Supplementary Information

Pd^{II}-mediated Integration of Isocyanides and Azide Ion Might Proceed via Formal 1,3-Dipolar Cycloaddition between RNCs Ligands and Uncomplexed Azide

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Table S1. Crystal Data.

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empirical formula	$C_{47}H_{53}ClN_4OP_2Pd$
fw	893.72
temp (K)	123(2)
λ(Å)	0.71073
cryst syst	Monoclinic
space group	$P2_1/c$
a (Å)	12.9196(3)
b (Å)	13.3903(3)
c (Å)	25.3747(4)
β (deg)	95.4960(10)
V (Å^3)	4369.57(16)
Z	4
ρ_{calc} (Mg/m^3)	1.359
μ(Mo Kα) (mm^{-1})	0.599
No. reflns.	31011
Unique reflns.	11689
GOOF (F^2)	1.060
R_{int}	0.0354
R1[a] ($I \geq 2\sigma$)	0.0411
wR2[b] ($I \geq 2\sigma$)	0.0860

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]]^{1/2}$.

$$\Delta S_1 = R \ln V^s_{m,liq} / V_{m,gas} \quad (1)$$

$$\Delta S_2 = R \ln V^o_m / V^s_{m,liq} \quad (2)$$

$$\alpha = \frac{S^{o,s}_{liq} - (S^{o,s}_{gas} + R \ln V^s_{m,liq} / V_{m,gas})}{(S^{o,s}_{gas} + R \ln V^s_{m,liq} / V_{m,gas})} \quad (3)$$

$$S_s = S_g + \Delta S_{sol} = S_g + [\Delta S_1 + \alpha(S_g + \Delta S_1) + \Delta S_2] =$$

$$S_g + [(-11.80 \text{ cal/mol•K}) - 0.21(S_g - 11.80 \text{ cal/mol•K}) + 5.45 \text{ cal/mol•K}] \quad (4),$$

where S_g = gas-phase entropy of solute, ΔS_{sol} = solvation entropy, $S^{\circ,s}_{liq}$, $S^{\circ,s}_{gas}$, and $V^s_{m,liq}$ = standard entropies and molar volume of the solvent in liquid or gas phases (173.84 and 270.28 J/mol•K and 64.15 mL/mol, respectively, for CH_2Cl_2), $V_{m,gas}$ = molar volume of the ideal gas at 25 °C (24450 mL/mol), V°_m = molar volume of the solution corresponding to the standard conditions (1000 mL/mol). The enthalpies and Gibbs free energies in solution (H_s and G_s) were estimated using the expressions (5) and (6)

$$H_s = E_s(\text{6-311+G(d,p)}) - E_g(\text{6-311+G(d,p)}) + H_g(\text{6-31G(d)}) \quad (5)$$

$$G_s = H_s - TS_s \quad (6),$$

where E_s, E_g and H_g are the total energies in solution and in gas phase and gas-phase enthalpy calculated at the corresponding level.

Table S2. Calculated total energies (E_g, E_s), enthalpies (H_g, H_s), Gibbs free energies (G_g, G_s) (in Hartree) and entropies (S_g, S_s) (in cal/mol•K) in gas phase and CH_2Cl_2 solution, respectively.

