Experimental Details and Spectroscopic Data

All preparations and manipulations were carried out using standard Schlenk techniques and a dry-box under argon atmosphere. Solvents (n-pentane, n-hexane, tetrahydrofuran, toluene and benzene were distilled over sodium/benzophenone while dichloromethane (DCM), 1,2-difluorobenzene, C_6D_6, $CDCl_3$, CD_3CN, CD_2Cl_2, were distilled over CaH_2. All solvents were stored over 4 Å molecular sieves prior to use. The commercial products aluminium trichloride and sodium hexafluoroanitmonate were used without further purification. Phosphines such as (PCl_3 and $^tBuPCl_2$) were distilled prior to use, and $MeN(PCl_2)_2$ was purchased from Sigma Aldrich and used without further purification. $PhN(PCl_2)_2$, $NaBAr^{Cl}{}_4$ (Ar^{Cl} = 3,5-Cl_2-C_6H_3) and the ligands carbodiphosphorane and carbodicarbene were prepared by literature methods.[S1] NMR spectra were obtained on a Brüker Avance III 400 and JEOL ECA 400 instrument. Chemical shifts (δ) are reported in parts per million (ppm) downfield from internal - tetramethylsilane (for ^1H and $^{13}C\{^1H\}$) and external standard - 85% phosphoric acid (for $^{31}P\{^1H\}$). Mass spectra were obtained on Waters Q-TOF Premier MS mass spectrometer using the electrospray ionization (ESI) mode.

Synthesis of $[(PPh_3)_2C{\cdot}PCl_2][AlCl_4]$, [**1**·**PCl$_2$**][**AlCl$_4$**]

The chloride salt of this compound was synthesized by adding 80 mL of toluene solution of $(PPh_3)_2C$ (**1**) 0.10 g (0.19 mmol) to 2.0 equivalents of $MeN(PCl_2)_2$ or $PhN(PCl_2)_2$. The reaction was stirred overnight followed by filtration. The resulting white solid was dissolved in 1,2-difluorobenzene and quantitative counterion conversion was achieved by adding 1.0 equivalent of $AlCl_3$. Single crystals of [**1**·**PCl$_2$**][**AlCl$_4$**] suitable for X-ray analysis were obtained by layering the above solution with n-hexane. Note: The compound [**1**·**PCl$_2$**][**Cl**] can also be synthesized from the reaction of **1** with PCl_3 (See reference 8 in the main text). ^1H NMR (300 MHz, CD_2Cl_2): δ 7.19-7.72 (m, 30H, Ph). $^{13}C\{^1H\}$ (100 MHz, CD_2Cl_2): δ 124.0 (br, m, *ipso-C*, $Ph_{(carbone)}$), 129.9 (virtual triplet, *o-C*, $Ph_{(carbone)}$), 133.6 (s, *p-C*, $Ph_{(carbone)}$), 134.3 (virtual triplet, *m-C*, $Ph_{(carbone)}$). $^{31}P\{^1H\}$ (CD_2Cl_2, 121 MHz): δ 23.85 (d, $P_{(carbone)}$), 173.53 (t, $P_{(central)}$). $^{27}Al\{^1H\}$ (104 MHz, CD_2Cl_2): δ 107.05 (s).

Synthesis of $[(PPh_3)_2C{\cdot}P(^tBu)Cl][Cl]$, [**1**·**P(^{t}Bu)Cl**][**Cl**]

A benzene solution of $(PPh_3)_2C$ 0.10 g (0.19 mmol) was added to a toluene solution (20 mL) containing 3.0 equivalents of $^tBuPCl_2$. The reaction was stirred overnight and it resulted in the formation of white precipitate. The solution was filtered off and white precipitate was washed with toluene twice and finally with n-hexane and dried in vacuo to yield [**1**·**P(^{t}Bu)Cl**][**Cl**] as a white solid. Yield: 0.11 g (90 %). ^1H NMR (400 MHz, $CDCl_3$): δ 7.40-7.69 (m, 30H, Ph), 0.57 (d, 9H, $^3J_{PH}$ = 15.6 Hz, C*C*H_3). $^{13}C\{^1H\}$ (CD_2Cl_2, 100.6 MHz): δ 27.94 (d, $^2J_{P(central)C}$ = 33.6 Hz, C*C*H3), 40.40 (dt, $^1J_{P(central)C}$ = 72.0 Hz, $^3J_{P(central)C}$ = 11.2 Hz, *C*CH3), 124.40 (br m, *ipso-C*, $Ph_{(carbone)}$), 129.11 (virtual triplet, *o-C*, $Ph_{(carbone)}$), 133.72 (s, *p-C*, $Ph_{(carbone)}$), 134.60 (virtual triplet, *m-C*, $Ph_{(carbone)}$). $^{31}P\{^1H\}$ (CD_2Cl_2, 202 MHz): δ 23.42 (multiplet – a set of second order doublets, $P_{(carbone)}$), 131.55 (second order triplet, $P_{(central)}$). ES-MS Calculated for $[C_{41}H_{39}ClP_3]^+$ (**1**·**P(^{t}Bu)Cl$^+$**): m/z 659.1953. Found: 659.1955.

Synthesis of $[\{C_6H_4(MeN)_2C\}_2C{\cdot}PCl_2][X]$, [**2**·**PCl$_2$**][X] (X = Cl^-, SbF_6^- or $BAr^{Cl}{}_4$)

The chloride salt of this compound was synthesized by adding 80 mL of benzene solution of 0.10 g (0.33 mmol) of $\{C_6H_4(MeN)_2C\}_2C$ (**2**) to 2.0 equivalents of $MeN(PCl_2)_2$. The reaction was stirred overnight followed by filtration. The resulting light - yellow solid was dried under vacuum to yield 0.14 g (98%) of [**2**·**PCl$_2$**][Cl]. The most adequate counterion for crystallization of this species was found to be SbF_6^- which was quantitatively exchanged with the chloride anion by the addition of 1 equiv of $NaSbF_6$ to a DCM solution containing [**2**·**PCl$_2$**][Cl] followed by layering with n-hexane ([**2**·**PCl$_2$**][SbF_6]).

[**2**·**PCl$_2$**][Cl]: $^{31}P\{^1H\}$ (CD_2Cl_2, 160 MHz): δ 159.99 (s). ES-MS Calculated for $[C_{19}H_{20}Cl_2N_4P]^+$ (**2**·**PCl$_2^+$**): m/z 405.0803. Found: 405.0804. Note: Due to surprisingly high insolubility of [**2**·**PCl$_2$**][X] (X = Cl^- and SbF_6^-) in common organic solvents (C_6D_6, CD_2Cl_2, CD_3CN,) we quantitatively converted [**2**·**PCl$_2$**][Cl] to [**2**·**PCl$_2$**][$BAr^{Cl}{}_4$] (Ar^{Cl} = 3,5-Cl_2-C_6H_3). This conversion was achieved by addition of 1.0 equivalent of $NaBAr^{Cl}{}_4$ to the THF solution of [**2**·**PCl$_2$**][Cl] followed by precipitation with n-pentane, and subsequently filtered and dried in vacuo to yield [**2**·**PCl$_2$**][$BAr^{Cl}{}_4$] as a yellow solid. ^1H NMR (400 MHz, CD_2Cl_2): δ 7.38-7.52 (m, 8H, $Ph_{(carbone)}$), 6.80-6.94 (m, 12H, $Ph_{(BArCl4)}$), 3.68 (s, 12H, NCH_3). $^{11}B\{^1H\}$ (128 MHz, CD_2Cl_2): δ -7.69 (s). $^{13}C\{^1H\}$ (100 MHz, CD_2Cl_2): δ 32.8 (s, NCH_3), 111.8 (s, CH arom.), 122.9 (s, *p-C*, $BAr^{Cl}{}_4$), 127.3 (br s, C arom.), 132.0 (s, *m-C*, $BAr^{Cl}{}_4$), 132.9 (q, $^2J_{CB}$ = 4 Hz, *o-C*, $BAr^{Cl}{}_4$), 164.7 (q, $^1J_{CB}$ = 49 Hz, *ipso-C*, $BAr^{Cl}{}_4$). Signals that correspond to the N*C*N and C*C*C resonances were not observed in the $^{13}C\{^1H\}$ Spectrum.

Crystallographic methods

Single crystals were mounted on quartz fiber and the X-ray intensity data were collected at 103(2) K on a Bruker X8 APEX system, using Mo Kα radiation, with the SMART suite of programs.[S2] Data were processed and corrected for Lorentz and polarization effects with SAINT[S3] and for absorption effects with SABADS.[S4] Structural solution and refinement were carried out with the SHELXTL suite of programs.[S5] The structure was solved by direct method and refined for all data by full-matrix least-squares methods on F^2. All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were generated geometrically and allowed to ride on their respective parent atoms; they were assigned appropriate isotopic thermal parameters.

Crystallographic data for [**1**·**PCl_2**][$AlCl_4$]: $C_{37}H_{30}AlCl_6P_3$, M_r 807.20, triclinic, P-1, a = 10.7482(3), b = 11.7146(3) Å, and c = 16.2326(5) Å, α = 108.1778(13)°, β = 100.8287(13)°, and γ = 99.8863(13)°, 1848.28(9) Å^3, Z = 2, ρ_c = 1.450 gcm^{-3}, T = 103(2) K, λ = 0.71073 Å; 54649 reflections collected, 11898 independent [R(int) = 0.0370], which were used in all calculations; R1 = 0.0326, wR2 = 0.0786 for I > 2σ(I), and R1 = 0.0433, wR2 = 0.0845 for all unique reflections; max and min residual electron densities 1.034 eÅ^{-3} and -0.886 eÅ^{-3}. CCDC 1058665.

Crystallographic data for [**2**·**PCl_2**][SbF_6]: $C_{19}H_{20}Cl_2F_6N_4PSb$, M_r 642.01, orthorhombic, P_{bca}, a = 11.6300(9), b = 19.1931(14), and c = 21.1940(13) Å, α = 90, β =90, and γ = 90°, V = 4730.8(6) Å^3, Z = 8, ρ_c = 1.803 gcm^{-3}, T = 103(2) K, λ = 0.71073 Å; 69640 reflections collected, 4854 independent [R_{int} = 11.68 %], which were used in all calculations; R1 = 0.0640, wR2 = 0.1577 for I > 2σ(I), and R1 = 0.1188, wR2 = 0.2044 for all unique reflections; max and min residual electron densities 1.703 e$^-$/Å^3 and - 1.035 e$^-$/Å^3. CCDC 1058666.

Computational details

All quantum chemical calculations were performed with the Gaussian program package[S6] at the B3LYP/6-31G(d) level. Frequency calculations performed on the optimized structures revealed absence of imaginary frequency for the stable species, and a single imaginary frequency for each transition state. Intrinsic reaction coordinate calculations confirmed that the optimized transition states connect the structures of interest. Analysis of electron density and its Laplacian in the bond critical points and computation of delocalization index were performed with the AIMAll program package.[S7]

R = Ph_3P (**1**), NHC (**2**)

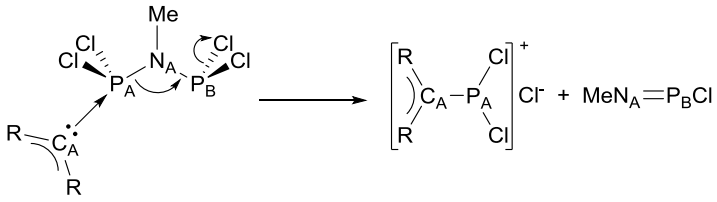


Table S1. Activation energy values.

L	E_a - kJ/mol (kcal/mol)
1	54 (12.9)
2	44 (10.4)

Table S2. Change in various bond distances (r), their electron densities (ρ_{BCP}), Laplacians ($\nabla^2\rho_{BCP}$) and delocalization indexes (DI) as **1** is approaching P_A of $MeN(PCl_2)_2$. Values highlighted in green are for the transition state while those ones in orange are for the final product(s).

P_A-C_A				P_A-N_A				P_B-N_A			
r	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI	R	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI	r	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI
1.845	0.152	-0.157	0.93	/	/	/	/	1.534	0.208	1.236	1.58
2.071	0.105	-0.097	0.77	2.254	0.066	0.060	0.48	1.608	0.190	0.798	1.09
2.100	0.100	-0.074	0.73	2.179	0.075	0.044	0.53	1.616	0.188	0.758	1.07
2.200	0.082	-0.017	0.63	2.017	0.100	-0.030	0.65	1.640	0.181	0.658	1.00
2.300	0.068	0.018	0.54	1.933	0.115	-0.068	0.70	1.655	0.177	0.592	0.97
2.400	0.056	0.037	0.47	1.882	0.124	-0.044	0.73	1.666	0.174	0.551	0.95
2.500	0.047	0.047	0.40	1.848	0.130	0.006	0.75	1.675	0.172	0.515	0.93
3.000	0.020	0.039	0.18	1.770	0.147	0.203	0.81	1.698	0.165	0.429	0.89
3.500	0.009	0.020	0.08	1.744	0.153	0.282	0.83	1.708	0.162	0.394	0.87
4.000	0.004	0.010	0.03	1.733	0.155	0.316	0.84	1.713	0.161	0.380	0.86
∞	/	/	/	1.720	0.159	0.358	0.85	1.720	0.159	0.358	0.85

Table S3. Change in various bond distances (r), their electron densities (ρ_{BCP}), Laplacians ($\nabla^2\rho_{BCP}$) and delocalization indexes (DI) as **2** is approaching P_A of $MeN(PCl_2)_2$. Values highlighted in green are for the transition state while those ones in orange are for the final product(s).

