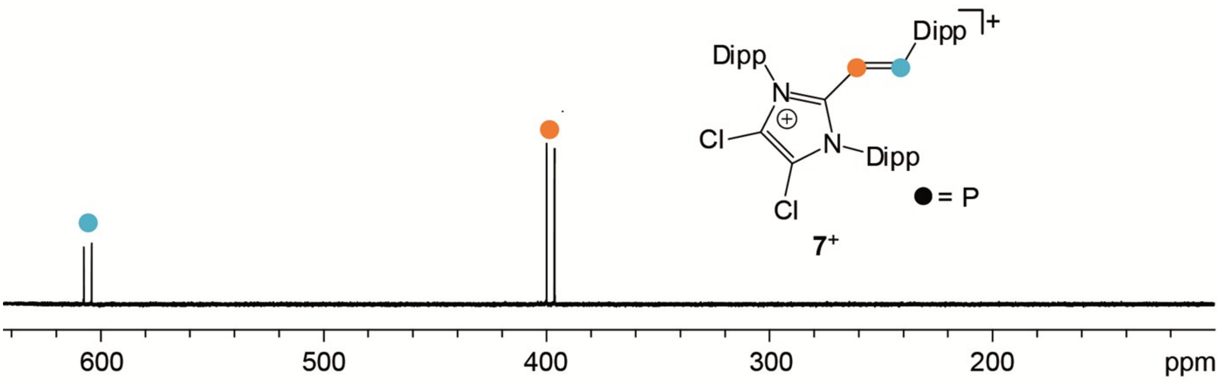
### S2.1. Preparation of $[(^{Cl}Im^{Dipp})P{=}PDipp][GaCl_4]$ (7$[GaCl_4]$)



**7**$[GaCl_4]$

A solution of **6** (130 mg, 0.2 mmol, 1.0 eq.) in benzene (10 mL) was stirred at ambient temperature. A solution of $GaCl_3$ (35 mg, 0.2 mmol, 1.0 eq.) in benzene (5 mL) was added dropwise within 10 min. The instant formation of a red precipitate and a red supernatant was observed. *n*-Hexane was added (10 mL) to complete precipitation. The red material was isolated by filtration and removal of all volatiles *in vacuo* yielded **7**$[GaCl_4]$ as analytically pure, microcrystalline red solid (**7**$[GaCl_4]$: 76%, 125 mg). Single crystals of **7**$[GaCl_4]$•$(C_6H_5F)$, suitable for X-ray single crystal structure determination, were obtained by slow diffusion of *n*-hexane into a $C_6H_5F$ solution of the respective compound at –35 °C.

**m.p.:** 176.8 - 178.8 °C; **Raman (100 mW, r.t., in cm$^{-1}$)**: $\nu$ = 3068 (10), 2970 (8), 2910 (29), 2868 (8), 1585 (11), 1556 (20), 1467 (6), 1444 (12), 1397 (8), 1365 (35), 1321 (17), 1297 (100), 1240 (18), 1167(5), 1105 (8), 1048 (10), 991 (8), 886 (9), 763 (8), 735 (7), 665 (12), 598 (43), 502 (5), 359 (6), 344 (25), 297 (6), 259 (5), 172 (7), 114 (67), 77 (28); **IR (ATR, r.t., in cm$^{-1}$)**: $\nu$ = 2966 (s), 2929 (vw), 1568 (m), 1461 (m), 1422 (vw), 1389 (w), 1366 (w), 1309 (vw), 1237 (w), 1153 (s), 1085 (vw), 1058 (w), 981 (m), 806 (vs), 764 (w), 747 (m), 670 (vw); 542 (w), 432 (m); **$^1$H NMR ($CD_2Cl_2$, 300 K, in ppm)**: $\delta$ = 0.90 (12H, d, H14, $^3J$(HH) = 6.6 Hz), 1.26 (12H, d, H8, $^3J$(HH) = 6.6 Hz), 1.36 (12H, d, H8, $^3J$(HH) = 6.6 Hz), 2.02 (2H, s(br), H13, $\Delta\nu_{1/2}$ = 22 Hz), 2.50 (4H, sept., H7, $^3J$(HH) = 6.6 Hz), 7.11 (2H, d, H11, $^3J$(HH) = 7.8 Hz), 7.38 (1H, t, H12, $^3J$(HH) = 7.8 Hz), 7.49 (4H, d, H5, $^3J$(HH) = 7.8 Hz), 7.75 (2H, t, H6, $^3J$(HH) = 7.8 Hz); **$^{13}$C{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: $\delta$ = 23.3 (4C, s, C14), 23.4 (4C, s(br), C8, $\Delta\nu_{1/2}$ = 5 Hz), 25.0 (4C, s, C8), 30.3 (4C, s, C7), 35.2 (2C, d, C13, $^3J$(CP) = 9.2 Hz), 124.7 (2C, s, C11), 125.8 (2C, d, C2, $^2J$(CP) = 2.5 Hz), 126.5 (4C, s, C5), 128.1 (2C, s, C3), 132.8 (1C, s, C12), 133.0 (1C, d, C9, $^1J$(CP) = 80 Hz), 134.3 (2C, s, C6), 146.2 (4C, s, C4), 150.5 (2C, s(br), C10, $\Delta\nu_{1/2}$ = 15 Hz), 154.5 (1C, dd, C1, $^1J$(CP) = 113 Hz, $^2J$(CP) = 12 Hz), **$^{31}$P{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: AX spin system: $\delta(P_A)$ = 398.1, $\delta(P_X)$ = 605.8, $^1J(P_AP_X)$ = –577.9 Hz; **$^{71}$Ga{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: $\delta$ = 250.4 (s); **MS-ESI-MS:** 679.29070 [M$^+$]. calcd.: for $C_{39}H_{51}Cl_2N_2P_2$ 679.29040; **UV/vis (2.7x10-4 M, $C_6H_5F$, in nm)**: $\nu$ = 490 ($\varepsilon$ = 429 cm$^2$/mol), 395 (sh, $\varepsilon$ = 4254 cm$^2$/mol), 349 ($\varepsilon$ = 4995 cm$^2$/mol); **elemental analysis for $C_{39}H_{51}N_2GaCl_6P_2$**: calcd.: C 52.5, H 5.8, N 3.1; found: C 51.4, H 5.6, N 2.9.

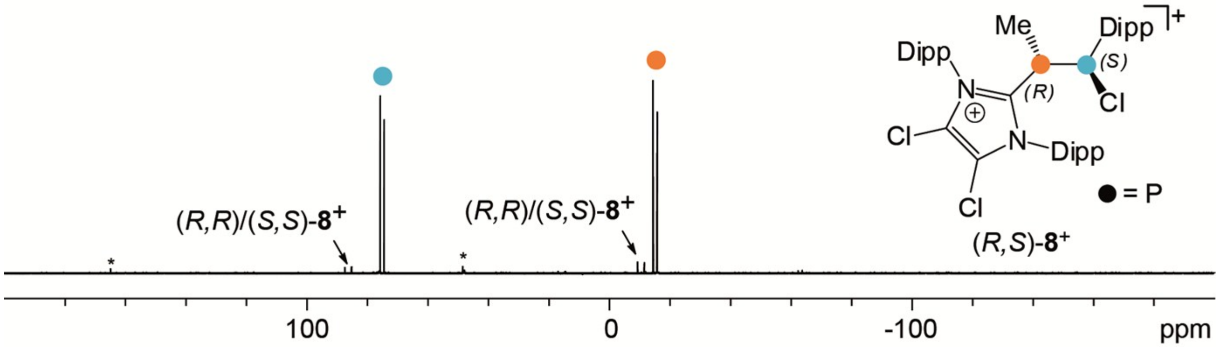


$^{31}P\{^1H\}$ NMR spectrum of **7**[GaCl$_4$] (CD$_2$Cl$_2$, 300 K)

## S2.2. Preparation of (*R*,*S*)/(*S*,*R*)-[($^{Cl}$Im$^{Dipp}$)PMe-PClDipp][OTf] (8[OTf])

A solution of **6** (190 mg, 0.27 mmol, 1.0 eq.) in benzene (5 mL) was stirred at ambient temperature. A solution of MeOTf (116 mg, 0.71 mmol, 2.6 eq.) in benzene (5 mL) was added dropwise within 5 min. The formation of a yellowish reaction mixture was observed which was investigated by means of $^{31}P\{^1H\}$ NMR spectroscopy.