Compound	E_g (6-31G(d))	E_g (6-311+G(d,p))	E_s	H_g (6-31G(d))	H_s	S_g (6-31G(d))	S_s	G_g (6-31G(d))	G_s
Metal-free									
N_3^-	-164.213093	-164.287117	-164.388756	-164.198438	-164.300077	50.75	36.22	-164.222550	-164.317286
CNMe	-132.716573	-132.759464	-132.770337	-132.666337	-132.677211	60.92	44.26	-132.695283	-132.698238
TS_metal-free	-296.905176	-297.016460	-297.107218	-296.841934	-296.932692	76.09	56.24	-296.878086	-296.959411
CN_4Me	-296.947371	-297.055136	-297.157429	-296.880387	-296.982680	72.65	53.52	-296.914906	-297.008110
TS5_metal-free	-296.930296	-297.037320	-297.134113	-296.866355	-296.963148	78.79	58.37	-296.903789	-296.990882
N_2	-109.524129	-109.560542	-109.561290	-109.515226	-109.515974	45.79	32.30	-109.536981	-109.531322
$N{=}C{=}NMe^-$	-187.504976	-187.585540	-187.684234	-187.450586	-187.549280	67.14	49.17	-187.482488	-187.572642
Pd									
trans-$[PdCl(PH_3)_2CNMe]^+$	-1407.036570	-1407.164141	-1407.236197	-1406.916083	-1406.988139	120.88	91.62	-1406.973515	-1407.031671
OC1	-1571.419278	-1571.599233	-1571.624758	-1571.282839	-1571.308364	135.09	102.85	-1571.347026	-1571.357231
OC2	-1571.425821	-1571.606221	-1571.622197	-1571.290193	-1571.306169	145.35	110.95	-1571.359255	-1571.358887
TS1	-1571.411935	-1571.593010	-1571.619287	-1571.276903	-1571.303180	132.59	100.87	-1571.339901	-1571.351109
INT-NNNCN	-1571.447361	-1571.626060	-1571.643297	-1571.311236	-1571.328473	136.27	103.78	-1571.375982	-1571.377783
TS2	-1571.428912	-1571.605925	-1571.623621	-1571.294380	-1571.312076	130.49	99.22	-1571.356381	-1571.359217
P	-1571.474857	-1571.648538	-1571.677871	-1571.336921	-1571.366254	129.23	98.22	-1571.398322	-1571.412921
A	-1571.449659	-1571.624298	-1571.641658	-1571.311802	-1571.329161	124.33	94.35	-1571.370875	-1571.373989
B	-1571.428758	-1571.606040	-1571.628851	-1571.291221	-1571.314032	124.15	94.21	-1571.350209	-1571.358793
C	-1571.401113	-1571.579115	-1571.614315	-1571.264436	-1571.299636	127.24	96.64	-1571.324889	-1571.345555
trans-$[PdCl(PH_3)_2N_3]$	-1438.698880	-1438.840921	-1438.855526	-1438.615727	-1438.630332	115.09	87.05	-1438.670411	-1438.671692
TS3	-1571.383292	-1571.562594	-1571.577229	-1571.249443	-1571.264078	133.26	101.40	-1571.312759	-1571.312258

TS4	-1571.368673	-1571.546602	-1571.566858	-1571.235639	-1571.255894	143.34	109.37	-1571.303744	-1571.307857
trans-[PdCl(PH_3)$_2$N=C=NMe]	-1461.999160	-1462.148848	-1462.165292	-1461.874269	-1461.890713	129.96	98.80	-1461.936018	-1461.937654
trans-[PdCl(PH_3)$_2$$N_2$]$^+$	-1383.775386	-1383.90006	-1383.975992	-1383.697333	-1383.773265	107.07	80.71	-1383.748208	-1383.811614
TS5	-1571.422202	-1571.599578	-1571.617885	-1571.288668	-1571.306975	132.34	100.67	-1571.351546	-1571.354808

Table S3. Calculated total activation and reaction energies (E_a and ΔE), enthalpies and Gibbs free energies of activation ($\Delta H^{\neq}$ and $\Delta G^{\neq}$) and reaction (ΔH and ΔG) (in kcal/mol) for the gas phase and CH_2Cl_2 solution (in parentheses).

Process	E_a	$\Delta H^{\neq}$	$\Delta G^{\neq}$	ΔE	ΔH	ΔG
N_3^- + *trans*-$[PdCl(PH_3)_2CNMe]^+$ → **OC1**				-92.9	-105.6	-94.7
				(0.1)	(-12.6)	(-5.2)
OC1 → INT-NNNCN	3.9	3.7	4.5	-16.8	-17.8	-18.2
	(3.4)	(3.3)	(3.8)	(-11.6)	(-12.6)	(-12.9)
INT-NNNCN → P	12.6	10.6	12.3	-14.1	-16.1	-14.0
	(12.4)	(10.3)	(11.7)	(-21.7)	(-23.7)	(-22.1)
CNMe + *trans*-$[PdCl(PH_3)_2N_3]$ → N_2 + *trans*-$[PdCl(PH_3)_2N{=}C{=}NMe]$	23.7	20.5	33.2	-68.4	-67.4	-67.3
	(30.5)	(27.3)	(36.2)	(-63.2)	(-62.2)	(-62.2)
CNMe + *trans*-$[PdCl(PH_3)_2N_3]$ → *trans*-$[PdCl(PH_3)_2N_2]^+$ + $N{=}C{=}NMe^-$	33.8	29.1	38.9	72.0	84.2	84.7
	(37.0)	(32.4)	(39.0)	(-21.6)	(-9.4)	(-9.0)
P → N_2 + *trans*-$[PdCl(PH_3)_2N{=}C{=}NMe]$	30.7	30.3	29.4	-38.2	-33.0	-46.9
	(37.6)	(37.2)	(36.5)	(-30.6)	(-25.4)	(-35.2)
OC1 → OC2				-4.4	-4.6	-7.7
				(1.6)	(1.4)	(-1.0)
N_3^- + CNMe → N_2 + $N{=}C{=}NMe^-$	18.9	14.3	24.9	-62.4	-63.4	-63.8
	(32.6)	(28.0)	(35.2)	(-54.2)	(-55.2)	(-55.5)
N_3^- + CNMe → CN_4Me				-5.4	-9.8	1.8
				(1.0)	(-3.4)	(4.7)