P_A-C_A				P_A-N_A				P_B-N_A			
r	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI	R	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI	r	ρ_{BCP}	$\nabla^2\rho_{BCP}$	DI
1.860	0.152	-0.199	0.83	/	/	/	/	1.534	0.208	1.236	1.58
2.008	0.119	-0.154	0.73	2.264	0.065	0.061	0.47	1.608	0.190	0.791	1.09
2.100	0.100	-0.077	0.64	2.067	0.092	-0.002	0.61	1.633	0.183	0.687	1.02
2.200	0.083	-0.021	0.56	1.966	0.109	-0.058	0.68	1.649	0.179	0.616	0.98
2.300	0.069	0.013	0.49	1.905	0.120	-0.062	0.72	1.662	0.175	0.567	0.96
2.400	0.057	0.035	0.42	1.863	0.128	-0.018	0.74	1.671	0.173	0.530	0.94
2.500	0.047	0.045	0.36	1.833	0.133	0.038	0.76	1.678	0.171	0.502	0.92
3.000	0.019	0.037	0.16	1.762	0.148	0.228	0.81	1.700	0.164	0.423	0.89
3.500	0.008	0.018	0.07	1.737	0.154	0.305	0.83	1.710	0.161	0.389	0.87
4.000	/	/	0.02	1.720	0.159	0.359	0.85	1.725	0.157	0.340	0.85
∞	/	/	/	1.720	0.159	0.358	0.85	1.720	0.159	0.358	0.85

Optimized structures for:

- **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003694	-0.015597	-0.855562
2	15	0	1.547070	-0.016637	-0.284834
3	15	0	-1.538479	-0.000859	-0.284539
4	6	0	-2.127918	1.590707	0.480782
5	6	0	-2.723388	-0.259902	-1.679485
6	6	0	-2.022033	-1.278457	0.969583
7	6	0	-3.205804	1.674837	1.375090
8	6	0	-3.611150	2.910667	1.883761
9	6	0	-2.946817	4.077763	1.502984
10	6	0	-1.872186	4.004171	0.614191
11	6	0	-1.465035	2.768687	0.109484
12	1	0	-3.721698	0.773701	1.693699
13	1	0	-4.443264	2.959738	2.581697
14	1	0	-3.262519	5.039058	1.900300
15	1	0	-1.348887	4.908950	0.315205
16	1	0	-0.622272	2.701850	-0.573617
17	6	0	-1.640066	-1.115340	2.311735
18	6	0	-1.873255	-2.125498	3.244566
19	6	0	-2.486739	-3.317007	2.851119
20	6	0	-2.861848	-3.493522	1.518585
21	6	0	-2.629592	-2.482808	0.583945
22	1	0	-1.156175	-0.196748	2.630955
23	1	0	-1.572411	-1.981224	4.278995
24	1	0	-2.668918	-4.103742	3.578705
25	1	0	-3.338366	-4.418597	1.203929
26	1	0	-2.926192	-2.631980	-0.449790
27	6	0	-4.113287	-0.170383	-1.512658
28	6	0	-4.968610	-0.366442	-2.597067
29	6	0	-4.443879	-0.649098	-3.860615
30	6	0	-3.061608	-0.733427	-4.034699
31	6	0	-2.205426	-0.538995	-2.949243
32	1	0	-4.534488	0.055977	-0.537419
33	1	0	-6.044100	-0.294817	-2.456398
34	1	0	-5.111240	-0.798922	-4.705580
35	1	0	-2.648155	-0.948864	-5.016810
36	1	0	-1.125689	-0.590785	-3.061297
37	6	0	2.539906	1.407881	-0.934111
38	6	0	1.846643	0.046458	1.544647
39	6	0	2.510390	-1.499077	-0.846819
40	6	0	3.706180	1.881725	-0.315149
41	6	0	4.423187	2.942311	-0.873112

42	6	0	3.984466	3.539119	-2.056239
43	6	0	2.821864	3.076147	-2.676392
44	6	0	2.102690	2.019618	-2.116975
45	1	0	4.048529	1.439591	0.616240
46	1	0	5.321051	3.305259	-0.379237
47	1	0	4.542848	4.365116	-2.489305
48	1	0	2.472297	3.540885	-3.594888
49	1	0	1.186118	1.659897	-2.577067
50	6	0	2.176512	-1.100584	2.280441
51	6	0	2.255535	-1.052608	3.674389
52	6	0	2.004526	0.140949	4.351526
53	6	0	1.669173	1.289654	3.628695
54	6	0	1.587841	1.242084	2.237582
55	1	0	2.372035	-2.035948	1.765622
56	1	0	2.514721	-1.950652	4.229341
57	1	0	2.068823	0.178310	5.435928
58	1	0	1.472253	2.223594	4.148858
59	1	0	1.317949	2.138941	1.686654
60	6	0	3.901630	-1.608019	-0.700134
61	6	0	4.571352	-2.749130	-1.141730
62	6	0	3.858985	-3.792906	-1.737985
63	6	0	2.475947	-3.689523	-1.891820
64	6	0	1.806169	-2.546879	-1.449866
65	1	0	4.469711	-0.801265	-0.246466
66	1	0	5.649600	-2.821992	-1.024352
67	1	0	4.382525	-4.680472	-2.084226
68	1	0	1.917318	-4.496806	-2.358768
69	1	0	0.731429	-2.441046	-1.570981

- $MeN(PCl_2)_2$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000006	0.030210	1.692252
2	7	0	0.000001	-0.047106	0.214801
3	15	0	1.415986	-0.019267	-0.760955
4	17	0	2.529515	-1.597606	0.081825
5	15	0	-1.415981	-0.019262	-0.760956
6	17	0	-2.529524	-1.597606	0.081830
7	17	0	-2.457638	1.615394	0.065232
8	17	0	2.457639	1.615390	0.065236
9	1	0	0.000075	1.074160	2.015744
10	1	0	0.886801	-0.476283	2.077852
11	1	0	-0.886857	-0.476167	2.077852

Partially optimized structures as **1** is approaching P_A of $MeN(PCl_2)_2$.

- $r(P_A\text{-}C_A)$ = 4.000 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003896	-3.758882	-1.148907
2	6	0	-0.155782	-2.366518	-1.105684
3	6	0	0.697634	-1.562215	-1.872952
4	6	0	1.681133	-2.136945	-2.681107
5	6	0	1.829724	-3.524998	-2.720886
6	6	0	0.991066	-4.333766	-1.951651
7	15	0	-1.450140	-1.515697	-0.081697
8	6	0	-1.573715	-2.561228	1.443000
9	6	0	-2.294407	-3.764178	1.488411
10	6	0	-2.342029	-4.516567	2.663964
11	6	0	-1.671350	-4.075228	3.805954
12	6	0	-0.957596	-2.875374	3.770982
13	6	0	-0.912082	-2.121930	2.597676
14	6	0	-1.062861	0.045760	0.233327
15	15	0	-1.561388	1.600411	0.084486
16	6	0	-2.203086	2.363162	1.649524
17	6	0	-2.250967	3.752117	1.845385
18	6	0	-2.749717	4.281780	3.036350
19	6	0	-3.199303	3.428841	4.047294
20	6	0	-3.144374	2.046083	3.864588
21	6	0	-2.645943	1.517298	2.672545
22	6	0	-2.872131	1.971090	-1.178900
23	6	0	-2.739533	1.396851	-2.454264
24	6	0	-3.705473	1.609124	-3.436708
25	6	0	-4.829505	2.389599	-3.156612
26	6	0	-4.979169	2.954033	-1.890157
27	6	0	-4.007321	2.748724	-0.907981
28	6	0	-0.169124	2.745305	-0.341254
29	6	0	-0.120079	3.492567	-1.524501
30	6	0	0.995660	4.282866	-1.819659
31	6	0	2.069428	4.341513	-0.932972
32	6	0	2.024352	3.608851	0.258053
33	6	0	0.915021	2.816691	0.550086
34	6	0	-3.036558	-1.895162	-0.969364
35	6	0	-3.071783	-2.400965	-2.275996
36	6	0	-4.291003	-2.584837	-2.933619
37	6	0	-5.488481	-2.266446	-2.293843
38	6	0	-5.464572	-1.759689	-0.991579
39	6	0	-4.248878	-1.572484	-0.337190
40	15	0	2.839537	-0.459147	0.951908
41	17	0	2.902531	0.379068	2.903793
42	7	0	4.457075	-0.127870	0.426316
43	6	0	5.675537	-0.545950	1.151555
44	17	0	3.020562	-2.492446	1.478827
45	15	0	4.454518	0.609305	-1.119407
46	17	0	5.773385	2.235727	-0.807708
47	17	0	5.765981	-0.660863	-2.192369
48	1	0	-1.891131	4.422621	1.069408
49	1	0	-2.780442	5.359133	3.177896
50	1	0	-3.582947	3.841760	4.976755
51	1	0	-3.482329	1.378087	4.652768
52	1	0	-2.574755	0.442262	2.530825
53	1	0	-4.141684	3.193749	0.072169

54	1	0	-5.854856	3.556210	-1.661325
55	1	0	-5.586244	2.550868	-3.919989
56	1	0	-3.584884	1.157549	-4.417853
57	1	0	-1.879449	0.770057	-2.671689
58	1	0	0.887178	2.250176	1.476392
59	1	0	2.851497	3.660756	0.961347
60	1	0	2.936229	4.955453	-1.162213
61	1	0	1.020060	4.853535	-2.744579
62	1	0	-0.949992	3.461416	-2.223135
63	1	0	-2.836110	-4.108394	0.611826
64	1	0	-2.908996	-5.443782	2.688319
65	1	0	-1.710065	-4.661005	4.720792
66	1	0	-0.437082	-2.523878	4.658045
67	1	0	-0.378457	-1.176041	2.563976
68	1	0	-2.147086	-2.656552	-2.783817
69	1	0	-4.301758	-2.980001	-3.946371
70	1	0	-6.436541	-2.410934	-2.805376
71	1	0	-6.393826	-1.508208	-0.487004
72	1	0	-4.239337	-1.170648	0.672720
73	1	0	-0.632467	-4.401130	-0.547827
74	1	0	1.108353	-5.414223	-1.970756
75	1	0	2.599733	-3.973633	-3.343004
76	1	0	2.332222	-1.502235	-3.277140
77	1	0	0.586707	-0.482802	-1.810568
78	1	0	6.491898	0.137129	0.909229
79	1	0	5.486327	-0.498396	2.225712
80	1	0	5.951195	-1.565506	0.870198

- $r(P_A\text{-}C_A) = 3.500$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.321358	1.524232	-2.551702
2	6	0	-2.396577	2.151826	-1.297024
3	6	0	-3.413064	3.093210	-1.079373
4	6	0	-4.321426	3.406533	-2.093032
5	6	0	-4.226474	2.787677	-3.339230
6	6	0	-3.222629	1.843952	-3.566320
7	15	0	-1.161874	1.651649	0.002150
8	6	0	-0.814049	0.045053	0.141965
9	15	0	-1.591235	-1.398926	-0.060594
10	6	0	-3.292151	-1.441043	-0.809850
11	6	0	-3.545512	-1.979558	-2.078762
12	6	0	-4.827704	-1.923434	-2.631331
13	6	0	-5.871419	-1.328160	-1.923847
14	6	0	-5.629325	-0.785324	-0.659050
15	6	0	-4.350681	-0.840160	-0.108316
16	6	0	0.347632	2.646255	-0.396506
17	6	0	0.592196	3.168420	-1.673255
18	6	0	1.787201	3.837771	-1.950948
19	6	0	2.751790	3.996737	-0.956249
20	6	0	2.514490	3.486860	0.323696
21	6	0	1.321333	2.819058	0.601000
22	6	0	-1.760956	2.495483	1.546487
23	6	0	-1.697841	3.887361	1.721781
24	6	0	-2.169902	4.475811	2.895772
25	6	0	-2.704067	3.679829	3.912185
26	6	0	-2.758866	2.294686	3.751959
27	6	0	-2.286602	1.707359	2.576381
28	6	0	-1.838132	-2.345234	1.514506
29	6	0	-2.783032	-3.376014	1.639408
30	6	0	-2.925046	-4.064265	2.845732
31	6	0	-2.127937	-3.728664	3.941814
32	6	0	-1.193100	-2.697945	3.829101
33	6	0	-1.050984	-2.009028	2.623749
34	6	0	-0.610810	-2.540646	-1.143099
35	6	0	0.298100	-1.963611	-2.039826
36	6	0	1.048055	-2.762253	-2.904662
37	6	0	0.904669	-4.150554	-2.874401
38	6	0	0.009178	-4.735289	-1.976761
39	6	0	-0.745415	-3.935776	-1.116541
40	15	0	2.579826	-0.573820	0.732397
41	7	0	4.302364	-0.454027	0.490829
42	15	0	4.641958	0.348131	-0.978585
43	17	0	5.876929	-1.066677	-1.964732
44	17	0	2.418619	-2.653076	1.063674
45	17	0	2.475787	0.058541	2.761924
46	6	0	5.321896	-1.101868	1.341263
47	17	0	6.150484	1.710521	-0.375336
48	1	0	-1.270829	4.514365	0.943603
49	1	0	-2.114368	5.554306	3.019852
50	1	0	-3.067176	4.138402	4.828342
51	1	0	-3.160808	1.668998	4.544695
52	1	0	-2.300260	0.627525	2.457667
53	1	0	-3.506598	3.581537	-0.115634
54	1	0	-5.105825	4.135121	-1.904220
55	1	0	-4.933626	3.033412	-4.127197
56	1	0	-3.146415	1.348906	-4.530841
57	1	0	-1.558342	0.771380	-2.726958
58	1	0	1.144174	2.433653	1.600201
59	1	0	3.256296	3.613864	1.107723
60	1	0	3.681082	4.516854	-1.171997
61	1	0	1.959795	4.237723	-2.946837
62	1	0	-0.150042	3.059567	-2.457238
63	1	0	-3.423909	-3.632992	0.800673
64	1	0	-3.663608	-4.857425	2.930287
65	1	0	-2.240498	-4.263909	4.881189
66	1	0	-0.573323	-2.426952	4.679792
67	1	0	-0.339972	-1.193429	2.534228
68	1	0	-2.742831	-2.448353	-2.638909
69	1	0	-5.008181	-2.348047	-3.615699
70	1	0	-6.868702	-1.285294	-2.353868
71	1	0	-6.437557	-0.318912	-0.101782
72	1	0	-4.172987	-0.411384	0.874531
73	1	0	-1.427986	-4.406217	-0.415785
74	1	0	-0.098675	-5.816317	-1.940720
75	1	0	1.493556	-4.774946	-3.541284
76	1	0	1.749897	-2.301752	-3.595425
77	1	0	0.419759	-0.883558	-2.029274
78	1	0	6.247312	-0.523829	1.299888
79	1	0	4.965721	-1.120815	2.372795
80	1	0	5.508438	-2.122743	0.997606