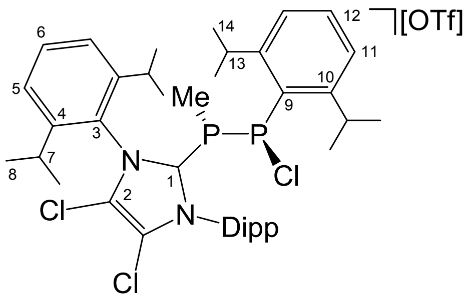
**$^{31}P\{^1H\}$ NMR ($C_6D_6$-capillary, benzene, 300 K, in ppm)**: δ = –15.1 (A part of the AX spin system of (*R,S*)/(*S,R*)-**8**$^+$, $^1J(P_AP_X)$ = –218.2 Hz), –10.5 (A part of the AX spin system of (*S,S*)/(*R,R*)-**8**$^+$, $^1J(P_AP_X)$ = –354.8 Hz), 75.1 ppm (X part of the AX spin system of (*R,S*)/(*S,R*)-**8**$^+$), 86.4 ppm (X part of the AX spin system of (*S,S*)/(*R,R*)-**8**$^+$).



$^{31}P\{^1H\}$ NMR spectrum of the reaction mixture of **6** and MeOTf ($C_6H_6$, $C_6D_6$-capillary, 300 K), small amounts of unidentified side products are marked with asterisks.

*n*-Hexane was added (10 mL) to the reaction mixture giving a yellowish precipitate which was isolated by filtration. Removal of all volatiles *in vacuo* yielded (*R,S*)/(*S,R*)-**8**[OTf] as colourless, microcrystalline solid (77%, 183 mg). Single crystals of **8**[OTf]•2(1,2-$C_6H_4F_2$), suitable for X-ray single crystal structure determination, were obtained by slow diffusion of *n*-hexane into $CH_2Cl_2$ and 1,2-$C_6H_4F_2$ solutions of the respective compounds at –35 °C.

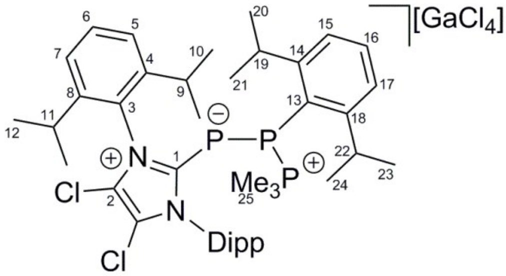
## S2.3. Characterization data of (*R*/*S*)/(*S*/*R*)-[($^{Cl}$Im$^{Dipp}$)PMe-PClDipp][OTf] (8[OTf])



*(R,S)*-**8**[OTf]

**m.p.:** 166.5 - 168.9 °C; **Raman (100 mW, r.t., in cm$^{-1}$)**: *ν* = 3063 (43), 2971 (16), 2918 (56), 1585 (42), 1566 (14), 1464 (24), 1356 (50), 1321 (20), 1285 (38), 1226 (21), 1177 (11), 1104 (16), 1030 (49), 992 (100), 886 (26), 754 (13), 67 (20), 515 (14), 463 (35), 347 (16), 312 (16), 244 (18); **IR (ATR, r.t., in cm$^{-1}$)**: *ν* = 3068 (vw), 2965 (w), 1583 (vw), 1562 (w), 1463 (w), 1387 (w), 1369 (vw), 1320 (vw), 1257 (vs), 1222 8w), 1148 (m), 1059 (w), 1029 (vs), 935 (vw), 890 (w), 810 (m), 765 (vw), 750 (vw), 680 8s), 636 (vs); **$^1$H NMR ($CD_2Cl_2$, 300 K, in ppm)**: δ = 0.69 (3H, dd, Me, $^2J$(HP) = 8.7 Hz, $^3J$(HP) = 5.2 Hz), 0.99 (3H, d, H14, $^3J$(HH) = 6.6 Hz), 1.01 (3H, d, H14, $^3J$(HH) = 6.6 Hz), 1.10 (3H, d, H14, $^3J$(HH) = 6.6 Hz), 1.15 (3H, d, H14, $^3J$(HH) = 6.6 Hz), 1.31 (6H, d, H8, $^3J$(HH) = 6.7 Hz), 1.32 (6H, d, H8, $^3J$(HH) = 6.7 Hz), 1.44 (6H, d, H8, $^3J$(HH) = 6.7 Hz), 1.44 (6H, d, H8, $^3J$(HH) = 6.7 Hz), 2.42 (2H, sept., H7, $^3J$(HH) = 6.7 Hz), 2.44 (2H, sept., H7, $^3J$(HH) = 6.7 Hz), 3.11 (1H, sept., H13, $^3J$(HH) = 6.6 Hz), 3.46 (2H, sept., H7, $^3J$(HH) = 6.6 Hz), 7.13 (1H, d, H11, $^3J$(HH) = 7.9 Hz), 7.16 (1H, d, H11, $^3J$(HH) = 7.9 Hz), 7.41 (1H, t, H12, $^3J$(HH) = 7.9 Hz), 7.54 (2H, d, H5, $^3J$(HH) = 7.9 Hz), 7.54 (2H, d, H5, $^3J$(HH) = 7.9 Hz), 7.79 (2H, t, H6, $^3J$(HH) = 7.9 Hz); **$^{13}$C{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: δ = 7.7 (1C, dd, Me, $^1J$(CP) = 22.0 Hz, $^2J$(CP) = 13.0 Hz), 23.0 (1C, s, C14), 23.6 (2C, s, C8), 23.7 (2C, s, C8), 24.8 (2C, s, C8), 25.0 (1C, s, C14), 25.2 (2C, s, C8), 25.6 (1C, s, C14), 25.6 (1C, s, C14), 30.2 (2C, s, C7), 30.3 (2C, s, C7), 32.2 (1C, d, C13, $^3J$(CP) = 17.5 Hz), 32.6 (1C, d, C13, $^3J$(CP) = 12.3 Hz), 121.5 (1C, s, $CF_3$, $^1J$(CF) = 321.6 Hz), 124.6 (1C, d, C11, $^3J$(CP) = 12.3 Hz), 126.3 (2C, d, C2, $^3J$(CP) = 2.7 Hz), 126.5 (2C, s, C5), 126.6 (2C, s, C5), 127.2 (1C, s, C11), 127.2 (1C, dd, C9, $^1J$(CP) = 51.7 Hz, $^2J$(CP) = 4.6 Hz), 128.4 (2C, s, C3), 134.0 (1C, s, C12), 134.4 (2C, s, C6), 146.3 (2C, s, C4), 146.4 (2C, s, C4), 151.7 (1C, dd, C1, $^1J$(CP) = 95.4 Hz, $^2J$(CP) = 24.4 Hz), 155.3 (1C, dd, C10, $^2J$(CP) = 40.6 Hz, $^2J$(CP) = 3.7 Hz), 155.8 (1C, s, C10); **$^{31}$P{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: AX spin system: δ($P_A$) = –15.1, δ($P_X$) = 75.1, $^1J$($P_AP_X$) = –217.8 Hz; **$^{19}$F{$^1$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: δ = –78.8 (s); **elemental analysis for $C_{42}H_{54}N_2O_3F_3P_2SCl_3$**: calcd.: C 57.9, H 6.2, N 3.4; found: C 58.9, H 6.4, N 2.8.

