Supporting Information:

Heterobimetallic Scandium-Group 10 Metal Complexes with LM→Sc (LM = Ni, Pd, Pt) Dative Bond

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1. Spectroscopic Data

NMR spectra

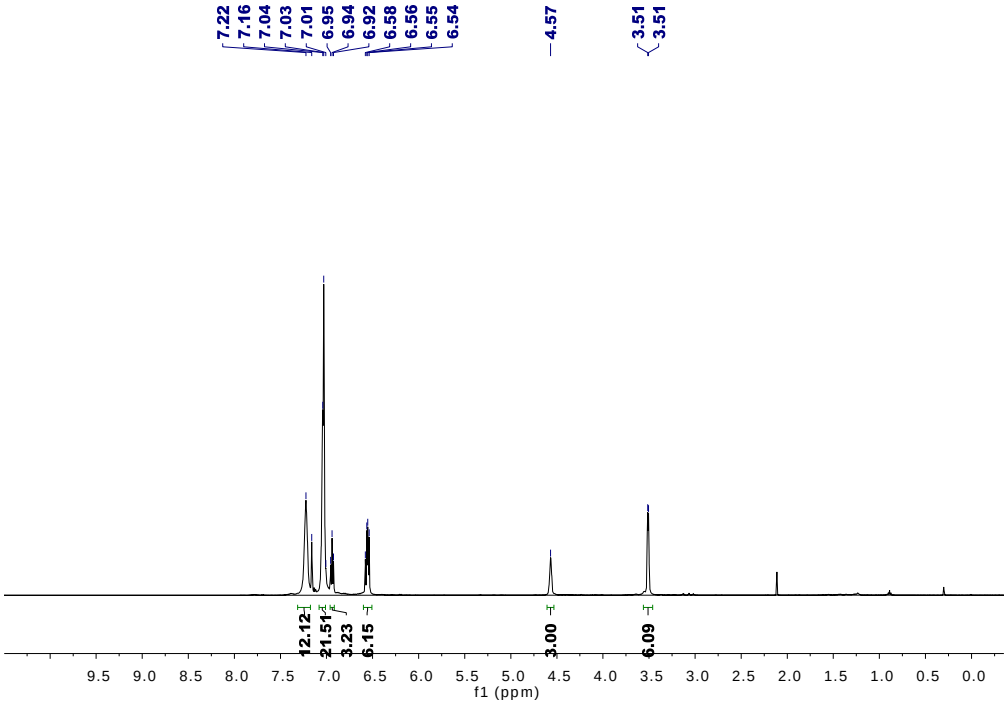


Figure S1. ^{1}H NMR spectrum of **LH$_3$** in C_6D_6 at 25 °C.

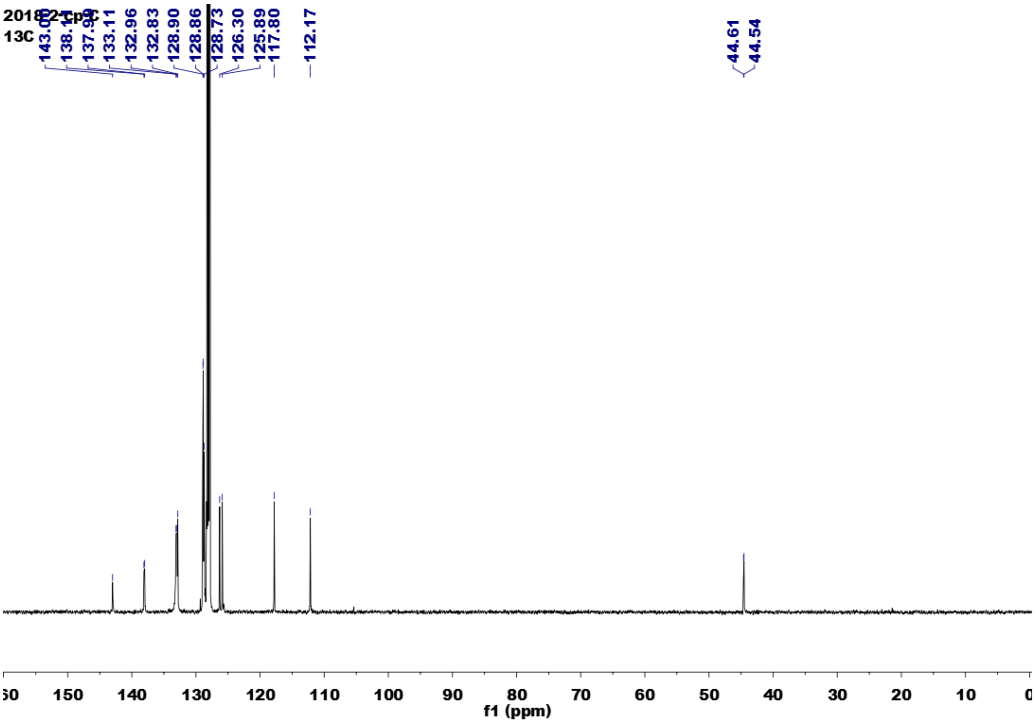


Figure S2. ^{13}C{^{1}H} NMR spectrum of **LH$_3$** in C_6D_6 at 25 °C.