- $r(P_A\text{-}C_A) = 3.000$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.300850	-3.953813	-1.076933
2	6	0	-0.938164	-2.601438	-1.146410
3	6	0	-0.019955	-2.195845	-2.123863
4	6	0	0.514866	-3.117668	-3.024596
5	6	0	0.143863	-4.461257	-2.951663
6	6	0	-0.761829	-4.877280	-1.974005
7	15	0	-1.641416	-1.299616	-0.030925
8	6	0	-2.019305	-2.181479	1.556771
9	6	0	-3.127813	-3.033199	1.694686
10	6	0	-3.378818	-3.680694	2.905363
11	6	0	-2.530225	-3.480729	3.996105

12	6	0	-1.433643	-2.626546	3.871639
13	6	0	-1.180695	-1.980236	2.660494
14	6	0	-0.586877	-0.013785	0.123505
15	15	0	-0.821578	1.626813	-0.041480
16	6	0	-1.343263	2.547680	1.488401
17	6	0	-1.246000	3.944313	1.608857
18	6	0	-1.663814	4.586152	2.775049
19	6	0	-2.176320	3.840794	3.840135
20	6	0	-2.261211	2.452334	3.736394
21	6	0	-1.842740	1.811207	2.568201
22	6	0	-2.018760	2.197467	-1.349285
23	6	0	-2.001354	1.540694	-2.590941
24	6	0	-2.854134	1.933406	-3.621774
25	6	0	-3.753947	2.982327	-3.424742
26	6	0	-3.796380	3.628945	-2.190005
27	6	0	-2.936147	3.241260	-1.160459
28	6	0	0.748570	2.505886	-0.485958
29	6	0	1.076669	2.785168	-1.820741
30	6	0	2.292457	3.389519	-2.144709
31	6	0	3.202090	3.722131	-1.139982
32	6	0	2.886982	3.450175	0.192699
33	6	0	1.668304	2.850867	0.517667
34	6	0	-3.352221	-1.038303	-0.711418
35	6	0	-3.751092	-1.536057	-1.959221
36	6	0	-5.034452	-1.280343	-2.448778
37	6	0	-5.933822	-0.523188	-1.699209
38	6	0	-5.545726	-0.020071	-0.454702
39	6	0	-4.266133	-0.275172	0.034124
40	15	0	2.312826	-0.603672	0.617223
41	17	0	2.148865	0.025393	2.652368
42	7	0	4.078524	-0.700087	0.551814
43	6	0	4.932567	-1.464143	1.481648
44	17	0	1.937666	-2.663708	0.923629
45	15	0	4.638260	0.036417	-0.872201
46	17	0	6.263356	1.203551	-0.150327
47	17	0	5.770405	-1.527215	-1.769491
48	1	0	-0.833568	4.533712	0.794427
49	1	0	-1.582808	5.667163	2.855045
50	1	0	-2.497600	4.341676	4.749678
51	1	0	-2.643437	1.864573	4.566863
52	1	0	-1.878582	0.728420	2.495684
53	1	0	-2.992397	3.753649	-0.206832
54	1	0	-4.502660	4.438001	-2.021882
55	1	0	-4.422541	3.287006	-4.225587
56	1	0	-2.821379	1.413113	-4.575377
57	1	0	-1.323371	0.706322	-2.743930
58	1	0	1.432932	2.657483	1.558497
59	1	0	3.588570	3.704633	0.982373
60	1	0	4.149675	4.190292	-1.391666
61	1	0	2.525730	3.603401	-3.184448
62	1	0	0.378601	2.544167	-2.615232
63	1	0	-3.810784	-3.179115	0.862883
64	1	0	-4.242567	-4.334158	2.997732
65	1	0	-2.728070	-3.982812	4.939642
66	1	0	-0.771323	-2.460075	4.717081
67	1	0	-0.337881	-1.304530	2.567293
68	1	0	-3.062766	-2.129967	-2.551533
69	1	0	-5.329064	-1.676559	-3.417245
70	1	0	-6.932290	-0.325299	-2.080208
71	1	0	-6.240826	0.570749	0.136050
72	1	0	-3.976817	0.120600	1.004015
73	1	0	-1.993403	-4.296347	-0.315093
74	1	0	-1.045530	-5.924206	-1.903825
75	1	0	0.564947	-5.182733	-3.646975
76	1	0	1.229340	-2.788871	-3.774823
77	1	0	0.286990	-1.153745	-2.147822
78	1	0	5.915915	-0.992641	1.545802
79	1	0	4.475105	-1.457468	2.472453
80	1	0	5.041763	-2.495790	1.135930

- $r(P_A\text{-}C_A) = 2.500$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.301989	1.466507	-2.782132
2	6	0	-1.582385	2.077955	-1.547969
3	6	0	-2.604075	3.036497	-1.497253
4	6	0	-3.304401	3.392517	-2.652304
5	6	0	-2.993530	2.802017	-3.876329
6	6	0	-1.990816	1.832488	-3.937406
7	15	0	-0.573831	1.565574	-0.071284
8	6	0	-0.366665	-0.097075	0.164905
9	15	0	-1.620810	-1.234807	0.014558
10	6	0	-3.286526	-0.686666	-0.597071
11	6	0	-3.712639	-0.940141	-1.908043
12	6	0	-4.961782	-0.495307	-2.346451
13	6	0	-5.800474	0.207583	-1.482065
14	6	0	-5.384208	0.468884	-0.174575
15	6	0	-4.137781	0.026065	0.264219
16	6	0	1.043884	2.438011	-0.321401
17	6	0	1.567485	2.674572	-1.601367
18	6	0	2.791316	3.325027	-1.760793
19	6	0	3.515507	3.745117	-0.644535
20	6	0	3.005202	3.516582	0.633698
21	6	0	1.776892	2.874527	0.794727
22	6	0	-1.275838	2.536999	1.349443
23	6	0	-1.291960	3.942537	1.362145
24	6	0	-1.816448	4.635168	2.452861
25	6	0	-2.318155	3.933926	3.552974
26	6	0	-2.284276	2.539894	3.559895
27	6	0	-1.762898	1.846636	2.464468
28	6	0	-2.087872	-2.094070	1.588679
29	6	0	-3.287674	-2.817199	1.708089
30	6	0	-3.613868	-3.459079	2.902895
31	6	0	-2.751522	-3.380959	3.998538
32	6	0	-1.566995	-2.651828	3.894358
33	6	0	-1.237428	-2.011254	2.698196
34	6	0	-1.169063	-2.585786	-1.171104
35	6	0	-0.228374	-2.302709	-2.169665
36	6	0	0.109488	-3.261875	-3.124709
37	6	0	-0.485769	-4.523346	-3.088039
38	6	0	-1.415827	-4.819999	-2.090187
39	6	0	-1.756478	-3.858523	-1.138076
40	15	0	2.050041	-0.618381	0.536086
41	7	0	3.876869	-0.888613	0.607078
42	15	0	4.562866	-0.179386	-0.746038
43	17	0	5.641567	-1.798060	-1.654130
44	17	0	1.612039	-2.688172	0.752614
45	17	0	1.926580	-0.058825	2.614853
46	6	0	4.618104	-1.724003	1.564717
47	17	0	6.257149	0.852120	0.065681
48	1	0	-0.882980	4.499414	0.523558
49	1	0	-1.825231	5.721975	2.448438
50	1	0	-2.721369	4.474966	4.404938
51	1	0	-2.653200	1.988248	4.420454
52	1	0	-1.708139	0.762607	2.481714
53	1	0	-2.869321	3.503584	-0.556091
54	1	0	-4.096771	4.133785	-2.589903
55	1	0	-3.534845	3.086493	-4.774696
56	1	0	-1.749324	1.353599	-4.882680
57	1	0	-0.548417	0.687390	-2.836247
58	1	0	1.393113	2.709459	1.794786
59	1	0	3.563274	3.833673	1.510003

60	1	0	4.472915	4.242741	-0.769374
61	1	0	3.178557	3.500670	-2.760689
62	1	0	1.019724	2.365358	-2.483668
63	1	0	-3.983742	-2.863807	0.876196
64	1	0	-4.546201	-4.012481	2.979136
65	1	0	-3.007382	-3.879108	4.930028
66	1	0	-0.893131	-2.577528	4.743571
67	1	0	-0.323474	-1.434719	2.628200
68	1	0	-3.072407	-1.490594	-2.589132
69	1	0	-5.278163	-0.703078	-3.365171
70	1	0	-6.774100	0.549225	-1.823374
71	1	0	-6.032201	1.013896	0.506795
72	1	0	-3.831087	0.229874	1.285280
73	1	0	-2.468824	-4.114618	-0.361711
74	1	0	-1.873150	-5.804928	-2.046005
75	1	0	-0.218669	-5.275181	-3.825885
76	1	0	0.848459	-3.028028	-3.886379
77	1	0	0.259168	-1.332753	-2.168502
78	1	0	5.565460	-1.242150	1.824262
79	1	0	4.024484	-1.839788	2.472771
80	1	0	4.819260	-2.711136	1.136709

- $r(P_A\text{-}C_A)$ = 2.400 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.333114	-0.115593	0.155520
2	15	0	-1.629712	-1.218432	0.019849
3	15	0	-0.520227	1.557890	-0.073261
4	15	0	1.985199	-0.645734	0.478587
5	7	0	3.833972	-0.985172	0.577279
6	15	0	4.569185	-0.228126	-0.711553
7	6	0	4.532086	-1.864678	1.525228
8	17	0	1.526039	-2.716196	0.661639
9	17	0	1.896423	-0.106143	2.572275
10	17	0	6.254455	0.757490	0.192673
11	17	0	5.675817	-1.813426	-1.658572
12	6	0	1.104836	2.406585	-0.356372
13	6	0	1.599797	2.641236	-1.648198
14	6	0	2.823606	3.283726	-1.835508
15	6	0	3.576700	3.697029	-0.736218
16	6	0	3.095011	3.470785	0.553302
17	6	0	1.866260	2.837643	0.743081
18	6	0	-1.177243	2.531147	1.365486
19	6	0	-1.183531	3.936837	1.377148
20	6	0	-1.668645	4.633206	2.483465
21	6	0	-2.139745	3.935671	3.599359
22	6	0	-2.114611	2.541442	3.606526
23	6	0	-1.632586	1.844124	2.495843
24	6	0	-1.548689	2.082156	-1.528910
25	6	0	-2.557471	3.052509	-1.457969
26	6	0	-3.269565	3.423681	-2.600942
27	6	0	-2.982823	2.837263	-3.832773
28	6	0	-1.993040	1.855932	-3.913631
29	6	0	-1.293075	1.474256	-2.770204
30	6	0	-2.090940	-2.092205	1.587329
31	6	0	-3.309010	-2.784502	1.710015
32	6	0	-3.638582	-3.436846	2.897997
33	6	0	-2.762580	-3.398877	3.984878
34	6	0	-1.560459	-2.699985	3.878127
35	6	0	-1.226326	-2.050431	2.687976
36	6	0	-1.256102	-2.554040	-1.209179
37	6	0	-0.320123	-2.287030	-2.216582
38	6	0	-0.045645	-3.233102	-3.204374
39	6	0	-0.701394	-4.464680	-3.193011
40	6	0	-1.627569	-4.745492	-2.186992
41	6	0	-1.903955	-3.797572	-1.201244
42	6	0	-3.289089	-0.598912	-0.535315
43	6	0	-3.755578	-0.805658	-1.840862
44	6	0	-5.001425	-0.312842	-2.234884
45	6	0	-5.797043	0.390740	-1.331213
46	6	0	-5.341069	0.603716	-0.028286
47	6	0	-4.097661	0.113534	0.366559
48	1	0	-0.796680	4.490784	0.526343
49	1	0	-1.670219	5.719993	2.478751
50	1	0	-2.511694	4.479776	4.463476
51	1	0	-2.458756	1.992783	4.479105
52	1	0	-1.582846	0.760015	2.512274
53	1	0	-2.803685	3.517608	-0.510777
54	1	0	-4.051493	4.174418	-2.522799
55	1	0	-3.532735	3.134234	-4.721776
56	1	0	-1.770229	1.379993	-4.864913
57	1	0	-0.549805	0.686486	-2.839393
58	1	0	1.505549	2.674871	1.751977
59	1	0	3.676348	3.781669	1.416460
60	1	0	4.534788	4.187344	-0.882681
61	1	0	3.188431	3.457551	-2.844050
62	1	0	1.030543	2.337089	-2.518348
63	1	0	-4.017077	-2.798101	0.887187
64	1	0	-4.584526	-3.966307	2.975983
65	1	0	-3.021495	-3.904477	4.911452
66	1	0	-0.875387	-2.656212	4.720385
67	1	0	-0.296899	-1.499981	2.618590
68	1	0	-3.150203	-1.357061	-2.552368
69	1	0	-5.348867	-0.483717	-3.250263
70	1	0	-6.768438	0.769228	-1.638221
71	1	0	-5.955908	1.147206	0.684253
72	1	0	-3.761524	0.278747	1.385204
73	1	0	-2.614543	-4.041092	-0.419500
74	1	0	-2.132080	-5.707764	-2.162857
75	1	0	-0.484363	-5.206232	-3.957166
76	1	0	0.691150	-3.012917	-3.972105
77	1	0	0.214214	-1.342341	-2.198337
78	1	0	4.746720	-2.833763	1.062896
79	1	0	5.471001	-1.402516	1.845819
80	1	0	3.902100	-2.019042	2.402811