$CN_4Me \rightarrow N_2 + N{=}C{=}NMe^-$	11.2	8.8	7.0	-57.1	-53.6	-65.6
	(14.6)	(12.3)	(10.8)	(-55.3)	(-51.8)	(-60.2)

Table S4. Cartesian atomic coordinates of the calculated equilibrium structures.

Atom	X	Y	Z
N_3^-			
N	0.000000	0.000000	-1.190246
N	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.190246
CNMe			
C	1.488263	0.000000	-0.000101
N	0.310865	-0.000002	0.000189
C	-1.109253	-0.000001	-0.000033
H	-1.483532	0.876361	0.537944
H	-1.483042	0.027902	-1.028099
H	-1.483537	-0.904246	0.489631
TS_metal-free			
N	-1.189169	-1.078643	0.000036
N	-1.610184	0.125368	-0.000095
N	-1.456455	1.281930	0.000036
N	0.845942	0.140190	0.000088
C	0.358850	-1.036246	-0.000007
C	2.278497	0.303634	-0.000043
H	2.833437	-0.651955	-0.000942
H	2.605949	0.882101	0.881100
H	2.605592	0.883608	-0.880320
CN_4Me			
C	0.236478	1.208270	0.000053
N	-0.552180	0.074368	0.000409
N	0.173936	-1.093375	0.000122
N	1.407262	-0.702931	-0.000161
N	1.488263	0.672493	-0.000099
C	-1.989058	0.011908	-0.000193
H	-2.352842	1.042590	-0.000750
H	-2.376781	-0.508406	0.888062
H	-2.375862	-0.509137	-0.888363
TS5_metal-free			
C	-0.192581	-1.186166	-0.003889
N	0.607038	-0.111975	-0.018853
N	-1.445195	-0.921264	0.006565
C	2.030730	0.020855	0.008495
H	2.527617	-0.432568	-0.866252
H	2.494464	-0.414218	0.910633
H	2.254774	1.096011	0.001604
N	-0.321090	1.200083	-0.003655
N	-1.455860	0.796391	0.005426
N_2			
N	0.000000	0.000000	0.552772
N	0.000000	0.000000	-0.552772
$N=C=NMe^-$			
N	-1.884851	0.273617	-0.000057
N	0.429435	-0.651026	-0.000070