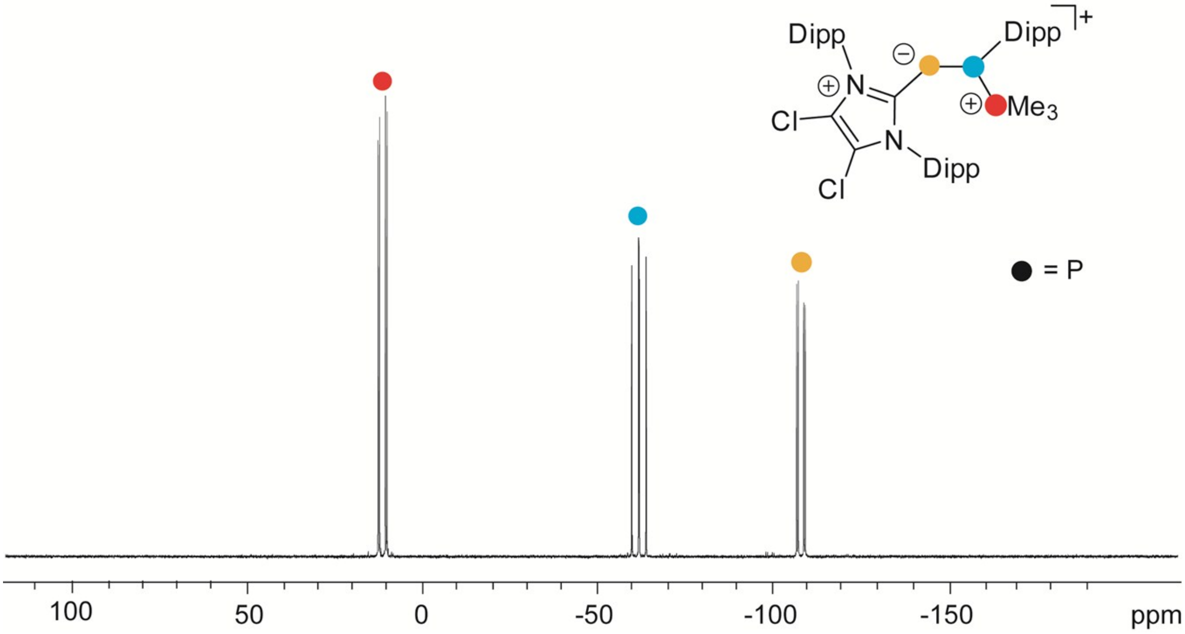
## S2.4. Preparation of [($^{Cl}$Im$^{Dipp}$)P-PDipp-PMe$_3$][GaCl$_4$] 9[GaCl$_4$]



A solution of **7** (76 mg, 0.08 mmol, 1.0 eq.) in *o*-difluorobenzene (1.5 mL) was stirred at ambient temperature. A solution of PMe$_3$ (10 mg, 0.13 mmol, 1.0 eq.) in *o*-difluorobenzene (1 mL) was added dropwise, accompanied by a color change to deep yellow. The solvent was removed in *vacuo*. The oily residue was washed with *n*-hexane (2 x 2 mL) and the formation of a yellow powder was observed. After removal of all volatiles *in vacuo*, **9**[GaCl$_4$] was isolated as microcrystalline yellow solid (**9**[GaCl$_4$]: 96%, 79 mg). Single crystals of **X**[GaCl$_4$], suitable for X-ray single crystal structure determination, were obtained by slow diffusion of *n*-pentane into a CH$_2$Cl$_2$ solution of the respective compound at –35 °C.

**m.p.:** decomp. 170-172 °C; **Raman (60 mW, r.t., in cm$^{-1}$)**: $v$ = 3070(10), 3055(5), 2962(34), 2938(29), 2914(91), 2867(51), 2761(8), 2713(6), 1596 (15), 1585(12), 1467(24), 1443(21), 1399(9), 1296(100), 1267(9), 1225(11), 1102(12), 1048(10), 1024(5), 956(8), 885(17), 765(9), 734(6), 674(14), 607(10), 442(12), 346(36), 298(9), 224(9); **IR (ATR, r.t., in cm$^{-1}$)**: $v$ = 2968(vw), 2958(vw), 2930(vw), 2867(vw), 1595(m), 1464(w), 1442(w), 1407(vw), 1384(w), 1360(m), 1292(vs), 1269(vw), 1183(vw), 1107(vw), 1061(vw), 1045(vw), 953(vs), 856(vw), 813(w), 801(m), 763(vw), 751(vw), 733(vw), 668(m), 650(vw), 606(vw), 543(vw), 515(w), 482(w), 437(w); **$^1$H NMR (CD$_2$Cl$_2$, 300 K, in ppm)**: δ = 0.94 (3H, d, H21, $^3J$(HH) = 5.9 Hz), 1.01 (3H, d, H24, $^3J$(HH) = 6.0 Hz), 1.03 (3H, d, H23, $^3J$(HH) = 6.0 Hz), 1.14 (3H, d, $^3J$(HH) = 5.9 Hz), 1.23 (12H, d, H12 $^3J$(HH) = 6.8 Hz), 1.27 (12H, d, H10, $^3J$(HH) = 6.8 Hz), 1.39 (9H, d, H25, $^2J$(HP) = 12.4 Hz), 2.53 (2H, *pseudo* sept., H9, $^3J$(HH) = 6.8 Hz), 2.61-2.71 (2H, m, H19, 22), 2.72 (2H, *pseudo* sept., H11, $^3J$(HH) = 6.8 Hz), 7.08 (1H, t, H17, $^3J$(HH) = 7.4 Hz), 7.11 (1H, t, H15, $^3J$(HH) = 7.4 Hz), 7.36 (1H, t, H16, $^3J$(HH) = 7.4 Hz), 7.40-7.47 (4H, *pseudo* t(br), H5, 7), 7.64(2H, t(br), H6, $^3J$(HH) = 7.5 Hz); **$^{13}$C{$^1$H} NMR (CD$_2$Cl$_2$, 300 K, in ppm)**: δ = 10.64 (3C, dd, C25, $^1J$(CP) = 45 Hz, $^2J$(CP) = 9 Hz), 24.08 (4C, s, C10), 24.30 (4C, s, C12), 24.39 (1C, d, C20, $^4J$(CP) = 5 Hz), 25.25 (1C, s, C23), 25.88 (1C, s, C24), 27.56 (1C, d, $^4J$(CP) = 5 Hz), 29.88 (2C, s, C11), 30.08 (2C, s, C9), 32.74 (1C, d, C22, $^3J$(CP) = 33 Hz), 35.38 (1C, d, C19, $^3J$(CP) = 29 Hz), 120.02 (2C, d, C2, $^3J$(CP) = 4 Hz), 125.19 (1C, d, C15, $^3J$(CP) = 8 Hz), 125.80 (1C, s, C17), 125.94 (4C, s, C5, 7), 130.64 (2C, s, C3), 132.21 (1C, s, C16), 132.66 (2C, s, C6), 146.87 (2C, s, C8), 147.23 (2C, s, C4), 155.29 (1C, dd, C13, $^1J$(CP = 36 Hz, $^2J$(CP) = 9 Hz), 155.90 (2C, s, C14, 18), 168.86 (1C, ddd, C1, $^1J$(CP) = 142 Hz, $^2J$(CP) = 34 Hz, $^3J$(CP) = 13 Hz); **$^{31}$P{$^1$H} NMR (CD$_2$Cl$_2$, 300 K, in ppm)**: AMX spin system: δ(P$_A$) = -108.1,

$\delta(\mathrm{P_M}) = -62.1$, $\delta(\mathrm{P_X}) = 11.2$, ${}^{1}J(\mathrm{P_AP_M}) = -322.1$ Hz, ${}^{1}J(\mathrm{P_MP_X}) = 343.3$ Hz, ${}^{2}J(\mathrm{P_AP_X}) = 72.8$ Hz; **${}^{71}$Ga{${}^{1}$H} NMR ($CD_2Cl_2$, 300 K, in ppm)**: $\delta = 250.4$; **elemental analysis for $C_{42}H_{60}N_2GaCl_6P_3$**: calcd.: C 52.1, H 6.2, N 2.9; found: C 51.7, H 6.0, N 2.8.