- $r(P_A\text{-}C_A)$ = 2.300 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.300697	-0.124102	0.166916
2	15	0	-0.507592	1.552512	-0.083904
3	15	0	-1.604981	-1.229698	0.029222
4	15	0	1.925627	-0.603525	0.488837
5	7	0	3.823524	-0.945799	0.627220
6	15	0	4.547617	-0.253530	-0.690521
7	6	0	4.514848	-1.793435	1.604640
8	17	0	1.509924	-2.685111	0.679083
9	17	0	1.844473	-0.057304	2.587209
10	17	0	6.265339	0.754930	0.143661
11	17	0	5.638371	-1.881301	-1.605552
12	6	0	1.113394	2.422034	-0.312105
13	6	0	1.662341	2.641631	-1.584816
14	6	0	2.882308	3.301664	-1.728409
15	6	0	3.575854	3.750665	-0.604286
16	6	0	3.037621	3.543726	0.665821
17	6	0	1.813662	2.891199	0.812322

18	6	0	-1.230415	2.521632	1.322904
19	6	0	-1.291900	3.925997	1.304552
20	6	0	-1.817225	4.625105	2.390338
21	6	0	-2.271189	3.932675	3.516494
22	6	0	-2.188306	2.541224	3.554697
23	6	0	-1.667571	1.840414	2.463784
24	6	0	-1.493406	2.035635	-1.580853
25	6	0	-2.538916	2.968577	-1.552383
26	6	0	-3.219169	3.309817	-2.723577
27	6	0	-2.864202	2.730073	-3.940735
28	6	0	-1.837171	1.785244	-3.979521
29	6	0	-1.167844	1.433409	-2.808588
30	6	0	-2.085957	-2.092417	1.595174
31	6	0	-3.313633	-2.770130	1.704839
32	6	0	-3.662822	-3.419428	2.888648
33	6	0	-2.796996	-3.393110	3.984010
34	6	0	-1.586232	-2.707527	3.890445
35	6	0	-1.231845	-2.060650	2.704693
36	6	0	-1.234441	-2.566981	-1.197804
37	6	0	-0.303459	-2.302644	-2.210673
38	6	0	-0.031666	-3.252601	-3.195131
39	6	0	-0.685266	-4.485186	-3.175320
40	6	0	-1.606216	-4.763087	-2.163867
41	6	0	-1.879990	-3.811574	-1.180913
42	6	0	-3.248031	-0.583377	-0.538561
43	6	0	-3.689159	-0.756745	-1.857789
44	6	0	-4.921547	-0.243333	-2.266134
45	6	0	-5.730275	0.445759	-1.362736
46	6	0	-5.300296	0.624133	-0.045979
47	6	0	-4.069527	0.114257	0.363517
48	1	0	-0.915626	4.477098	0.447275
49	1	0	-1.862361	5.710549	2.362171
50	1	0	-2.674197	4.479325	4.364879
51	1	0	-2.517345	1.997720	4.436224
52	1	0	-1.572615	0.760076	2.505002
53	1	0	-2.838982	3.425160	-0.616769
54	1	0	-4.030504	4.031451	-2.679173
55	1	0	-3.389935	3.004039	-4.851471
56	1	0	-1.560816	1.314728	-4.919299
57	1	0	-0.394900	0.672851	-2.846872
58	1	0	1.411228	2.739451	1.806811
59	1	0	3.572182	3.882865	1.548318
60	1	0	4.532113	4.253149	-0.716797
61	1	0	3.291724	3.459714	-2.722184
62	1	0	1.140312	2.309566	-2.473851
63	1	0	-4.013750	-2.773833	0.875221
64	1	0	-4.615666	-3.937664	2.956572
65	1	0	-3.070658	-3.896980	4.907239
66	1	0	-0.909417	-2.672129	4.739653
67	1	0	-0.295198	-1.521244	2.648087
68	1	0	-3.073772	-1.297026	-2.568805
69	1	0	-5.248624	-0.387594	-3.292231
70	1	0	-6.691917	0.839591	-1.680892
71	1	0	-5.925601	1.155744	0.666348
72	1	0	-3.754609	0.252366	1.392595
73	1	0	-2.584876	-4.054949	-0.393972
74	1	0	-2.108087	-5.726477	-2.132333
75	1	0	-0.469620	-5.230135	-3.936483
76	1	0	0.702839	-3.035026	-3.965664
77	1	0	0.232103	-1.358832	-2.199313
78	1	0	4.731359	-2.778960	1.177901
79	1	0	5.454141	-1.324113	1.915800
80	1	0	3.880580	-1.918181	2.484442

- $r(P_A\text{-}C_A) = 2.200$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.281376	-0.134672	0.152709
2	15	0	-0.480049	1.554447	-0.090494
3	15	0	-1.610539	-1.227172	0.030046
4	15	0	1.847427	-0.603491	0.450038
5	7	0	3.818587	-0.993452	0.621457
6	15	0	4.559424	-0.306350	-0.669852
7	6	0	4.487691	-1.815839	1.630281
8	17	0	1.454095	-2.691471	0.619167
9	17	0	1.807037	-0.075076	2.560942
10	17	0	5.701229	-1.922239	-1.575234
11	17	0	6.270779	0.733995	0.180225
12	6	0	1.147143	2.408586	-0.317914
13	6	0	1.700041	2.618224	-1.590853
14	6	0	2.924341	3.269517	-1.733726
15	6	0	3.617141	3.719943	-0.609751
16	6	0	3.073304	3.525134	0.659711
17	6	0	1.845270	2.881207	0.806700
18	6	0	-1.194288	2.511729	1.324650
19	6	0	-1.264174	3.915911	1.307672
20	6	0	-1.779374	4.610774	2.400843
21	6	0	-2.213354	3.914859	3.532679
22	6	0	-2.119707	2.524105	3.569736
23	6	0	-1.609556	1.826837	2.471705
24	6	0	-1.465454	2.037276	-1.584292
25	6	0	-2.505389	2.976393	-1.555132
26	6	0	-3.179442	3.325745	-2.727420
27	6	0	-2.824040	2.747906	-3.945402
28	6	0	-1.802696	1.797005	-3.984428
29	6	0	-1.138698	1.437525	-2.812840
30	6	0	-2.095718	-2.084498	1.596138
31	6	0	-3.339989	-2.731450	1.708740
32	6	0	-3.697644	-3.380706	2.889850
33	6	0	-2.824260	-3.384548	3.979525
34	6	0	-1.596968	-2.729712	3.882846
35	6	0	-1.233139	-2.083461	2.699601
36	6	0	-1.282451	-2.560953	-1.210378
37	6	0	-0.372652	-2.305632	-2.244712
38	6	0	-0.138507	-3.255949	-3.238210
39	6	0	-0.808882	-4.479253	-3.206402
40	6	0	-1.708801	-4.747780	-2.173866
41	6	0	-1.945158	-3.796253	-1.181338
42	6	0	-3.238413	-0.532045	-0.516958
43	6	0	-3.693966	-0.685931	-1.833862
44	6	0	-4.919298	-0.144828	-2.226774
45	6	0	-5.706526	0.551878	-1.310231
46	6	0	-5.262534	0.709456	0.004436
47	6	0	-4.038689	0.171912	0.399114
48	1	0	-0.901125	4.470293	0.446914
49	1	0	-1.831378	5.695867	2.374011
50	1	0	-2.608168	4.458537	4.386735
51	1	0	-2.431219	1.978219	4.456038
52	1	0	-1.504417	0.747672	2.513608
53	1	0	-2.806623	3.430985	-0.618999
54	1	0	-3.986371	4.052192	-2.683097
55	1	0	-3.344889	3.028455	-4.856879
56	1	0	-1.525812	1.328404	-4.924915
57	1	0	-0.368783	0.674219	-2.851907
58	1	0	1.440357	2.735519	1.800958
59	1	0	3.608064	3.864573	1.541803
60	1	0	4.578421	4.212544	-0.721786
61	1	0	3.339072	3.417389	-2.726721
62	1	0	1.179896	2.283574	-2.479898
63	1	0	-4.045151	-2.712105	0.883708
64	1	0	-4.662700	-3.875383	2.960005
65	1	0	-3.104611	-3.888268	4.900766
66	1	0	-0.913695	-2.718067	4.727420
67	1	0	-0.282500	-1.569609	2.642567

68	1	0	-3.095676	-1.232110	-2.554718	75	1	0	-0.621735	-5.224612	-3.974570
69	1	0	-5.257955	-0.273830	-3.251049	76	1	0	0.580949	-3.046328	-4.024835
70	1	0	-6.662966	0.967074	-1.616545	77	1	0	0.178404	-1.371105	-2.244312
71	1	0	-5.871605	1.245887	0.727031	78	1	0	4.887709	-2.733017	1.182145
72	1	0	-3.713823	0.292788	1.427013	79	1	0	5.311682	-1.260153	2.092957
73	1	0	-2.633175	-4.033008	-0.377757	80	1	0	3.772586	-2.088754	2.409400
74	1	0	-2.222916	-5.704243	-2.132722						

- $r(P_A\text{-}C_A)$ = 2.100 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.271447	-2.075689	2.710887
2	6	0	-2.124808	-2.067026	1.600002
3	6	0	-3.380079	-2.694536	1.702270
4	6	0	-3.758886	-3.332866	2.882609
5	6	0	-2.896203	-3.344945	3.980723
6	6	0	-1.657558	-2.710626	3.893135
7	15	0	-1.617504	-1.234798	0.030939
8	6	0	-0.282156	-0.133015	0.149746
9	15	0	1.746582	-0.575086	0.464066
10	17	0	1.415951	-2.669648	0.632945
11	6	0	-3.222303	-0.515319	-0.542140
12	6	0	-4.030222	0.198402	0.359186
13	6	0	-5.246078	0.739167	-0.055485
14	6	0	-5.672860	0.574592	-1.374967
15	6	0	-4.877263	-0.132261	-2.276528
16	6	0	-3.659962	-0.676619	-1.864261
17	6	0	-1.286053	-2.577779	-1.194215
18	6	0	-0.395110	-2.327578	-2.246415
19	6	0	-0.167221	-3.290039	-3.229408
20	6	0	-0.824598	-4.519357	-3.169215
21	6	0	-1.704751	-4.782172	-2.118513
22	6	0	-1.935268	-3.819264	-1.135680
23	15	0	-0.478556	1.567510	-0.101032
24	6	0	-1.222988	2.512885	1.300675
25	6	0	-1.316949	3.915648	1.271020
26	6	0	-1.848959	4.609893	2.356296
27	6	0	-2.275258	3.915663	3.492105
28	6	0	-2.157249	2.527157	3.541559
29	6	0	-1.631127	1.829415	2.451482
30	6	0	-1.435347	2.028585	-1.615218
31	6	0	-2.487782	2.954202	-1.610323
32	6	0	-3.134975	3.297656	-2.799135
33	6	0	-2.740663	2.726573	-4.008395
34	6	0	-1.707606	1.787592	-4.022627
35	6	0	-1.068902	1.434739	-2.835332
36	6	0	1.157021	2.408019	-0.293414
37	6	0	1.756913	2.577984	-1.551467
38	6	0	2.992034	3.212730	-1.666030
39	6	0	3.648296	3.686157	-0.529528
40	6	0	3.055438	3.534462	0.723497
41	6	0	1.816968	2.906186	0.843814
42	17	0	1.750377	-0.060928	2.580313
43	7	0	3.875072	-0.996583	0.659071
44	15	0	4.585960	-0.353809	-0.642644
45	17	0	5.779931	-1.972857	-1.531194
46	6	0	4.531485	-1.786611	1.693421
47	17	0	6.316973	0.775970	0.129719
48	1	0	-0.958376	4.469457	0.408163
49	1	0	-1.919107	5.693583	2.320563
50	1	0	-2.682528	4.459349	4.340182
51	1	0	-2.461876	1.983249	4.431326
52	1	0	-1.508557	0.752831	2.504171
53	1	0	-2.820478	3.401286	-0.681353
54	1	0	-3.951737	4.013823	-2.774445
55	1	0	-3.240713	3.002897	-4.932626
56	1	0	-1.400377	1.324830	-4.956423
57	1	0	-0.286971	0.683253	-2.856806
58	1	0	1.378086	2.788084	1.827055
59	1	0	3.562477	3.890913	1.615000
60	1	0	4.621463	4.158979	-0.618833
61	1	0	3.446608	3.325333	-2.645825
62	1	0	1.268055	2.221975	-2.449626
63	1	0	-4.074984	-2.670216	0.868903
64	1	0	-4.731568	-3.813238	2.945024
65	1	0	-3.193055	-3.840460	4.901146
66	1	0	-0.981640	-2.706862	4.743524
67	1	0	-0.310391	-1.580588	2.663111
68	1	0	-3.054799	-1.231206	-2.572765
69	1	0	-5.203643	-0.267378	-3.303894
70	1	0	-6.623466	0.991402	-1.696643
71	1	0	-5.862336	1.282639	0.655519
72	1	0	-3.718733	0.322896	1.390570
73	1	0	-2.605929	-4.052560	-0.316548
74	1	0	-2.207002	-5.743544	-2.054506
75	1	0	-0.641147	-5.273906	-3.929109
76	1	0	0.538533	-3.084932	-4.029329
77	1	0	0.147957	-1.389154	-2.270775
78	1	0	4.934663	-2.719948	1.279911
79	1	0	5.356516	-1.223207	2.147937
80	1	0	3.812208	-2.035893	2.478880

Optimized structure of the transition state for the formation of **[1-PCl_2]**[Cl].