C	-0.761244	-0.124839	0.000120
C	1.523644	0.287058	0.000032
H	1.565828	0.967779	0.883036
H	1.567900	0.965561	-0.884774
H	2.479784	-0.264790	0.001720
trans-[PdCl(PH_3)$_2$CNMe]$^+$			
Pd	-0.221209	-0.000096	0.000038
C	1.748228	-0.001715	0.000058
N	2.910081	-0.002251	0.000084
C	4.339756	-0.001547	-0.000017
Cl	-2.548113	0.002094	0.000066
P	-0.464564	2.340250	-0.000080
P	-0.469364	-2.339831	-0.000080
H	4.695755	0.522516	0.890292
H	4.697509	-1.033782	0.008792
H	4.695563	0.507250	-0.899209
H	-1.196162	2.828045	-1.095128
H	0.659699	3.189372	0.000013
H	-1.196546	2.828322	1.094580
H	0.652754	-3.191759	-0.000243
H	-1.202277	-2.826366	1.094643
H	-1.202323	-2.825717	-1.095062
OC1			
C	1.025116	1.111696	-0.421592
N	2.038493	1.679097	-0.496746
C	3.367153	2.195654	-0.523479
Pd	-0.653728	0.122474	-0.165960
Cl	-2.635248	-1.139753	0.044058
P	0.387440	-1.893756	-0.731313
P	-2.014706	1.942485	0.547049
H	3.609219	2.521658	-1.538446
H	4.033239	1.391406	-0.198023
H	3.437641	3.044719	0.161117
H	-0.011471	-3.083105	-0.112163
H	1.719663	-2.012543	-1.180138
H	-0.220624	-2.134485	-2.005409
H	-1.548763	3.270105	0.698703
H	-3.155492	2.188530	-0.240992
H	-2.623996	1.767990	1.804653
N	3.606575	-0.783422	0.745698
N	2.557159	-1.210101	1.033524
N	1.467300	-1.655187	1.278992
OC2			
Pd	-0.837909	0.066561	-0.157174
Cl	-2.561300	-1.314438	0.681469
P	0.234301	-1.889903	-0.792740
P	-2.101787	1.908117	0.553237
N	2.675193	0.794275	-1.738015
N	1.624882	1.040284	-1.318103
N	0.542772	1.398399	-0.898811

H	0.382539	-2.874257	0.194773
H	1.527722	-1.830344	-1.349168
H	-0.449988	-2.612491	-1.791244
H	-1.605867	3.204855	0.303644
H	-3.408772	2.029506	0.040748
H	-2.385871	2.002626	1.930385
N	3.506996	-0.369628	1.307385
C	2.623495	-1.137433	1.378926
C	4.560616	0.572136	1.144298
H	5.525764	0.072102	1.266217
H	4.468535	1.363312	1.893837
H	4.490590	1.003588	0.141822
TS1			
C	-1.039107	0.900281	0.147698
N	-1.881396	1.658428	0.481364
C	-3.218967	2.171422	0.410622
Pd	0.722813	0.023575	0.081970
Cl	2.822344	-1.052484	-0.026381
P	-0.275425	-2.081105	0.360954
P	1.940739	1.993812	-0.255754
H	-3.223508	3.224599	0.701244
H	-3.854826	1.590925	1.083050
H	-3.595036	2.059839	-0.610377
H	-0.251406	-2.886036	-0.786679
H	-1.583131	-2.236206	0.859947
H	0.442651	-2.899325	1.262690
H	1.322945	3.263357	-0.290329
H	2.965750	2.241470	0.675932
H	2.672851	2.042459	-1.456686
N	-3.921286	-1.061049	0.053609
N	-2.993072	-0.875439	-0.634115
N	-1.998079	-0.681101	-1.284979
INT-NNNCN			
C	1.408765	0.000048	0.208472
N	2.122820	-0.000109	1.254424
C	1.536336	-0.000411	2.580585
Pd	-0.607224	0.000008	-0.031923
Cl	-3.010443	0.000009	-0.341158
P	-0.702259	2.320900	-0.088652
P	-0.702204	-2.320894	-0.088991
N	4.413429	0.000055	-1.216468
N	3.286363	0.000179	-1.081361
N	2.036410	0.000308	-1.084552
H	0.435425	-0.000179	2.579461
H	1.887787	0.879676	3.132956
H	1.887411	-0.881003	3.132398
H	-1.215492	2.856849	-1.285474
H	0.430470	3.148852	0.073920
H	-1.573781	2.926850	0.836926
H	-1.215026	-2.856640	-1.286084