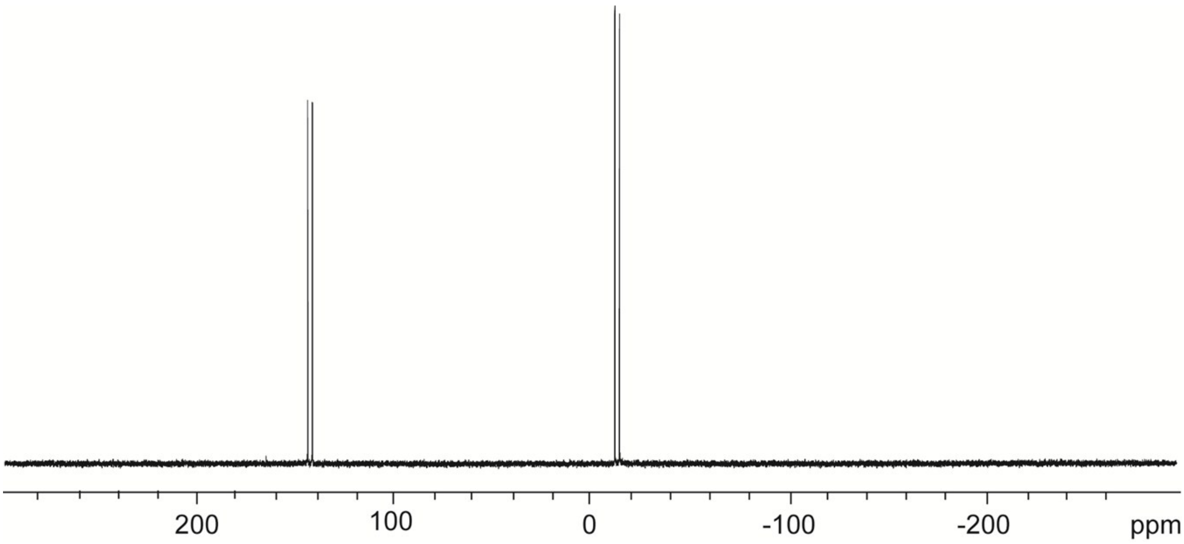


${}^{31}$P{${}^{1}$H} NMR spectrum of **9**[$GaCl_4$] ($CD_2Cl_2$, 300 K).

## S2.5. Reaction of [($^{Cl}$Im$^{Dipp}$)P-PDipp][$GaCl_4$] with [($^n$Bu)$_4$N][Cl]

To a solution of **7**[$GaCl_4$] (20 mg, 0.02 mmol, 1.0 eq.) in *o*-difluorobenzene (1.5 mL), a solution of [(*n*-Bu)$_4$N][Cl] (6.2 mg, 0.02 mmol, 1.0 eq.) in *o*-difluorobenzene (0.5 mL) was added. The immediate formation of a yellowish reaction mixture was observed. The formation of **6** was unambiguously identified by the investigation of the $^{31}P\{^1H\}$ NMR spectrum.

**$^{31}P\{^1H\}$ NMR ($C_6D_6$-capillary, *o*-difluorobenzene, 300K °C, in ppm)**: AX spin system: $\delta(P_A) = -13.3$, $\delta(P_X) = 142.1$, $^1J(P_AP_X) = 381.6$ Hz.



$^{31}P\{^1H\}$ NMR spectrum of **6** (*o*-difluorobenzene, C6D6-capillary, 300 K)

## 3. Crystallographic Details

**Table S1**. Crystallographic data of **6**•0.5(Et2O)•0.5(n-hexane), **7**[GaCl$_4$]•(C$_6$H$_5$F), **8**[OTf]•2(1,2-C$_6$H$_4$F$_2$) and **9**[GaCl$_4$]

| | **6**•0.5(Et$_2$O) •0.5(*n*-hexane) | **7**[GaCl$_4$]•(C$_6$H$_5$F) | **8**[OTf]•2(1,2-C$_6$H$_4$F$_2$) | **9**[GaCl$_4$] |
|---|---|---|---|---|
| Formula | $C_{44}H_{63}Cl_3N_2O_{0.5}P_2$ | $C_{45}H_{56}Cl_6FGaN_2P_2$ | $C_{53}H_{61}Cl_3F_7N_2O_3P_2S$ | C42 H60 Cl6 Ga N2 P3 |
| MW in g mol$^{-1}$ | 796.25 | 988.28 | 1107.39 | 968.25 |
| Colour | yellow, plate | red, block | colourless, block | yellow, block |
| Crystal System | monoclinic | monoclinic | monoclinic | triclinic |
| Space group | *C*2/c | *P*2$_1$/c | *P*2$_1$/c | *P-1* |
| *a* in Å | 27.4843(3) | 10.7484(6) | 12.2639(2) | 13.8028(4) |
| *b* in Å | 17.6558(2) | 13.6179(7) | 12.5384(2) | 17.4286(5) |
| *c* in Å | 21.9216(3) | 33.648(2) | 36.3192(7) | 21.7529(6) |
| $\alpha$ in ° | 90 | 90 | 90 | 107.6090(10) |
| $\beta$ in ° | 118.269(1) | 94.250(1) | 99.262(1) | 98.7010(10) |
| $\gamma$ in ° | 90 | 90 | 90 | 97.4200(10) |
| *V* in Å$^3$ | 9368.7(2) | 4911.6(5) | 5511.9(2) | 4844.6(2) |
| Z | 8 | 4 | 4 | 4 |
| *T* in K | 153(2) | 153(1) | 153(1) | 153(2) |
| Crystal size mm$^3$ | 0.18x0.11x0.03 | 0.10x0.06x0.03 | 0.37x0.17x0.15 | 0.095x0.088x0.031 |
| $\rho_c$ in mg m$^{-3}$ | 1.129 | 1.337 | 1.334 | |
| *F*(000) | 3408 | 2048 | 2308 | 2016 |
| $\lambda_{MoK\alpha}$, Å | 1.54178 | 0.71073 | 0.71073 | 0.71073 |
| $\theta_{min}$ in ° | 3.10 | 1.61 | 1.14 | 1.643 |
| $\theta_{max}$ in ° | 68.02 | 28.28 | 27.88 | 27.945 |
| Index range | $-33 \le h \le 33$<br>$-18 \le k \le 20$<br>$-26 \le l \le 24$ | $-14 \le h \le 14$<br>$-18 \le k \le 18$<br>$-44 \le l \le 44$ | $-16 \le h \le 16$<br>$-16 \le k \le 16$<br>$-47 \le l \le 47$ | $-18 \le h \le 17$<br>$-17 \le k \le 22$<br>$-28 \le l \le 28$ |
| $\mu$ in mm$^{-1}$ | 2.645 | 0.988 | 0.329 | 1.029 |
| Absorption correction | multi-scan | multi-scan | multi-scan | multi-scan |
| Reflection collected | 26436 | 50535 | 54790 | 45789 |
| Reflection unique | 8324 | 12176 | 13138 | 22824 |
| $R_{int}$ | 0.0501 | 0.0346 | 0.0508 | 0.0503 |
| Reflection obs. [F > 2σ(F)] | 7039 | 9475 | 9459 | 14837 |
| Residual density in e Å$^{-3}$ | 0.835/-0.421 | 1.435/-1.059 | 0.824/-0.744 | 1.455/-0.843 |
| Parameters | 475 | 526 | 663 | 1049 |
| GooF | 1.051 | 1.117 | 1.087 | 1.007 |
| $R_1$ [I > 2σ(I)] | 0.0522 | 0.0663 | 0.0483 | 0.1069 |
| w$R_2$ (all data) | 0.1655 | 0.1849 | 0.1833 | 0.1246 |
| CCDC | 1429021 | 1429022 | 1429023 | 1429024 |

### 3.1 Structure solution and refinement

Single crystals were coated with Paratone-N oil, mounted using a glass fibre pin and frozen in the cold nitrogen stream of the goniometer. All data sets were collected at 153(2) K on Bruker equipped with either a rotation anode at 153(2) Kwith a scan width of 0.3° using graphite-monochromated Cu Kα radiation ($\lambda$ = 1.54178 Å) (**6**) or with a microfocus sealed tube Mo$K_\alpha$ source ($\lambda$ = 0.71073 Å) (**7**, **8**, **9**). Data reduction and absorption correction were done using the Bruker SMART[S3] software package. Data sets were corrected for absorption effects using SADABS routine (empirical multi-scan method). Structure solutions were found with the SHELXS-97 (**6**, **7**, **8**) or SHELXT-2013[S8] (**9**) package using the direct method and were refined with SHELXL-97[S4] (**6**, **7**, **8**) or SHELXL-2013[S8] (**9**) against $F^2$ using first isotropic and anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms bonded to carbon atoms were added to the structure models on calculated positions using the riding model. Images of the Structures depicted were produced with Diamond[S9] software.

## 4. Computational Details

All calculations were carried out using the Gaussian 09 Package (Rev. B.01).[S10] Geometry optimizations were performed using M06-2X density functional[S11] on double zeta basis set level (def2svp[S12,13]). Analytical vibrational analysis was performed to confirm an energetic minimum structure. Orbitals were visualized and plotted using vmd program.[S14]

NBO 3.1[S15] was utilized as implemented in Gaussian 09 for NBO analysis. Dissociation curves were obtained by constrained optimization and subsequently fitted with QtiPlot[S16] using standard Morse potential: $V(r) = D_0(1 - e^{-a(r-r_0)})^2 - D_0$. The 2,6-diisopropylphenyl moieties were substituted by methyl groups (denoted as $\mathbf{6_{me}}$) resulting in a significant decrease of the computational costs.