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.032674	0.227575	0.357210
2	6	0	-3.226910	-0.488066	-0.544773
3	6	0	-3.655606	-0.629835	-1.872345
4	6	0	-4.860708	-0.063101	-2.289635
5	6	0	-5.653245	0.647263	-1.387957
6	6	0	-5.236034	0.791513	-0.063163
7	15	0	-1.635107	-1.233105	0.028598
8	6	0	-1.319031	-2.574386	-1.200505
9	6	0	-0.420502	-2.337522	-2.249208
10	6	0	-0.208656	-3.301520	-3.234168
11	6	0	-0.889515	-4.518272	-3.178826
12	6	0	-1.777595	-4.767531	-2.131478
13	6	0	-1.992182	-3.803234	-1.146541
14	6	0	-0.289745	-0.136598	0.147262
15	15	0	-0.473734	1.570541	-0.099570
16	6	0	-1.413477	2.033294	-1.621334
17	6	0	-2.455144	2.970717	-1.628658
18	6	0	-3.085662	3.319173	-2.824972
19	6	0	-2.684818	2.741035	-4.028748
20	6	0	-1.661488	1.791285	-4.030743
21	6	0	-1.038713	1.433871	-2.836266

22	6	0	1.168565	2.396023	-0.273209
23	6	0	1.776390	2.578885	-1.525717
24	6	0	3.019689	3.200267	-1.622760
25	6	0	3.674959	3.647301	-0.475059
26	6	0	3.072523	3.484759	0.772151
27	6	0	1.825995	2.870152	0.875761
28	6	0	-1.225380	2.507777	1.301966
29	6	0	-1.315974	3.910999	1.278555
30	6	0	-1.848823	4.601073	2.366052
31	6	0	-2.279355	3.902339	3.497449
32	6	0	-2.163737	2.513487	3.541014
33	6	0	-1.636090	1.819667	2.449266
34	6	0	-2.149435	-2.061149	1.596510
35	6	0	-3.414526	-2.669048	1.699964
36	6	0	-3.799399	-3.306771	2.878644
37	6	0	-2.933185	-3.338310	3.973664
38	6	0	-1.684569	-2.724190	3.884490
39	6	0	-1.292195	-2.089777	2.704045
40	15	0	1.706741	-0.586500	0.464587
41	17	0	1.739012	-0.105495	2.588961
42	7	0	3.907258	-1.036599	0.649322
43	6	0	4.554423	-1.838230	1.677443
44	17	0	1.389848	-2.681736	0.610060
45	15	0	4.609290	-0.367750	-0.633026
46	17	0	6.333756	0.794360	0.151250
47	17	0	5.844129	-1.953225	-1.549863
48	1	0	-0.953569	4.468903	0.420009
49	1	0	-1.915712	5.685087	2.335578
50	1	0	-2.687216	4.442884	4.347205
51	1	0	-2.470670	1.966249	4.427895
52	1	0	-1.513383	0.743085	2.499186
53	1	0	-2.792595	3.422466	-0.703675
54	1	0	-3.894280	4.044742	-2.810514
55	1	0	-3.171877	3.021018	-4.958772
56	1	0	-1.348920	1.324228	-4.960568
57	1	0	-0.262422	0.676206	-2.848389
58	1	0	1.378613	2.742803	1.854028
59	1	0	3.579057	3.820632	1.671768
60	1	0	4.655583	4.106472	-0.550892
61	1	0	3.482180	3.321282	-2.597761
62	1	0	1.288350	2.242414	-2.431837
63	1	0	-4.112020	-2.630785	0.869101
64	1	0	-4.779528	-3.771556	2.942123
65	1	0	-3.234950	-3.833264	4.892744
66	1	0	-1.005361	-2.735786	4.732121
67	1	0	-0.322905	-1.611344	2.656434
68	1	0	-3.052512	-1.185450	-2.581704
69	1	0	-5.179661	-0.182741	-3.321169
70	1	0	-6.594198	1.082300	-1.713747
71	1	0	-5.850394	1.336973	0.647903
72	1	0	-3.730836	0.335488	1.393213
73	1	0	-2.669100	-4.025067	-0.329408
74	1	0	-2.298182	-5.719318	-2.071693
75	1	0	-0.718069	-5.274128	-3.940187
76	1	0	0.503221	-3.107920	-4.031432
77	1	0	0.141444	-1.410269	-2.269178
78	1	0	4.982741	-2.755099	1.251470
79	1	0	5.360913	-1.274251	2.164634
80	1	0	3.823881	-2.119733	2.442182

Optimized structure for **[1-PCl_2]**[Cl].

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.579498	0.192128	-1.850252
2	6	0	3.001512	-0.459007	-0.749274
3	6	0	3.588314	-1.639510	-0.257500
4	6	0	4.727658	-2.158243	-0.868044
5	6	0	5.299449	-1.504669	-1.960164
6	6	0	4.724596	-0.330977	-2.447599
7	15	0	1.534282	0.222919	0.127570
8	6	0	1.939126	-0.133180	1.884133
9	6	0	3.088474	0.416145	2.480724
10	6	0	3.429695	0.079180	3.788983
11	6	0	2.644929	-0.827404	4.507284
12	6	0	1.529418	-1.408467	3.905964
13	6	0	1.179077	-1.068125	2.597041
14	6	0	0.045708	-0.523843	-0.456906
15	15	0	0.454138	-1.827705	-1.697360
16	17	0	-1.468425	-2.543624	-2.210640
17	15	0	-1.550897	-0.013351	0.098517
18	6	0	-2.413245	-1.160587	1.253103
19	6	0	-3.451999	-0.679148	2.073486
20	6	0	-4.142324	-1.547254	2.917346
21	6	0	-3.802638	-2.902212	2.958210
22	6	0	-2.770838	-3.381625	2.153076
23	6	0	-2.078048	-2.519887	1.298808
24	6	0	1.554582	2.042466	-0.133507
25	6	0	1.856248	2.966907	0.875777
26	6	0	1.891887	4.332488	0.588451
27	6	0	1.627731	4.787374	-0.703343
28	6	0	1.308358	3.872045	-1.708322
29	6	0	1.262153	2.506492	-1.429187
30	6	0	-2.733014	0.325136	-1.263662
31	6	0	-2.266181	0.915336	-2.446163
32	6	0	-3.163775	1.254384	-3.458903
33	6	0	-4.527721	1.009431	-3.302181
34	6	0	-4.994771	0.411290	-2.130297
35	6	0	-4.104664	0.066363	-1.114466
36	6	0	-1.484258	1.559609	1.060959
37	6	0	-1.808396	2.780528	0.450887
38	6	0	-1.801833	3.962003	1.192157
39	6	0	-1.476794	3.939630	2.548842
40	6	0	-1.154867	2.729083	3.164547
41	6	0	-1.160851	1.544828	2.428097
42	17	0	0.642384	-0.250635	-3.737887
43	17	0	0.871950	-3.724729	-0.047447
44	1	0	3.730479	1.089294	1.920828
45	1	0	4.316874	0.512862	4.241989
46	1	0	2.917900	-1.094996	5.524422
47	1	0	0.936196	-2.142586	4.443361
48	1	0	0.343461	-1.563034	2.116665
49	1	0	2.041026	2.635673	1.890373
50	1	0	2.122484	5.039389	1.380738
51	1	0	1.662989	5.850841	-0.924482
52	1	0	1.092763	4.216667	-2.715882
53	1	0	1.006362	1.801986	-2.219326
54	1	0	3.140031	-2.174132	0.570639
55	1	0	5.158873	-3.080876	-0.491341
56	1	0	6.188314	-1.912313	-2.434207
57	1	0	5.157843	0.178236	-3.303318
58	1	0	3.143446	1.095573	-2.253392
59	1	0	-3.720778	0.372453	2.061695
60	1	0	-4.941453	-1.163089	3.545537
61	1	0	-4.339688	-3.577194	3.619385
62	1	0	-2.491867	-4.430976	2.179408
63	1	0	-1.266786	-2.917298	0.697316
64	1	0	-2.074354	2.810469	-0.599623
65	1	0	-2.057547	4.899201	0.706300

66	1	0	-1.480411	4.860546	3.125726
67	1	0	-0.907725	2.700728	4.222173
68	1	0	-0.928088	0.610824	2.926378
69	1	0	-4.482320	-0.418780	-0.222257
70	1	0	-6.053399	0.199142	-2.008400
71	1	0	-5.223613	1.267737	-4.095909
72	1	0	-2.783219	1.686482	-4.379650
73	1	0	-1.204262	1.049775	-2.613120

- Optimized structure for MeNPCl (monomer):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.985732	-0.868401	0.000000
2	7	0	1.341052	0.416615	-0.000001
3	15	0	-0.072491	1.013551	0.000000
4	17	0	-1.573942	-0.548323	0.000000
5	1	0	2.633592	-0.941682	-0.881741
6	1	0	2.633552	-0.941698	0.881769
7	1	0	1.275486	-1.704304	-0.000023

Optimized structure for **2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.845483	0.697614	-0.793633
2	6	0	3.544220	0.449159	-0.375682
3	6	0	3.253040	-0.606569	0.515496
4	6	0	4.257487	-1.430677	1.005661
5	6	0	5.574801	-1.175380	0.587907
6	6	0	5.862330	-0.133173	-0.293872
7	7	0	2.344947	1.075471	-0.671497
8	6	0	1.274534	0.448568	-0.005264
9	7	0	1.880843	-0.594226	0.728145
10	6	0	0.000001	0.864214	-0.000021
11	6	0	-1.274532	0.448568	0.005242
12	7	0	-2.344934	1.075465	0.671498
13	6	0	-3.544213	0.449160	0.375693
14	6	0	-3.253048	-0.606558	-0.515500
15	7	0	-1.880854	-0.594217	-0.728168
16	6	0	-4.845470	0.697612	0.793666
17	6	0	-5.862325	-0.133167	0.293910
18	6	0	-5.574811	-1.175365	-0.587885
19	6	0	-4.257504	-1.430659	-1.005661
20	6	0	-2.176351	2.222266	1.531505
21	6	0	-1.170735	-1.465237	-1.633562
22	6	0	2.176380	2.222282	-1.531492
23	6	0	1.170711	-1.465259	1.633515
24	1	0	0.217808	-0.995495	1.887081
25	1	0	0.973160	-2.450940	1.191094
26	1	0	1.753871	-1.604938	2.550536
27	1	0	-1.753911	-1.604905	-2.550574
28	1	0	-0.217838	-0.995467	-1.887137
29	1	0	-0.973174	-2.450923	-1.191157
30	1	0	2.916696	2.992636	-1.286478
31	1	0	2.280997	1.956863	-2.591943
32	1	0	1.170021	2.612261	-1.358528
33	1	0	-2.916673	2.992621	1.286515
34	1	0	-2.280946	1.956833	2.591955
35	1	0	-1.169996	2.612248	1.358524
36	1	0	5.071537	1.504373	-1.484118
37	1	0	6.888271	0.040642	-0.605802
38	1	0	6.378203	-1.806959	0.956209
39	1	0	4.036241	-2.249398	1.683646
40	1	0	-5.071512	1.504365	1.484164
41	1	0	-6.888262	0.040647	0.605857
42	1	0	-6.378220	-1.806938	-0.956183
43	1	0	-4.036269	-2.249373	-1.683658

Partially optimized structures as **2** is approaching P_A of $MeN(PCl_2)_2$.