H	0.430374	-3.149004	0.073868
H	-1.574140	-2.926879	0.836171
TS2			
C	1.410187	0.007313	-0.045138
N	2.239508	0.548136	0.741739
C	1.985899	1.307862	1.941076
Pd	-0.621124	-0.033913	-0.009764
Cl	-3.022399	-0.104067	0.016637
P	-0.833687	2.217110	-0.553157
P	-0.564087	-2.329103	0.339042
H	2.483130	2.282170	1.873401
H	2.411423	0.785592	2.805739
H	0.913734	1.464169	2.126531
H	-1.479317	2.453287	-1.781700
H	0.275624	3.079152	-0.697162
H	-1.639864	2.998319	0.296837
H	0.600597	-2.985402	0.785633
H	-1.521281	-2.871606	1.218007
H	-0.834551	-3.082787	-0.819295
N	4.012280	-0.169942	-0.436482
N	3.193042	-0.644453	-1.106226
N	1.888471	-0.734442	-1.171253
P			
C	1.358650	-0.168375	-0.226042
N	2.340818	0.436246	0.493563
N	3.550943	0.031147	0.018259
N	3.306187	-0.790672	-0.945074
N	1.959765	-0.944770	-1.123047
C	2.273642	1.367508	1.605104
Pd	-0.636830	-0.038665	-0.015319
Cl	-3.015998	0.050585	0.184459
P	-0.769592	2.222161	-0.550777
P	-0.662109	-2.341692	0.270020
H	1.469330	1.076196	2.284460
H	2.103069	2.391421	1.254744
H	3.229496	1.329288	2.129287
H	-1.510005	2.477149	-1.719904
H	0.368479	3.016777	-0.813625
H	-1.447105	3.059008	0.356488
H	-0.772594	-3.054602	-0.938680
H	0.435525	-3.008223	0.847412
H	-1.732286	-2.893853	0.999750
A			
C	-2.105280	0.816504	0.000087
N	-3.256621	0.096688	0.000021
N	-3.049373	-1.260132	-0.000062
N	-1.784684	-1.426051	-0.000053
N	-1.190255	-0.184142	0.000041
C	-4.620370	0.596338	0.000038
Pd	0.814366	0.038078	0.000017

Cl	3.138538	0.331474	0.000045
P	0.511071	2.357013	-0.000071
P	1.116399	-2.280237	-0.000027
H	-4.570166	1.684878	-0.000049
H	-5.150151	0.248712	0.891259
H	-5.150226	0.248568	-0.891083
H	1.701018	3.115993	-0.000156
H	-0.175918	2.928214	1.083999
H	-0.175984	2.928014	-1.084203
H	0.582368	-3.009825	1.078630
H	0.582596	-3.009668	-1.078906
H	2.448856	-2.734762	0.000065
B			
C	3.089891	-1.374790	0.000174
N	3.252859	-0.001866	0.000086
N	2.096407	0.686300	-0.000084
N	1.202061	-0.257258	-0.000104
N	1.744110	-1.506590	0.000044
C	4.512847	0.719267	0.000043
H	5.300276	-0.034218	0.000414
H	4.596948	1.346465	0.892473
H	4.597242	1.345852	-0.892793
Pd	-0.798453	0.043720	-0.000023
Cl	-3.118349	0.319887	0.000155
P	-0.524647	2.363765	-0.000050
P	-1.053324	-2.289777	-0.000077
H	-1.702012	3.134724	0.000307
H	0.174116	2.940552	-1.078215
H	0.174828	2.940597	1.077618
H	-0.514494	-2.998015	-1.086848
H	-0.514519	-2.998151	1.086614
H	-2.386551	-2.747802	-0.000122
C			
C	-3.649067	0.066582	0.009961
N	-2.463546	0.586147	0.406190
N	-1.414108	-0.098100	-0.170829
N	-1.957009	-1.045447	-0.902269
N	-3.279666	-0.972454	-0.827721
C	-2.242836	1.665654	1.347164
H	-3.213992	1.895053	1.784977
H	-1.859728	2.562757	0.848031
H	-1.546106	1.357867	2.133544
Pd	0.625363	-0.040000	-0.003526
Cl	2.961743	-0.073021	0.198403
P	0.907124	2.224338	-0.552669
P	0.553216	-2.356728	0.259089
H	1.473805	3.062206	0.427324
H	-0.177156	3.027229	-0.969067
H	1.802353	2.445527	-1.614715
H	-0.554351	-2.940000	0.899974