### 4.1 Computational Results

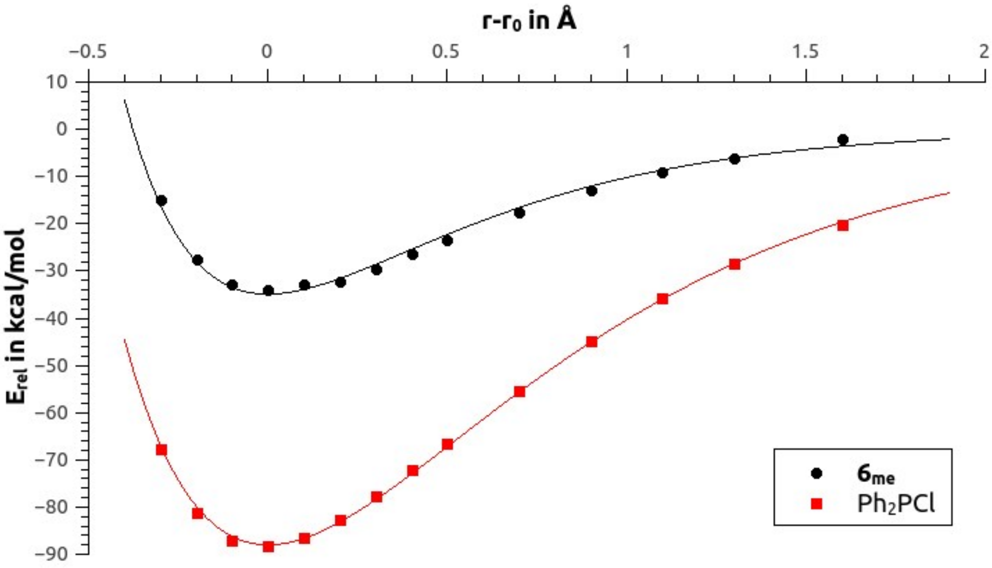
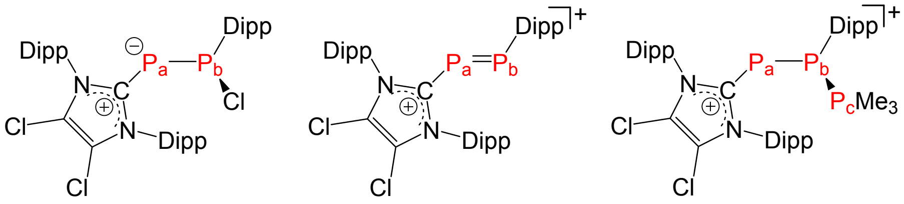


**Figure 4.1**: Energy Profile of P–Cl bond Dissociation of $6_{me}$ and $Ph_2PCl$.

**Table S2**. P-Cl Bond Dissociation of $\mathbf{6_{me}}$ and $Ph_2PCl$

| Compound | $D_0$ in kcal/mol | a in $Å^{-1}$ | k in N/m |
|---|---|---|---|
| $\mathbf{6_{me}}$ | 34.1 | 1.8059 | 154,4 |
| $Ph_2PCl$ | 88.2 | 1.3364 | 218,9 |

The general numbering scheme of compounds **6**, **7**⁺, and **9**⁺ is shown below. The energy threshold for donor-acceptor interactions in Tables S3 to S5 was declared 5 kcal/mol. Single bonds are denoted as BD(1), double bonds as BD(2) and lone pairs as LP.



**6** **$7^+$** **$9^+$**

Numbering Scheme of **6**, **$7^+$**, and **$9^+$**

**Table S3**. Natural Charges of Phosphorus Atoms

| **Compound** | **Natural Charge $P_a$** | **Natural Charge $P_b$** | **Natural Charge $P_c$** |
|---|---|---|---|
| **6** | -0.065 | 0.452 | - |
| **$7^+$** | 0.243 | 0.438 | - |
| **$9^+$** | -0.142 | 0.208 | 1.197 |

**Table S4**. NBO Analysis of compound **6**

| **Bondtype** | **Atom 1 (contrib. %)** | **Atom 2 (contrib. %)** | **Occupation** | **Acceptor Orbital** | **E in kcal/mol** |
|---|---|---|---|---|---|
| BD(1) | $P_a$ (47.8) | $P_b$ (52.2) | 1.94 | BD*(1) C-N | 5.1 |
| BD(1) | $P_a$ (31.8) | C (61.4) | 1.96 | - | - |
| BD(1) | $P_b$ (30.6) | Cl (69.4) | 1.98 | - | - |
| LP | $P_a$ | $sp^{0.7}$-type | 1.95 | BD*(1) C-N | 9.3 |
| LP | $P_a$ | p-type | 1.52 | BD*(1) $P_b$-Cl | 22.5 |
| LP | $P_b$ | p-type | 1.96 | - | - |
| LP | C | p-type | 0.95 | LPs of Ns (donor orbitals!) | 153.2/146.8 |

**Table S5**. NBO Analysis for **7**$^+$

| **Bondtype** | **Atom 1 (contrib. %)** | **Atom 2 (contrib. %)** | **Occupation** | **Acceptor Orbital** | **E in kcal/mol** |
|---|---|---|---|---|---|
| BD(1) | $P_a$ (51.7) | $P_b$ (48.3) | 1.96 | - | - |
| BD(2) | $P_a$ (57.4) | $P_b$ (42.6) | 1.88 | BD*(2) C-N | 18.5 |
| BD(1) | $P_a$ (32.0) | C (68.0) | 1.97 | - | - |
| LP | $P_a$ | $sp^{0.46}$-type | 1.96 | BD*(1) C-N | 9.2 |
| LP | $P_b$ | $sp^{0.47}$-type | 1.97 | - | - |

**Table S6**. NBO Analysis for **9**$^+$

| **Bondtype** | **Atom 1 (contrib. %)** | **Atom 2 (contrib. %)** | **Occupation** | **Acceptor Orbital** | **E in kcal/mol** |
|---|---|---|---|---|---|
| BD(1) | $P_a$ (43.5) | $P_b$ (56.5) | 1.93 | BD*(2) C-N | 6.8 |
| BD(1) | $P_a$ (31.8) | C (68.2) | 1.96 | - | - |
| BD(1) | $P_b$ (43.4) | $P_c$ (56.6) | 1.95 | - | - |
| LP | $P_a$ | $sp^{0.39}$-type | 1.95 | BD*(1) C-N | 6.0 |
| LP | $P_a$ | p-type | 1.69 | BD*(2) C-N | 11.2 |
| LP | $P_b$ | $sp^{1.1}$-type | 1.91 | BD*(1) $P_c$-Me | 6.0 |