- $r(P_A\text{-}C_A)$ = 4.000 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.683685	0.901238	-0.560175
2	6	0	-5.420082	0.453225	-0.197519
3	6	0	-5.159863	-0.919877	0.000291
4	6	0	-6.159445	-1.870533	-0.166045
5	6	0	-7.438447	-1.417225	-0.527648
6	6	0	-7.696139	-0.059234	-0.720223
7	7	0	-4.229710	1.131021	0.033083
8	6	0	-3.204778	0.225060	0.375835
9	7	0	-3.825606	-1.034589	0.356854
10	6	0	-1.943529	0.474486	0.768247
11	15	0	1.474987	-1.506587	0.144475
12	17	0	0.651328	-2.730366	-1.376115
13	6	0	-3.134413	-2.260038	0.684992
14	6	0	-4.072387	2.565852	0.016494
15	6	0	-0.892938	1.269819	0.514868
16	7	0	0.015953	1.762317	1.471913
17	6	0	1.060143	2.434207	0.860409
18	6	0	0.830941	2.379427	-0.532900
19	7	0	-0.354024	1.681915	-0.724206
20	6	0	1.715852	2.964714	-1.429822
21	6	0	2.850233	3.608403	-0.904543

22	6	0	3.075057	3.664567	0.471597
23	6	0	2.176529	3.078364	1.379778
24	6	0	-0.151464	1.565680	2.893052
25	6	0	-0.921666	1.338428	-2.007263
26	17	0	1.274153	-2.834769	1.776156
27	7	0	3.154725	-1.651569	-0.193693
28	6	0	3.883036	-2.933895	-0.298610
29	15	0	3.897223	-0.095392	-0.253405
30	17	0	4.973231	-0.241963	-2.068998
31	17	0	5.498341	-0.371044	1.100923
32	1	0	-1.575972	0.473902	-1.875776
33	1	0	-1.505185	2.164145	-2.435477
34	1	0	-0.123199	1.074427	-2.708962
35	1	0	-4.955347	3.040726	0.457907
36	1	0	-3.195244	2.824952	0.613571
37	1	0	-3.936627	2.956885	-1.000737
38	1	0	0.789833	1.232103	3.344348
39	1	0	-0.477679	2.485622	3.395812
40	1	0	-0.914787	0.794785	3.025577
41	1	0	-3.793474	-2.912100	1.267667
42	1	0	-2.801350	-2.798637	-0.211527
43	1	0	-2.258251	-1.996440	1.282928
44	1	0	2.349948	3.131468	2.450129
45	1	0	3.954392	4.175425	0.853138
46	1	0	3.555340	4.075934	-1.585611
47	1	0	1.537296	2.936690	-2.500355
48	1	0	-5.961063	-2.928520	-0.025360
49	1	0	-8.236830	-2.141111	-0.663778
50	1	0	-8.692828	0.265087	-1.005362
51	1	0	-6.884743	1.955837	-0.722285
52	1	0	4.737999	-2.807985	-0.965579
53	1	0	4.228563	-3.253664	0.687828
54	1	0	3.219071	-3.691093	-0.720118

- $r(P_A\text{-}C_A) = 3.500$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.071686	4.477516	1.408999
2	6	0	1.839605	3.398787	0.564622
3	6	0	1.420548	3.590843	-0.767923
4	6	0	1.224904	4.866006	-1.285109
5	6	0	1.456374	5.955443	-0.431863
6	6	0	1.870544	5.765286	0.888743
7	7	0	1.947623	2.027625	0.762172
8	6	0	1.599775	1.333630	-0.407177
9	7	0	1.284506	2.333819	-1.334506
10	6	0	1.449964	-0.005080	-0.600564
11	15	0	-1.954754	-0.054647	0.209025
12	17	0	-1.883021	2.051160	0.199492
13	6	0	0.845988	2.060282	-2.684395
14	6	0	2.232668	1.392657	2.030556
15	6	0	2.265648	-1.061341	-0.399135
16	7	0	1.868505	-2.406225	-0.306208
17	6	0	2.966832	-3.240310	-0.174932
18	6	0	4.116110	-2.422686	-0.209883
19	7	0	3.678849	-1.111064	-0.350366
20	6	0	5.389097	-2.969521	-0.108485
21	6	0	5.494072	-4.364066	0.024014
22	6	0	4.357163	-5.172192	0.060292
23	6	0	3.069997	-4.619039	-0.035397
24	6	0	0.495517	-2.837550	-0.413367
25	6	0	4.541651	0.024554	-0.578547
26	17	0	-1.335500	-0.409144	2.201762
27	7	0	-3.666061	-0.290943	0.391532
28	6	0	-4.497043	0.305384	1.458273
29	15	0	-4.228887	-1.440916	-0.742470
30	17	0	-5.909505	-0.450506	-1.554995
31	17	0	-5.229452	-2.821990	0.506051
32	1	0	4.033543	0.735152	-1.235075
33	1	0	4.814222	0.540854	0.351176
34	1	0	5.458670	-0.312543	-1.071360
35	1	0	1.709283	1.921834	2.833741
36	1	0	1.869938	0.364137	1.987402
37	1	0	3.307027	1.386131	2.253459
38	1	0	-0.052566	-2.068669	-0.962844
39	1	0	0.450195	-3.783302	-0.963475
40	1	0	0.027202	-2.975709	0.569914
41	1	0	-0.102964	2.569803	-2.887249
42	1	0	1.590680	2.387798	-3.420650
43	1	0	0.707300	0.979641	-2.764742
44	1	0	2.187450	-5.250042	0.003178
45	1	0	4.463847	-6.247529	0.170860
46	1	0	6.478914	-4.814701	0.107328
47	1	0	6.276730	-2.344371	-0.122000
48	1	0	0.904255	5.016025	-2.311317
49	1	0	1.311827	6.963506	-0.809676
50	1	0	2.045524	6.626847	1.526611
51	1	0	2.401413	4.333713	2.433278
52	1	0	-5.518705	0.430336	1.093708
53	1	0	-4.496669	-0.338217	2.341870
54	1	0	-4.095904	1.286821	1.717533

- $r(P_A\text{-}C_A) = 3.000$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.661243	4.246143	1.356195
2	6	0	2.214364	3.204631	0.551212
3	6	0	1.810295	3.429813	-0.779140
4	6	0	1.842058	4.702586	-1.337983
5	6	0	2.290883	5.753583	-0.526571
6	6	0	2.691931	5.530134	0.794421
7	7	0	2.068975	1.843908	0.792737
8	6	0	1.575575	1.195988	-0.342521
9	7	0	1.436093	2.200483	-1.299338
10	6	0	1.158002	-0.105492	-0.481685
11	15	0	-1.757584	0.106700	0.192360
12	17	0	-1.547364	2.212137	0.260246
13	6	0	0.922281	1.975965	-2.633479
14	6	0	2.285795	1.207321	2.075849
15	6	0	1.876467	-1.246359	-0.348608
16	7	0	1.361025	-2.551703	-0.286175
17	6	0	2.381688	-3.485628	-0.190896
18	6	0	3.599187	-2.776425	-0.224032
19	7	0	3.282293	-1.426736	-0.329191
20	6	0	4.818199	-3.439611	-0.154904
21	6	0	4.796994	-4.840450	-0.057792
22	6	0	3.591354	-5.542132	-0.024295
23	6	0	2.359712	-4.871223	-0.086581
24	6	0	-0.035822	-2.872285	-0.465807
25	6	0	4.249480	-0.383375	-0.583375
26	17	0	-1.189638	-0.359548	2.186122
27	7	0	-3.501864	0.032734	0.427925
28	6	0	-4.254532	0.653979	1.535215
29	15	0	-4.187230	-0.993722	-0.741755
30	17	0	-5.789904	0.182170	-1.477458
31	17	0	-5.304349	-2.343972	0.452140

32	1	0	3.828112	0.345959	-1.279751
33	1	0	4.556046	0.142539	0.329661
34	1	0	5.137348	-0.826192	-1.043670
35	1	0	1.805072	1.793066	2.866317
36	1	0	1.835101	0.215095	2.045493
37	1	0	3.354971	1.115444	2.302494
38	1	0	-0.486324	-2.101828	-1.095504
39	1	0	-0.121121	-3.840955	-0.967878
40	1	0	-0.577380	-2.919026	0.487065
41	1	0	0.034201	2.593260	-2.809445
42	1	0	1.679452	2.212874	-3.390461
43	1	0	0.653669	0.919901	-2.702969
44	1	0	1.424081	-5.420269	-0.047623
45	1	0	3.600116	-6.625082	0.059134
46	1	0	5.737458	-5.380792	0.000501
47	1	0	5.759564	-2.898763	-0.166222
48	1	0	1.530014	4.878406	-2.362623
49	1	0	2.327021	6.759283	-0.935041
50	1	0	3.036301	6.364168	1.398867
51	1	0	2.977100	4.075098	2.380524
52	1	0	-5.255523	0.923568	1.190530
53	1	0	-4.330016	-0.039082	2.377553
54	1	0	-3.738281	1.561500	1.853088

- $r(P_A\text{-}C_A) = 2.500$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.004742	-3.494807	0.926163
2	6	0	-3.245945	-2.421119	0.470483
3	6	0	-3.216814	-2.070682	-0.891343
4	6	0	-3.938561	-2.788396	-1.839878
5	6	0	-4.698589	-3.871472	-1.383699
6	6	0	-4.732978	-4.216084	-0.026544
7	7	0	-2.430229	-1.516441	1.135242
8	6	0	-1.882496	-0.610702	0.243548
9	7	0	-2.387578	-0.960698	-1.002780
10	6	0	-0.899527	0.333097	0.536317
11	15	0	1.376529	-0.684010	0.349046
12	17	0	0.497642	-2.481582	-0.389355
13	6	0	-1.944696	-0.396513	-2.263820
14	6	0	-2.228169	-1.480574	2.572088
15	6	0	-1.042816	1.673230	0.313680
16	7	0	-0.053061	2.662406	0.435893
17	6	0	-0.564277	3.911876	0.106673
18	6	0	-1.927728	3.743442	-0.190486
19	7	0	-2.213625	2.388913	-0.043122
20	6	0	-2.725589	4.824131	-0.546974
21	6	0	-2.124261	6.091284	-0.594456
22	6	0	-0.770184	6.258284	-0.298947
23	6	0	0.034838	5.165105	0.054943
24	6	0	1.234655	2.490773	1.079671
25	6	0	-3.565344	1.871837	0.011829
26	17	0	1.364104	-1.110225	2.445662
27	7	0	3.093836	-1.285701	0.126276
28	6	0	3.682431	-2.526733	0.655207
29	15	0	3.952650	-0.118505	-0.720682
30	17	0	4.879276	-1.240305	-2.282644
31	17	0	5.685317	0.173143	0.494437
32	1	0	-3.885033	1.410157	-0.929697
33	1	0	-3.647425	1.129421	0.809359
34	1	0	-4.244892	2.696697	0.242960
35	1	0	-1.760927	-2.408718	2.914817
36	1	0	-1.564321	-0.645165	2.793280
37	1	0	-3.187001	-1.345465	3.086106
38	1	0	2.037225	2.293983	0.360913
39	1	0	1.474648	3.404233	1.633704
40	1	0	1.170095	1.666406	1.791946
41	1	0	-1.607461	-1.198470	-2.928225
42	1	0	-2.750530	0.161609	-2.753749
43	1	0	-1.111360	0.277186	-2.063551
44	1	0	1.090028	5.297713	0.271258
45	1	0	-0.325544	7.247777	-0.350645
46	1	0	-2.725017	6.951540	-0.874853
47	1	0	-3.776050	4.699600	-0.791041
48	1	0	-3.916522	-2.521202	-2.891570
49	1	0	-5.272849	-4.453604	-2.098217
50	1	0	-5.334276	-5.061103	0.295360
51	1	0	-4.027431	-3.767765	1.976248
52	1	0	4.368261	-2.957272	-0.080230
53	1	0	4.224606	-2.326270	1.584339
54	1	0	2.885692	-3.246294	0.851050

- $r(P_A\text{-}C_A) = 2.400$ Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.129554	-3.359321	0.928663
2	6	0	-3.326888	-2.318303	0.471341
3	6	0	-3.297658	-1.958298	-0.887505
4	6	0	-4.063819	-2.633240	-1.833198
5	6	0	-4.867805	-3.682636	-1.375738
6	6	0	-4.901952	-4.036885	-0.020397
7	7	0	-2.462259	-1.457246	1.132900
8	6	0	-1.884408	-0.574366	0.241332
9	7	0	-2.417649	-0.888306	-1.000101
10	6	0	-0.849469	0.323519	0.526528
11	15	0	1.318907	-0.687988	0.339449
12	17	0	0.418420	-2.467437	-0.426382
13	6	0	-1.962083	-0.336840	-2.263114
14	6	0	-2.248110	-1.440625	2.569228
15	6	0	-0.956739	1.672678	0.318640
16	7	0	0.060357	2.632864	0.437690
17	6	0	-0.417909	3.895148	0.104524
18	6	0	-1.786208	3.764533	-0.184760
19	7	0	-2.110008	2.418802	-0.029725
20	6	0	-2.555811	4.865751	-0.540769
21	6	0	-1.919115	6.114864	-0.596233
22	6	0	-0.559121	6.244526	-0.308243
23	6	0	0.216459	5.130673	0.045795
24	6	0	1.339929	2.441779	1.096340
25	6	0	-3.478690	1.949309	0.049083
26	17	0	1.311760	-1.141776	2.435941
27	7	0	3.041577	-1.363127	0.124754
28	6	0	3.583927	-2.627556	0.643157
29	15	0	3.937557	-0.226145	-0.710177
30	17	0	4.840914	-1.364295	-2.281295
31	17	0	5.684970	0.008771	0.506633
32	1	0	-3.831019	1.498639	-0.885872
33	1	0	-3.574639	1.212216	0.849756
34	1	0	-4.123545	2.798762	0.290260
35	1	0	-1.794610	-2.380198	2.898246
36	1	0	-1.567978	-0.620399	2.796219
37	1	0	-3.201939	-1.294803	3.089074
38	1	0	2.146387	2.230399	0.386897
39	1	0	1.586709	3.354000	1.649653
40	1	0	1.256927	1.622773	1.812530
41	1	0	-1.664561	-1.149568	-2.933000