H	0.576837	-3.079695	-0.946861
H	1.628635	-2.948150	0.949509
trans-[PdCl(PH_3)$_2$$N_3$]			
Pd	-0.176305	-0.037037	0.000017
Cl	-2.033255	1.426514	-0.000290
P	1.156838	1.858456	0.000251
P	-1.678763	-1.834473	0.000055
N	3.630766	-0.814068	-0.000604
N	2.503670	-1.066148	-0.000141
N	1.338203	-1.424882	0.000448
H	0.977344	2.744656	-1.078428
H	2.562335	1.715331	0.000075
H	0.977582	2.743979	1.079526
H	-1.150366	-3.141379	0.000426
H	-2.585632	-1.916557	1.075304
H	-2.585516	-1.917106	-1.075250
TS3			
Pd	-0.810484	-0.055129	-0.054441
Cl	-3.062760	-0.674982	0.251676
P	-1.612262	2.123620	0.035721
P	-0.178434	-2.323944	-0.115912
N	2.669284	2.134693	0.017070
N	1.676462	1.560161	-0.172747
N	1.136085	0.431306	-0.356770
H	-2.556710	2.461160	-0.951835
H	-0.747963	3.235977	-0.054360
H	-2.336076	2.461746	1.194393
H	0.535650	-2.830397	-1.213920
H	0.532502	-2.887420	0.956773
H	-1.311786	-3.165658	-0.133812
N	3.469123	-0.217725	0.090146
C	2.436320	-0.828986	-0.104315
C	4.856927	-0.497099	0.335489
H	5.462885	-0.050115	-0.458621
H	5.057168	-1.574437	0.377150
H	5.157802	-0.037920	1.281916
TS4			
Pd	0.791310	-0.001482	-0.008634
Cl	3.145227	-0.026996	0.379885
P	0.895174	2.330933	0.002745
P	0.877155	-2.331126	-0.161399
N	-2.867668	0.179491	-1.820281
N	-1.745397	0.122586	-1.304287
N	-1.237489	0.011236	-0.189631
H	1.791422	2.927710	-0.905388
H	1.331046	2.944624	1.194518
H	-0.266171	3.091698	-0.252915
H	1.723772	-2.865078	-1.152779
H	1.366672	-3.030690	0.960059
H	-0.299963	-3.067961	-0.415803

N	-3.512937	-0.044989	0.585505
C	-3.964598	0.061264	-0.519372
C	-3.632397	-0.178813	1.999418
H	-3.171623	-1.116316	2.322329
H	-4.687765	-0.174271	2.295102
H	-3.115060	0.647312	2.494368
trans-[PdCl(PH_3)$_2$N=C=NMe]			
Pd	-0.517996	-0.023869	-0.108385
Cl	-2.665948	0.731432	0.532985
P	0.143626	2.195438	-0.197301
P	-1.177912	-2.264872	-0.011342
N	1.278011	-0.724891	-0.786944
N	3.487918	0.133856	-0.145012
C	2.360752	-0.323512	-0.388126
C	4.383480	-0.398610	0.871397
H	-0.396035	2.966230	-1.245913
H	1.516781	2.487151	-0.343582
H	-0.187716	3.014257	0.898871
H	-1.262559	-2.929822	-1.252022
H	-0.330346	-3.164364	0.667631
H	-2.424354	-2.613920	0.545362
H	5.252289	-0.864454	0.389832
H	3.910176	-1.142707	1.526157
H	4.758077	0.422765	1.492332
trans-[PdCl(PH_3)$_2$$N_2$]$^+$			
Pd	-0.000004	0.106902	0.000005
Cl	0.000238	-2.182938	0.000017
P	2.357652	-0.141389	-0.000014
P	-2.357629	-0.141854	-0.000013
N	-0.000382	3.260942	0.000028
N	-0.000237	2.154226	-0.000005
H	2.845202	-0.867259	-1.098460
H	2.845250	-0.867322	1.098364
H	3.179364	1.002936	-0.000026
H	-2.845030	-0.867678	-1.098557
H	-2.845056	-0.868043	1.098271
H	-3.179581	1.002297	0.000135
TS5			
C	-1.440107	0.013174	-0.074239
N	-2.255083	-0.643278	0.669312
N	-1.704103	0.844749	-1.043648
C	-2.042936	-1.528926	1.784883
Pd	0.642262	0.052667	-0.025014
Cl	3.010677	0.076237	0.141965
P	0.853431	-2.188490	-0.634553
P	0.533224	2.339887	0.328895
H	-1.524426	-2.457066	1.500086
H	-3.024020	-1.813351	2.177334
H	-1.479250	-1.053149	2.598644
H	1.621921	-2.398793	-1.794546

H	-0.270326	-2.987667	-0.935564
H	1.529007	-3.037769	0.262890
H	0.494908	3.100605	-0.853119
H	-0.555929	2.893258	1.027116
H	1.618461	2.941657	0.997238
N	-3.931713	0.130147	-0.280088
N	-3.400168	0.799398	-1.048693