**Table S7**. Molecular Structure and Selected Frontier Orbitals of **6** (hydrogen atoms omitted for clarity).

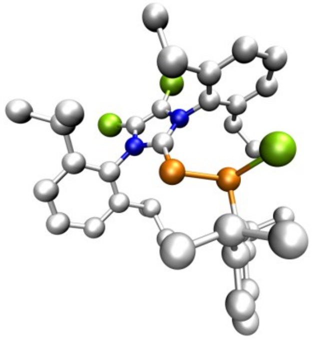
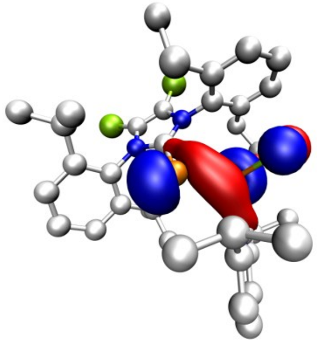
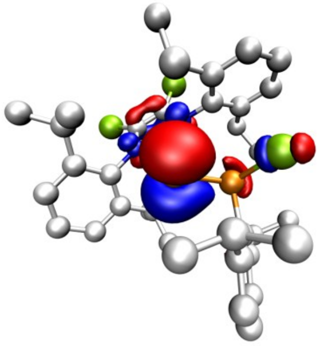
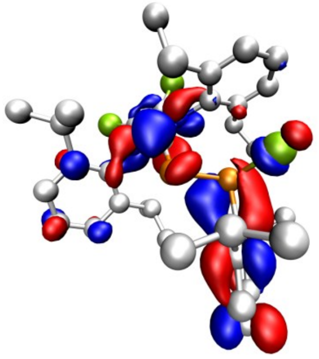
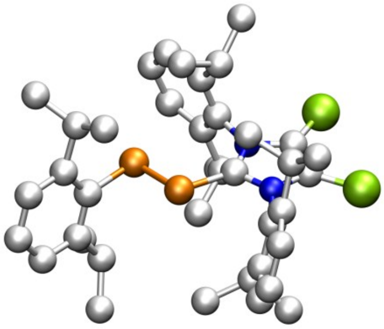
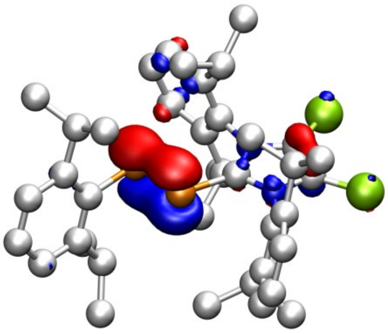
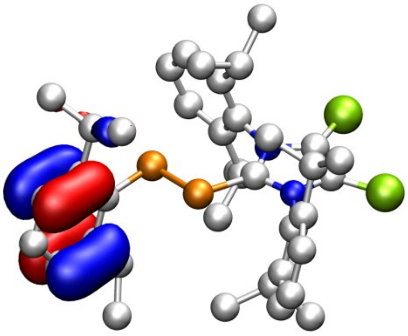
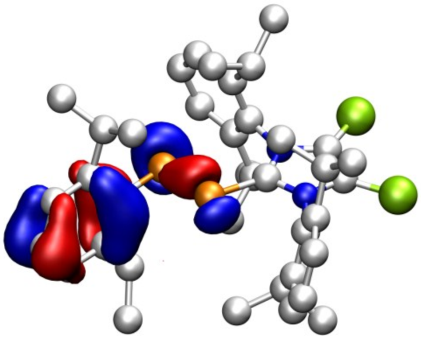
| **Description** | **Orbital Energy in H** | **Orbital** |
|---|---|---|
| Optimized Structure | - |  |
| HOMO -1 | -0.2503 |  |
| HOMO | -0.2190 |  |
| LUMO | -0.0058 |  |

**Table S8**. Molecular Structure and Selected Frontier Orbitals of **7**$^+$ (hydrogen atoms omitted for clarity).

| **Description** | **Orbital Energy in H** | **Orbital** |
|---|---|---|
| Optimized Structure | - |  |
| HOMO -2 | -0.3883 |  |
| HOMO -1 | -0.3806 |  |
| HOMO | -0.3787 |  |

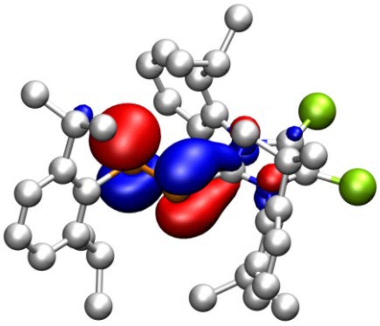
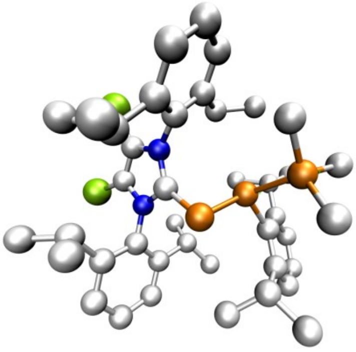
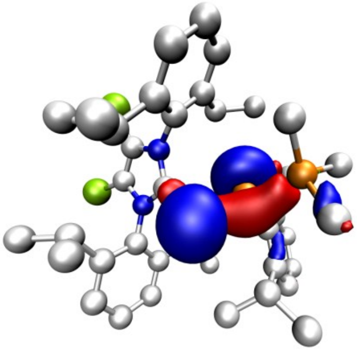
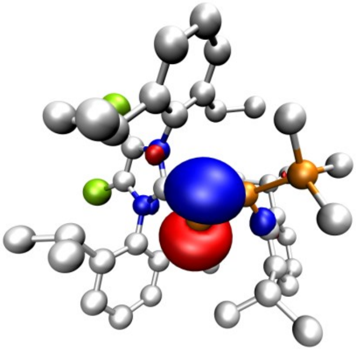
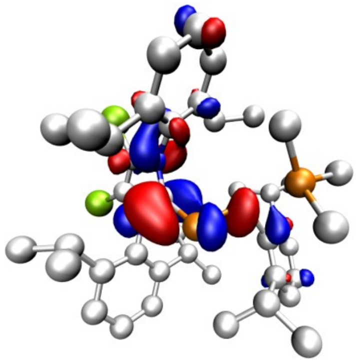
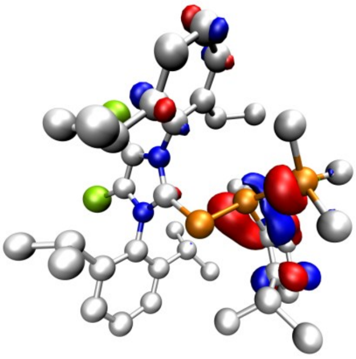
| | | |
|---|---|---|
| LUMO | -0.1911 |  |

**Table S9**. Molecular Structure and Selected Frontier Orbitals of **9**$^+$ (hydrogen atoms omitted for clarity).

| **Description** | **Orbital Energy in H** | **Orbital** |
|---|---|---|
| Optimized Structure | - |  |
| HOMO -1 | -0.3656 |  |
| HOMO | -0.3217 |  |

| | | |
|---|---|---|
| LUMO | -0.1065 |  |
| LUMO +1 | -0.0947 |  |

Optimized xyz-coordinates of **6**

97

| | | | |
|---|---|---|---|
| C | 3.20267 | -0.65972 | 0.23360 |
| C | 3.88885 | -0.96271 | -0.96945 |
| C | 3.54584 | -1.31970 | 1.43141 |
| P | 1.78406 | 0.52561 | 0.08187 |
| C | 4.85227 | -1.97306 | -0.96411 |
| C | 3.66568 | -0.14333 | -2.23357 |
| C | 4.53168 | -2.31334 | 1.39536 |
| C | 2.95122 | -0.99199 | 2.79063 |
| P | 0.27007 | -0.69551 | 0.99301 |
| Cl | 2.46288 | 2.04182 | 1.45456 |
| H | 5.37382 | -2.23140 | -1.88522 |
| C | 5.16533 | -2.65579 | 0.20896 |
| H | 2.58197 | 0.00462 | -2.36915 |
| C | 4.32371 | 1.22971 | -2.04289 |
| C | 4.19681 | -0.79430 | -3.50695 |
| H | 4.79883 | -2.82448 | 2.32265 |
| H | 2.15953 | -0.24420 | 2.68038 |
| C | 2.33641 | -2.22398 | 3.45476 |
| C | 4.02363 | -0.35253 | 3.67427 |
| C | -1.05578 | -0.01403 | -0.00425 |
| H | 5.91780 | -3.44640 | 0.19632 |
| H | 3.92943 | 1.74774 | -1.15457 |
| H | 4.15268 | 1.86689 | -2.92467 |
| H | 5.40770 | 1.09090 | -1.90505 |
| H | 5.29730 | -0.83300 | -3.49829 |
| H | 3.89017 | -0.19748 | -4.37876 |
| H | 3.81886 | -1.82117 | -3.62728 |
| H | 1.57843 | -2.68020 | 2.79998 |
| H | 1.85540 | -1.93520 | 4.40237 |
| H | 3.10781 | -2.97802 | 3.67876 |
| H | 4.86132 | -1.05114 | 3.83107 |
| H | 3.59834 | -0.09140 | 4.65598 |
| H | 4.40538 | 0.56194 | 3.19691 |
| N | -2.04023 | -0.80657 | -0.50374 |
| N | -1.39064 | 1.25874 | -0.35911 |
| C | -2.98238 | -0.04443 | -1.16804 |
| C | -2.03486 | -2.23381 | -0.41923 |
| C | -2.58501 | 1.24774 | -1.06514 |
| C | -0.79566 | 2.44622 | 0.18442 |
| Cl | -4.33349 | -0.72024 | -1.93746 |
| C | -1.11621 | -2.93640 | -1.20581 |
| C | -2.93468 | -2.84104 | 0.46655 |
| Cl | -3.35868 | 2.65471 | -1.60475 |
| C | -0.99899 | 2.69558 | 1.54881 |
| C | -0.08934 | 3.31545 | -0.65681 |
| C | -1.12828 | -4.32919 | -1.09762 |
| C | -0.16628 | -2.25177 | -2.16684 |