42	1	0	-2.749055	0.256214	-2.742170
43	1	0	-1.099393	0.300097	-2.068135
44	1	0	1.276045	5.234054	0.256082
45	1	0	-0.087009	7.220805	-0.366252
46	1	0	-2.496563	6.990763	-0.877021
47	1	0	-3.610611	4.770075	-0.778923
48	1	0	-4.041384	-2.359043	-2.883018
49	1	0	-5.477181	-4.231717	-2.087259
50	1	0	-5.538168	-4.855741	0.301837
51	1	0	-4.151668	-3.640317	1.976582
52	1	0	4.215819	-3.103297	-0.113214
53	1	0	4.174126	-2.448805	1.547571
54	1	0	2.759262	-3.301576	0.881139

- $r(P_A\text{-}C_A)$ = 2.300 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.740314	-2.151285	1.599202
2	6	0	-3.727789	-1.634965	0.794415
3	6	0	-3.583056	-2.032817	-0.545259
4	6	0	-4.449065	-2.955219	-1.126539
5	6	0	-5.465128	-3.475290	-0.319669
6	6	0	-5.606344	-3.082450	1.018836
7	7	0	-2.725072	-0.706815	1.044831
8	6	0	-1.954939	-0.509353	-0.091245
9	7	0	-2.501375	-1.329855	-1.061166
10	6	0	-0.777157	0.249797	-0.163685
11	15	0	1.270716	-0.794071	-0.082705
12	17	0	0.597465	-2.371460	-1.340864
13	6	0	-2.176104	-1.292521	-2.476982
14	6	0	-2.492798	-0.076990	2.332188
15	6	0	-0.767836	1.622920	-0.092125
16	7	0	0.264928	2.469412	0.330864
17	6	0	-0.086847	3.801541	0.121042
18	6	0	-1.389493	3.819111	-0.401390
19	7	0	-1.796558	2.490767	-0.514128
20	6	0	-2.031298	5.018247	-0.690078
21	6	0	-1.327779	6.207235	-0.450577
22	6	0	-0.031379	6.188591	0.068999
23	6	0	0.612017	4.978417	0.363348
24	6	0	1.361845	2.119763	1.221585
25	6	0	-2.964640	2.070299	-1.258942
26	17	0	0.726070	-1.621270	1.838425
27	7	0	3.005944	-1.570011	0.044973
28	6	0	3.354757	-2.940192	0.440522
29	15	0	4.115179	-0.378421	-0.287882
30	17	0	5.426470	-1.288530	-1.720234
31	17	0	5.459640	-0.451096	1.392492
32	1	0	-2.674311	1.394178	-2.069154
33	1	0	-3.703097	1.568467	-0.624501
34	1	0	-3.434218	2.951141	-1.699776
35	1	0	-2.579804	-0.825769	3.124295
36	1	0	-1.482264	0.328568	2.337368
37	1	0	-3.214892	0.727599	2.512215
38	1	0	2.307809	2.003663	0.685143
39	1	0	1.471878	2.913696	1.968614
40	1	0	1.126997	1.191114	1.743487
41	1	0	-1.906254	-2.289166	-2.833273
42	1	0	-3.039481	-0.924562	-3.045084
43	1	0	-1.325851	-0.627183	-2.617197
44	1	0	1.624477	4.965208	0.753499
45	1	0	0.491886	7.123591	0.245342
46	1	0	-1.804986	7.157027	-0.673315
47	1	0	-3.043939	5.045675	-1.080213
48	1	0	-4.338993	-3.263665	-2.161031
49	1	0	-6.157041	-4.198995	-0.739749
50	1	0	-6.405569	-3.507387	1.618592
51	1	0	-4.857341	-1.843833	2.633249
52	1	0	4.115485	-3.346639	-0.234028
53	1	0	3.736742	-2.958616	1.466748
54	1	0	2.465407	-3.570218	0.381190

- $r(P_A\text{-}C_A)$ = 2.200 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.762367	-2.036836	1.644326
2	6	0	-3.740102	-1.572582	0.819582
3	6	0	-3.609675	-2.018064	-0.505793
4	6	0	-4.499800	-2.937981	-1.054632
5	6	0	-5.524806	-3.405548	-0.228387
6	6	0	-5.651852	-2.965019	1.097323
7	7	0	-2.713049	-0.662353	1.035796
8	6	0	-1.945174	-0.522815	-0.107743
9	7	0	-2.513698	-1.358108	-1.048812
10	6	0	-0.746134	0.212465	-0.205943
11	15	0	1.222044	-0.767113	-0.124080
12	17	0	0.616252	-2.326098	-1.437708
13	6	0	-2.215237	-1.360774	-2.472482
14	6	0	-2.456394	-0.003835	2.305014
15	6	0	-0.735109	1.591439	-0.119469
16	7	0	0.286145	2.432412	0.330751
17	6	0	-0.064685	3.766169	0.124389
18	6	0	-1.357720	3.784810	-0.419038
19	7	0	-1.756887	2.455669	-0.554336
20	6	0	-2.000304	4.983937	-0.707239
21	6	0	-1.304483	6.172019	-0.446179
22	6	0	-0.015655	6.152573	0.093823
23	6	0	0.627208	4.942999	0.388175
24	6	0	1.372688	2.083322	1.238042
25	6	0	-2.900588	2.041306	-1.341222
26	17	0	0.679751	-1.664616	1.772314
27	7	0	3.005510	-1.581293	0.022545
28	6	0	3.338802	-2.963366	0.377561
29	15	0	4.112988	-0.387942	-0.242287
30	17	0	5.487083	-1.245752	-1.660888
31	17	0	5.425869	-0.487080	1.476766
32	1	0	-2.584585	1.342924	-2.121641
33	1	0	-3.676732	1.567486	-0.730660
34	1	0	-3.330919	2.921290	-1.822308
35	1	0	-2.596024	-0.720973	3.118124
36	1	0	-1.423627	0.340404	2.311981
37	1	0	-3.131804	0.846800	2.449974
38	1	0	2.326112	1.973368	0.714807
39	1	0	1.464763	2.875749	1.988800
40	1	0	1.136531	1.151214	1.753016
41	1	0	-1.950479	-2.366486	-2.805427
42	1	0	-3.092681	-1.010823	-3.029962
43	1	0	-1.369317	-0.699736	-2.650494
44	1	0	1.633328	4.929743	0.794082
45	1	0	0.501337	7.087798	0.286323
46	1	0	-1.780623	7.122526	-0.667799
47	1	0	-3.006819	5.010783	-1.112792
48	1	0	-4.400218	-3.283719	-2.078261
49	1	0	-6.235475	-4.125960	-0.621822
50	1	0	-6.458941	-3.350776	1.712729
51	1	0	-4.868737	-1.692639	2.667822

52	1	0	4.073000	-3.371749	-0.325744
53	1	0	3.749723	-3.013773	1.392172
54	1	0	2.436632	-3.576931	0.332108

- $r(P_A\text{-}C_A)$ = 2.100 Å

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.767435	-1.964347	1.684478
2	6	0	-3.742213	-1.538368	0.842064
3	6	0	-3.626462	-2.019683	-0.471410
4	6	0	-4.534007	-2.939429	-0.992561
5	6	0	-5.560891	-3.368336	-0.149300
6	6	0	-5.673643	-2.891406	1.165930
7	7	0	-2.697817	-0.641012	1.029010
8	6	0	-1.938160	-0.545017	-0.120857
9	7	0	-2.523613	-1.390588	-1.037708
10	6	0	-0.724229	0.177712	-0.243559
11	15	0	1.162946	-0.739969	-0.163356
12	17	0	0.638412	-2.292939	-1.515190
13	6	0	-2.245096	-1.429300	-2.466453
14	6	0	-2.417896	0.038485	2.283496
15	6	0	-0.721054	1.563924	-0.147101
16	7	0	0.284847	2.406591	0.321272
17	6	0	-0.077778	3.739129	0.123039
18	6	0	-1.365977	3.748369	-0.429792
19	7	0	-1.746421	2.415299	-0.585330
20	6	0	-2.022148	4.941942	-0.711757
21	6	0	-1.342062	6.134523	-0.435091
22	6	0	-0.055673	6.124813	0.113202
23	6	0	0.599744	4.921572	0.401328
24	6	0	1.384102	2.061369	1.218364
25	6	0	-2.872460	1.998368	-1.398072
26	17	0	0.649213	-1.705589	1.709304
27	7	0	3.040735	-1.587892	-0.001393
28	6	0	3.369139	-2.974053	0.324160
29	15	0	4.124602	-0.384402	-0.207565
30	17	0	5.582299	-1.177339	-1.600295
31	17	0	5.411024	-0.467400	1.555615
32	1	0	-2.537992	1.286326	-2.157450
33	1	0	-3.669906	1.540798	-0.802878
34	1	0	-3.279675	2.874829	-1.905150
35	1	0	-2.599171	-0.650796	3.111822
36	1	0	-1.369350	0.330382	2.293274
37	1	0	-3.052371	0.923968	2.400138
38	1	0	2.330187	1.946533	0.683955
39	1	0	1.482197	2.859092	1.961973
40	1	0	1.155438	1.132439	1.742675
41	1	0	-1.978750	-2.441708	-2.775956
42	1	0	-3.134872	-1.099837	-3.016276
43	1	0	-1.406301	-0.769192	-2.676419
44	1	0	1.603463	4.916904	0.812942
45	1	0	0.448847	7.064387	0.316837
46	1	0	-1.827125	7.081720	-0.651026
47	1	0	-3.025874	4.959955	-1.124462
48	1	0	-4.445076	-3.313634	-2.007031
49	1	0	-6.285029	-4.087502	-0.519581
50	1	0	-6.483237	-3.248760	1.794922
51	1	0	-4.862774	-1.592669	2.699327
52	1	0	4.093141	-3.378147	-0.393482
53	1	0	3.792849	-3.048500	1.333020
54	1	0	2.463113	-3.583862	0.280656

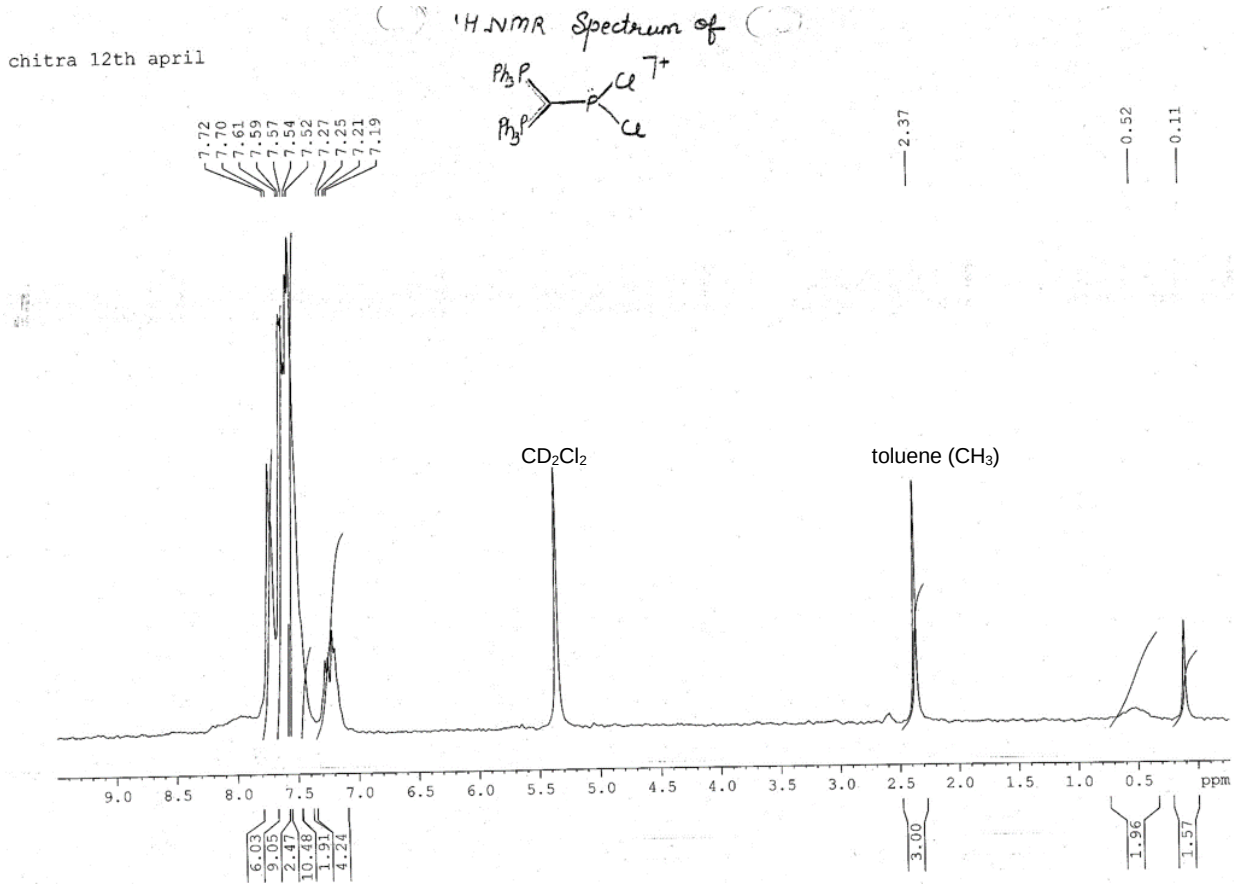
Optimized structure of the transition state for the formation of **[2-PCl$_2$]**[Cl].