| | | | |
|---|---|---|---|
| C | -2.91689 | -4.23532 | 0.53260 |
| C | -3.81234 | -1.99513 | 1.37043 |
| C | -0.41716 | 3.84423 | 2.08614 |
| C | -1.86338 | 1.81404 | 2.42562 |
| C | 0.47618 | 4.44975 | -0.07115 |
| C | 0.04381 | 3.10551 | -2.15268 |
| H | -0.42647 | -4.91263 | -1.69598 |
| C | -2.02070 | -4.97062 | -0.24351 |
| H | -0.16854 | -1.17099 | -1.96996 |
| C | 1.27158 | -2.73529 | -1.97893 |
| C | -0.65669 | -2.46772 | -3.60025 |
| H | -3.60496 | -4.75302 | 1.20107 |
| H | -4.10333 | -1.08723 | 0.82124 |
| C | -5.09760 | -2.70296 | 1.78518 |
| C | -3.01158 | -1.56062 | 2.60454 |
| H | -0.55232 | 4.05507 | 3.14872 |
| C | 0.32279 | 4.71018 | 1.28702 |
| H | -2.16658 | 0.92266 | 1.86335 |
| C | -1.10157 | 1.34524 | 3.66380 |
| C | -3.14642 | 2.55722 | 2.80173 |
| H | 1.04827 | 5.13510 | -0.69958 |
| H | -0.50483 | 2.19216 | -2.43301 |
| C | -0.56254 | 4.29445 | -2.90541 |
| C | 1.50411 | 2.93192 | -2.57070 |
| H | -2.01714 | -6.05968 | -0.17631 |
| H | 1.59093 | -2.60997 | -0.93330 |
| H | 1.94719 | -2.14711 | -2.61770 |
| H | 1.37186 | -3.79486 | -2.26417 |
| H | -0.67100 | -3.54344 | -3.83800 |
| H | 0.01283 | -1.96159 | -4.31280 |
| H | -1.67796 | -2.07443 | -3.72616 |
| H | -5.65260 | -3.06380 | 0.90613 |
| H | -5.73706 | -2.00993 | 2.35104 |
| H | -4.87771 | -3.56143 | 2.43856 |
| H | -2.78494 | -2.44147 | 3.22605 |
| H | -3.59220 | -0.84110 | 3.20467 |
| H | -2.05355 | -1.09527 | 2.33211 |
| H | 0.78208 | 5.59706 | 1.72581 |
| H | -0.14285 | 0.89029 | 3.37279 |
| H | -1.69939 | 0.60037 | 4.21240 |
| H | -0.90424 | 2.19505 | 4.33678 |
| H | -2.90839 | 3.46081 | 3.38530 |
| H | -3.79350 | 1.90880 | 3.41357 |
| H | -3.69788 | 2.86459 | 1.89922 |
| H | -1.59341 | 4.49699 | -2.58601 |
| H | -0.55271 | 4.09993 | -3.98860 |
| H | 0.03984 | 5.19703 | -2.71663 |
| H | 2.09787 | 3.80396 | -2.25222 |
| H | 1.57586 | 2.84759 | -3.66686 |
| H | 1.93461 | 2.03792 | -2.11087 |

Optimized xyz-coordinates of **7**$^+$

96

| | | | |
|---|---|---|---|
| C | 1.01207 | 0.15933 | -0.00146 |
| C | 2.68882 | 1.54462 | -0.48712 |
| C | 3.21021 | 0.28629 | -0.35481 |
| C | 0.40781 | 2.52401 | -0.18455 |
| C | -0.15026 | 3.01824 | -1.36998 |
| C | -1.16503 | 3.96613 | -1.22907 |
| C | -1.58670 | 4.37476 | 0.03748 |
| C | -0.98190 | 3.87647 | 1.18873 |
| C | 0.04685 | 2.93525 | 1.10095 |
| C | 0.29258 | 2.48634 | -2.72116 |
| C | -0.39970 | 1.15496 | -3.04296 |
| C | 0.04190 | 3.48456 | -3.84771 |
| C | 0.72030 | 2.40914 | 2.35283 |
| C | 1.42825 | 3.55785 | 3.07482 |
| C | -0.28002 | 1.70870 | 3.27308 |
| C | 2.22234 | -1.97388 | 0.07515 |
| C | 1.80797 | -2.72895 | -1.02497 |
| C | 1.82362 | -4.11795 | -0.87249 |
| C | 2.23886 | -4.69392 | 0.32444 |
| C | 2.65054 | -3.90041 | 1.39782 |
| C | 2.64727 | -2.50888 | 1.29729 |
| C | 1.36938 | -2.10109 | -2.33170 |
| C | -0.04411 | -2.54362 | -2.71956 |
| C | 2.37673 | -2.43131 | -3.43471 |
| C | 3.02908 | -1.59622 | 2.44852 |
| C | 3.92008 | -2.28796 | 3.47520 |
| C | 1.77650 | -1.03638 | 3.13663 |
| C | -3.33716 | -0.58724 | 0.17827 |
| C | -3.93292 | -0.76567 | 1.43799 |
| C | -4.93909 | -1.72833 | 1.56738 |
| C | -5.33730 | -2.48632 | 0.47164 |
| C | -4.74296 | -2.29121 | -0.77553 |
| C | -3.73786 | -1.33810 | -0.95040 |
| C | -3.45549 | 0.00168 | 2.65736 |
| C | -2.50769 | -0.86866 | 3.48529 |
| C | -4.60424 | 0.51579 | 3.52268 |
| C | -3.16409 | -1.04920 | -2.32874 |
| C | -3.83743 | 0.20160 | -2.90514 |
| C | -3.27771 | -2.21561 | -3.30298 |
| N | 1.33342 | 1.43525 | -0.27726 |
| N | 2.15926 | -0.54276 | -0.04577 |
| P | -0.58090 | -0.72725 | 0.32305 |
| P | -2.01091 | 0.68317 | -0.00439 |
| Cl | 3.44039 | 3.01682 | -0.82327 |
| Cl | 4.79468 | -0.26654 | -0.52072 |
| H | -1.63771 | 4.38668 | -2.11640 |
| H | -2.39180 | 5.10546 | 0.12564 |

| | | | |
|---|---|---|---|
| H | -1.30363 | 4.22177 | 2.17314 |
| H | 1.37899 | 2.30647 | -2.66767 |
| H | -1.49291 | 1.29011 | -3.03825 |
| H | -0.16224 | 0.36672 | -2.31684 |
| H | -0.09353 | 0.80472 | -4.04146 |
| H | -1.03764 | 3.59776 | -4.03098 |
| H | 0.50088 | 3.11797 | -4.77648 |
| H | 0.46189 | 4.47238 | -3.60865 |
| H | 1.48930 | 1.67048 | 2.07336 |
| H | 0.69474 | 4.31127 | 3.40081 |
| H | 2.15635 | 4.04697 | 2.41092 |
| H | 1.95197 | 3.17927 | 3.96495 |
| H | -1.07902 | 2.40424 | 3.57783 |
| H | 0.22895 | 1.34787 | 4.17951 |
| H | -0.74443 | 0.84846 | 2.77498 |
| H | 1.50700 | -4.74700 | -1.70656 |
| H | 2.24623 | -5.77987 | 0.42680 |
| H | 2.97929 | -4.37312 | 2.32318 |
| H | 1.36099 | -1.00665 | -2.22153 |
| H | -0.04281 | -3.59792 | -3.03902 |
| H | -0.41952 | -1.93365 | -3.55606 |
| H | -0.74634 | -2.44586 | -1.87802 |
| H | 2.42801 | -3.52062 | -3.58585 |
| H | 3.38190 | -2.07206 | -3.16746 |
| H | 2.06924 | -1.96429 | -4.38245 |
| H | 3.59858 | -0.75024 | 2.02834 |
| H | 3.35742 | -3.06536 | 4.01472 |
| H | 4.27308 | -1.55607 | 4.21508 |
| H | 4.79177 | -2.75714 | 2.99615 |
| H | 1.16965 | -1.86164 | 3.54122 |
| H | 1.13974 | -0.45443 | 2.45626 |
| H | 2.06632 | -0.37467 | 3.96786 |
| H | -5.40780 | -1.88902 | 2.53972 |
| H | -6.11914 | -3.23838 | 0.58671 |
| H | -5.07032 | -2.89295 | -1.62368 |
| H | -2.88851 | 0.88904 | 2.31251 |
| H | -3.04149 | -1.77228 | 3.81864 |
| H | -2.15387 | -0.31763 | 4.37041 |
| H | -1.63407 | -1.19205 | 2.89645 |
| H | -5.13834 | -0.32088 | 3.99766 |
| H | -5.32379 | 1.09486 | 2.92633 |
| H | -4.20812 | 1.15486 | 4.32575 |
| H | -2.09102 | -0.82961 | -2.22082 |
| H | -4.92062 | 0.03173 | -3.00053 |
| H | -3.42667 | 0.43323 | -3.90025 |
| H | -3.68686 | 1.07835 | -2.25274 |
| H | -4.32717 | -2.40139 | -3.57803 |
| H | -2.85952 | -3.13735 | -2.87130 |
| H | -2.72815 | -1.97861 | -4.22593 |

Optimized xyz-coordinates of **9**$^+$

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| | | | |
|---|---|---|---|
| P | -0.00064 | 0.33843 | 1.45342 |
| Cl | 3.69390 | -1.61027 | -2.24563 |
| P | -1.52433 | -0.68507 | 0.34496 |
| P | -2.33070 | -2.06358 | 1.81421 |
| Cl | 3.35228 | 1.86343 | -2.61931 |
| N | 1.73991 | -0.92576 | -0.48257 |
| N | 1.54597 | 1.20781 | -0.72199 |
| C | 1.10483 | 0.16270 | 0.00475 |
| C | 2.25549 | 3.14975 | 0.49554 |
| C | -3.55072 | 1.34467 | 0.88265 |
| C | 1.72001 | -2.23102 | 0.10719 |
| C | -3.79277 | -0.04961 | -1.12132 |
| C | 1.04137 | -3.26235 | -0.55059 |
| C | 1.31775 | 2.57834 | -0.36553 |
| C | 2.60136 | -0.55489 | -1.49979 |
| C | -3.08317 | 0.29851 | 0.05936 |
| C | 0.18042 | 3.22827 | -0.85123 |
| C | 3.39692 | 2.34356 | 1.08538 |
| C | 2.48659 | 0.79399 | -1.63910 |
| C | -2.87830 | 1.79342 | 2.16540 |
| C | -4.92810 | 0.68012 | -1.47575 |
| C | 0.16406 | -3.03120 | -1.76821 |
| C | -2.80052 | -1.31983 | 3.39691 |
| C | 2.04983 | 4.48552 | 0.84963 |
| C | -5.36370 | 1.74459 | -0.68943 |
| C | -0.82975 | 2.46496 | -1.68123 |
| C | 0.01744 | 4.56172 | -0.47519 |
| C | -4.68267 | 2.06355 | 0.47608 |
| C | 1.18216 | -4.54862 | -0.01560 |
| C | 0.94903 | 5.18420 | 0.35847 |
| C | 2.46259 | -2.40092 | 1.29023 |
| C | -3.31468 | -1.17832 | -2.02014 |
| C | -1.17527 | -3.75239 | -1.60709 |
| C | 3.18282 | -1.23947 | 1.95724 |
| C | -2.04659 | 3.05063 | 1.90406 |
| C | 1.91201 | -4.76241 | 1.14796 |
| C | 3.16773 | 2.13395 | 2.58365 |
| C | 4.74821 | 3.00067 | 0.81429 |
| C | 0.82334 | -3.51227 | -3.06261 |
| C | -1.04911 | -3.30014 | 2.13618 |
| C | -3.87671 | 2.04859 | 3.29859 |
| C | 2.52403 | -3.69556 | 1.80874 |
| C | 4.53469 | -0.95691 | 1.29518 |
| C | -4.41715 | -1.84151 | -2.83802 |
| C | 3.35532 | -1.44236 | 3.45831 |
| C | -3.82638 | -2.82108 | 1.11774 |
| C | -0.32419 | 2.25316 | -3.11101 |

| | | | |
|---|---|---|---|
| C | -2.19530 | -0.68570 | -2.94205 |
| C | -2.21131 | 3.10494 | -1.69477 |
| H | 3.42428 | 1.34475 | 0.62408 |
| H | -2.19797 | 1.00301 | 2.50094 |
| H | -5.48004 | 0.41999 | -2.37919 |
| H | -0.04332 | -1.95311 | -1.84315 |
| H | -3.59935 | -0.58617 | 3.22182 |
| H | -1.92063 | -0.80893 | 3.81694 |
| H | -3.14688 | -2.10487 | 4.08595 |
| H | 2.75605 | 4.97305 | 1.52463 |
| H | -6.24336 | 2.31884 | -0.98400 |
| H | -0.93576 | 1.48046 | -1.19767 |
| H | -0.86217 | 5.11056 | -0.81318 |
| H | -5.03207 | 2.89285 | 1.09287 |
| H | 0.69403 | -5.38868 | -0.51250 |
| H | 0.80209 | 6.22698 | 0.64318 |
| H | -2.89754 | -1.95454 | -1.36996 |
| H | -1.03812 | -4.84382 | -1.63254 |
| H | -1.84923 | -3.47909 | -2.43276 |
| H | -1.65484 | -3.47772 | -0.65822 |
| H | 2.56778 | -0.33954 | 1.83944 |
| H | -2.70846 | 3.86937 | 1.57445 |
| H | -1.29407 | 2.86670 | 1.12839 |
| H | -1.52588 | 3.36567 | 2.82176 |
| H | 2.00320 | -5.77105 | 1.55385 |
| H | 3.20881 | 3.09868 | 3.11302 |
| H | 3.95050 | 1.47640 | 2.99310 |
| H | 2.18389 | 1.67654 | 2.77557 |
| H | 4.79764 | 3.99336 | 1.28781 |
| H | 4.91256 | 3.12031 | -0.26668 |
| H | 5.55767 | 2.38216 | 1.23152 |
| H | 1.06254 | -4.58469 | -2.98350 |
| H | 1.74737 | -2.96783 | -3.28555 |
| H | 0.12554 | -3.37701 | -3.90350 |
| H | -0.99076 | -4.00179 | 1.29428 |
| H | -1.26046 | -3.84031 | 3.07005 |
| H | -0.08750 | -2.76150 | 2.20977 |
| H | -4.43391 | 2.98175 | 3.12908 |
| H | -3.33662 | 2.15765 | 4.25088 |
| H | -4.61571 | 1.23789 | 3.39720 |
| H | 3.07483 | -3.87974 | 2.73084 |
| H | 5.20975 | -1.81789 | 1.41628 |
| H | 4.99580 | -0.07642 | 1.77062 |
| H | 4.43743 | -0.74622 | 0.22155 |
| H | -4.79003 | -1.17104 | -3.62704 |
| H | -5.26719 | -2.13528 | -2.20337 |
| H | -4.01521 | -2.73968 | -3.33165 |
| H | 4.07554 | -2.24659 | 3.67348 |
| H | 2.39403 | -1.68874 | 3.93458 |
| H | 3.74216 | -0.51758 | 3.90946 |
| H | -4.49465 | -2.00188 | 0.80579 |

|  |  |  |  |
|---|---|---|---|
| H | -4.32413 | -3.45400 | 1.86678 |
| H | -3.56165 | -3.42086 | 0.23532 |
| H | -0.12299 | 3.22771 | -3.58182 |
| H | -1.08779 | 1.72958 | -3.70369 |
| H | 0.60080 | 1.65990 | -3.14233 |
| H | -2.60381 | 0.05227 | -3.65122 |
| H | -1.76761 | -1.52485 | -3.51562 |
| H | -1.38330 | -0.20099 | -2.37868 |
| H | -2.21092 | 4.02357 | -2.30315 |
| H | -2.54604 | 3.35093 | -0.67823 |
| H | -2.93466 | 2.39757 | -2.12843 |

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