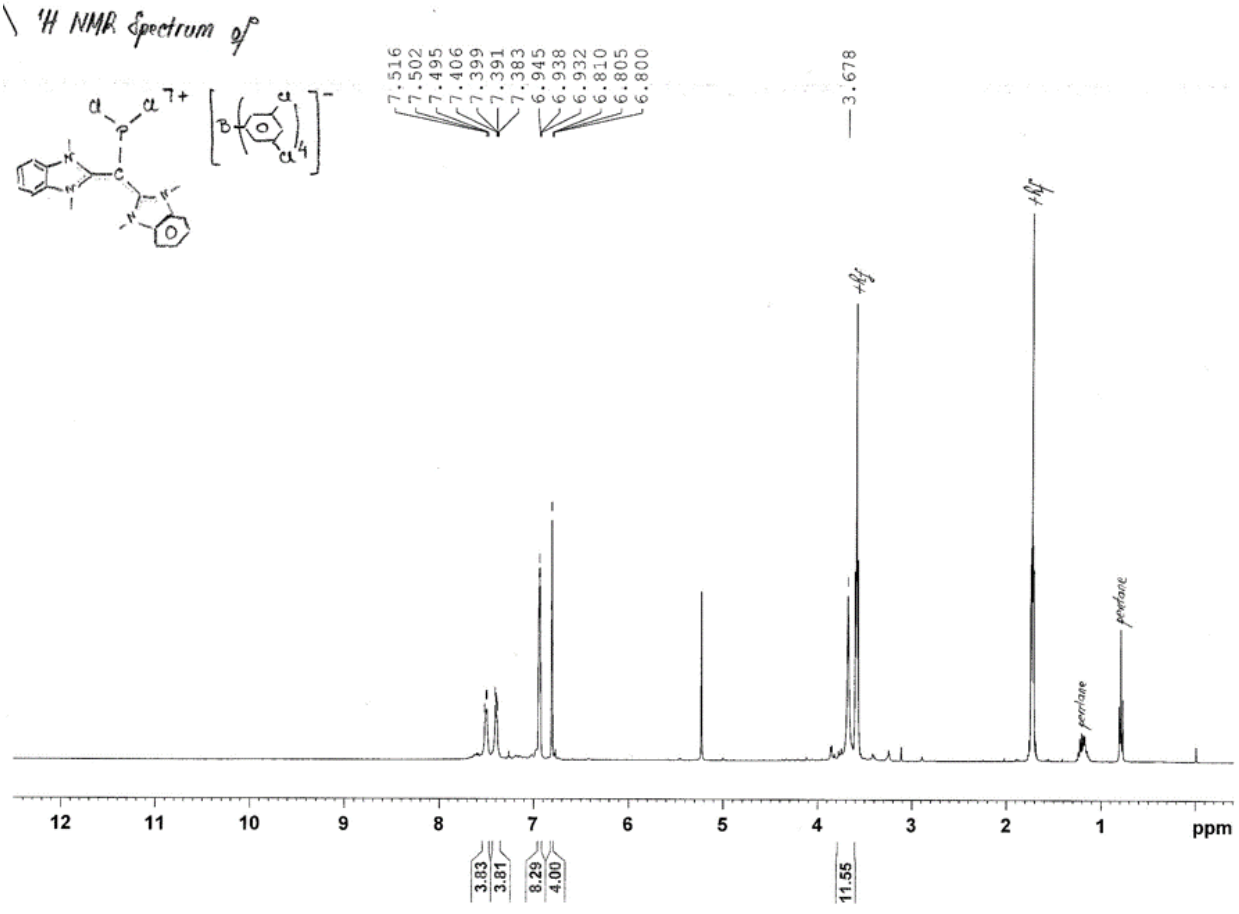
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.769103	4.835777	0.359264
2	6	0	0.049980	3.678221	0.076878
3	6	0	-1.243950	3.734949	-0.457442
4	6	0	-1.869283	4.950983	-0.714798
5	6	0	-1.148946	6.116819	-0.432611
6	6	0	0.145887	6.060076	0.096014
7	7	0	0.371917	2.331441	0.252712
8	6	0	-0.662921	1.534815	-0.214726
9	7	0	-1.664022	2.415448	-0.631290
10	6	0	-0.723337	0.140681	-0.324132
11	15	0	1.047032	-0.806535	-0.290932
12	17	0	0.592821	-1.826913	1.557117
13	6	0	-2.811847	2.044238	-1.438190
14	6	0	1.504094	1.934981	1.091087
15	6	0	-1.971299	-0.524101	-0.140356
16	7	0	-2.623796	-1.360594	-1.013714
17	6	0	-3.742216	-1.911338	-0.397422
18	6	0	-3.794888	-1.383143	0.901514
19	7	0	-2.696544	-0.540726	1.031022
20	6	0	-4.711470	-2.797378	-0.864508
21	6	0	-5.734720	-3.142142	0.019201
22	6	0	-5.785033	-2.617631	1.321081
23	6	0	-4.817635	-1.725508	1.784960
24	6	0	-2.389645	-1.460709	-2.449042
25	6	0	-2.330259	0.146788	2.260485
26	17	0	0.550859	-2.352464	-1.652552
27	7	0	3.103060	-1.743621	-0.143323
28	15	0	4.127095	-0.512775	-0.293792
29	17	0	5.081614	-0.197433	1.716543
30	6	0	3.401816	-3.097304	0.296114
31	17	0	5.894212	-1.336649	-1.254210
32	1	0	-2.513522	1.298147	-2.179006
33	1	0	-3.634414	1.645733	-0.834887
34	1	0	-3.166618	2.930985	-1.966504
35	1	0	-2.579715	-0.491711	3.110825
36	1	0	-1.255354	0.318840	2.257049
37	1	0	-2.861829	1.100078	2.350824
38	1	0	2.414459	1.781150	0.507826
39	1	0	1.673323	2.725848	1.827670
40	1	0	1.266800	1.015933	1.628811
41	1	0	-2.164911	-2.491766	-2.727092
42	1	0	-3.286177	-1.122259	-2.981408
43	1	0	-1.537250	-0.837193	-2.709172
44	1	0	1.778216	4.795722	0.754946
45	1	0	0.681436	6.981381	0.303274
46	1	0	-1.606790	7.081616	-0.628581
47	1	0	-2.877299	5.004019	-1.113596
48	1	0	-4.670546	-3.208632	-1.867554
49	1	0	-6.506192	-3.832777	-0.306902
50	1	0	-6.594526	-2.910991	1.982325
51	1	0	-4.864930	-1.317723	2.789160
52	1	0	4.271686	-3.499515	-0.238705
53	1	0	3.611712	-3.129254	1.373634
54	1	0	2.544062	-3.747245	0.092577

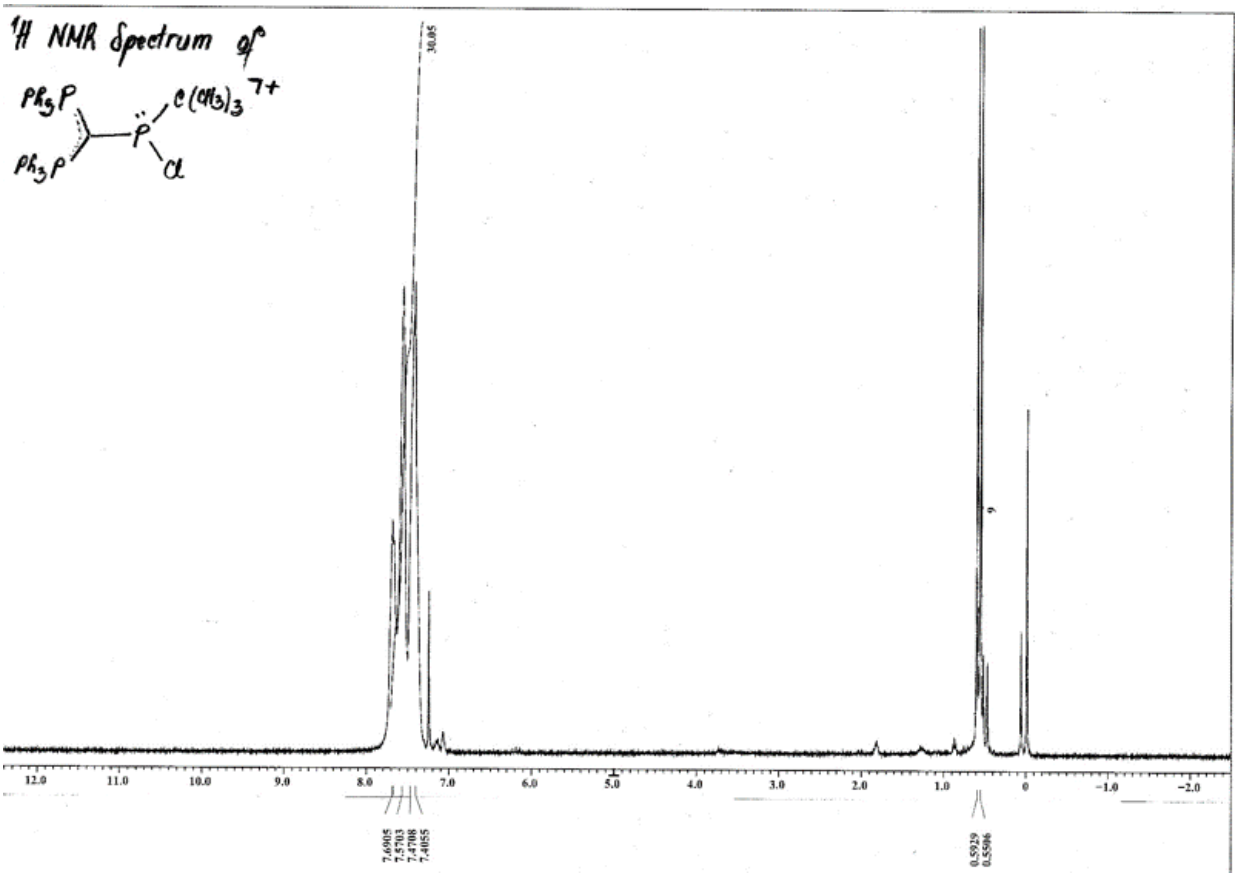
Optimized structure for **[2-PCl$_2$]**[Cl].

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029018	0.036130	-0.023814
2	6	0	-0.000948	0.003104	1.370840
3	6	0	1.182064	-0.009682	2.127108
4	6	0	2.438368	0.011129	1.521143
5	6	0	2.467780	0.043347	0.128377
6	6	0	1.283645	0.052781	-0.630251
7	7	0	-1.052950	-0.029813	2.279437
8	6	0	-0.556010	-0.041017	3.554227
9	7	0	0.806361	-0.020884	3.463971
10	6	0	-1.354546	-0.088928	4.747445
11	15	0	-1.344077	-1.564433	5.880260
12	17	0	-0.193430	-0.379485	7.609475
13	6	0	1.745826	0.180065	4.565654
14	6	0	-2.465156	-0.162332	1.924158
15	6	0	-2.308750	0.920453	4.955166
16	7	0	-3.480537	0.874746	5.682798
17	6	0	-4.083746	2.131340	5.686261
18	6	0	-3.291872	2.977189	4.898985
19	7	0	-2.197644	2.222820	4.471129
20	6	0	-3.643984	4.304457	4.675485
21	6	0	-4.816387	4.768392	5.280878
22	6	0	-5.605188	3.925660	6.073303
23	6	0	-5.250469	2.590902	6.291178
24	6	0	-4.131820	-0.300888	6.263646
25	6	0	-0.971831	2.834607	3.979618
26	17	0	0.338098	-2.643730	5.201769
27	17	0	-2.838334	-2.848761	4.162146
28	1	0	-0.117447	2.422986	4.521600
29	1	0	-0.831656	2.684339	2.904429
30	1	0	-1.019434	3.906712	4.179770
31	1	0	-2.526983	-0.646555	0.948180
32	1	0	-2.947861	-0.808507	2.661918
33	1	0	-2.946558	0.819957	1.876218
34	1	0	-3.790928	-0.470443	7.288820
35	1	0	-5.208841	-0.117727	6.265576
36	1	0	-3.939089	-1.181444	5.645479
37	1	0	2.429912	-0.667573	4.630410
38	1	0	2.311327	1.100322	4.380923
39	1	0	1.197568	0.256317	5.505526
40	1	0	-5.859140	1.947346	6.916762
41	1	0	-6.509757	4.313456	6.531673
42	1	0	-5.117240	5.800698	5.130583
43	1	0	-3.041723	4.959092	4.053778
44	1	0	3.351530	-0.003520	2.106428
45	1	0	3.426036	0.057925	-0.381628
46	1	0	1.346998	0.072497	-1.713874
47	1	0	-0.881040	0.046849	-0.613921

Selected NMR spectra:







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