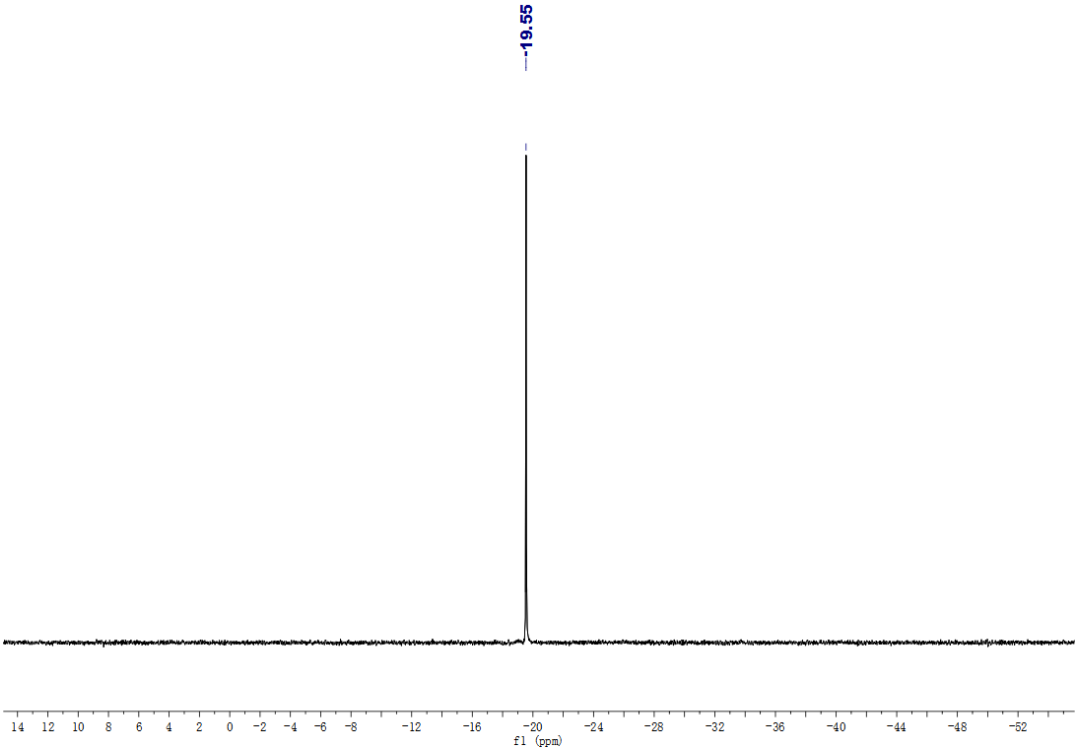


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of **LH_3** in C_6D_6 at 25 °C.

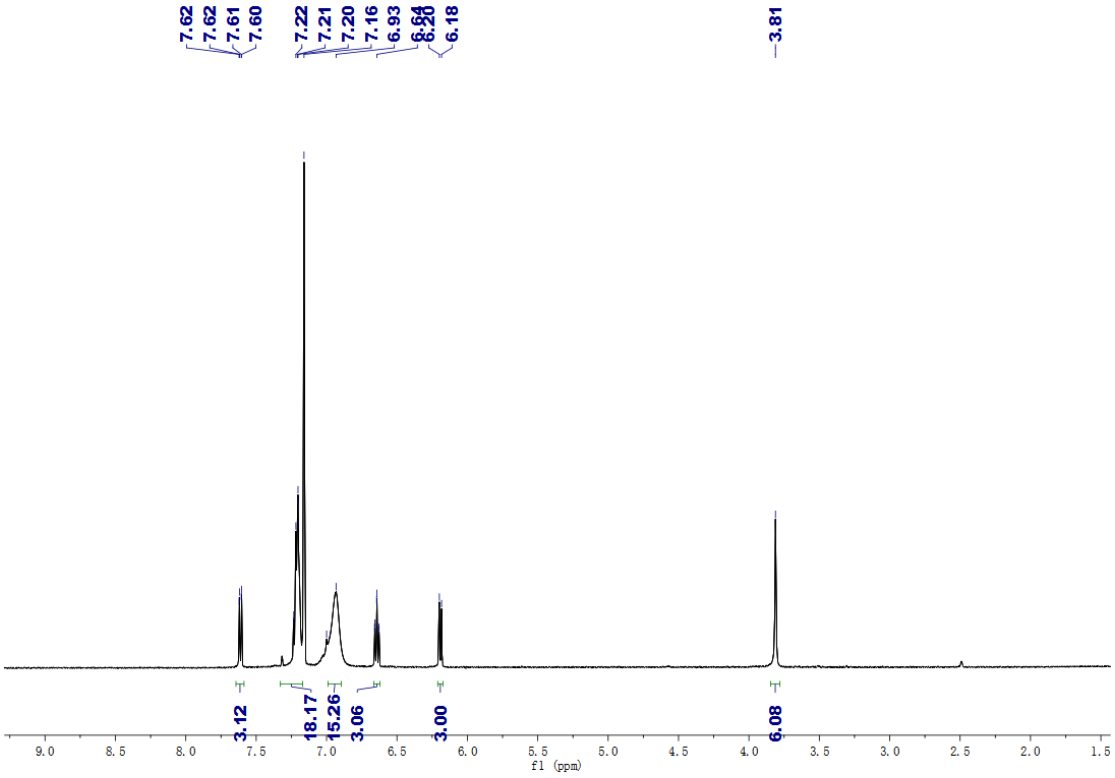


Figure S4. ^{1}H NMR spectrum of **1** in C_6D_6 at 25 °C.

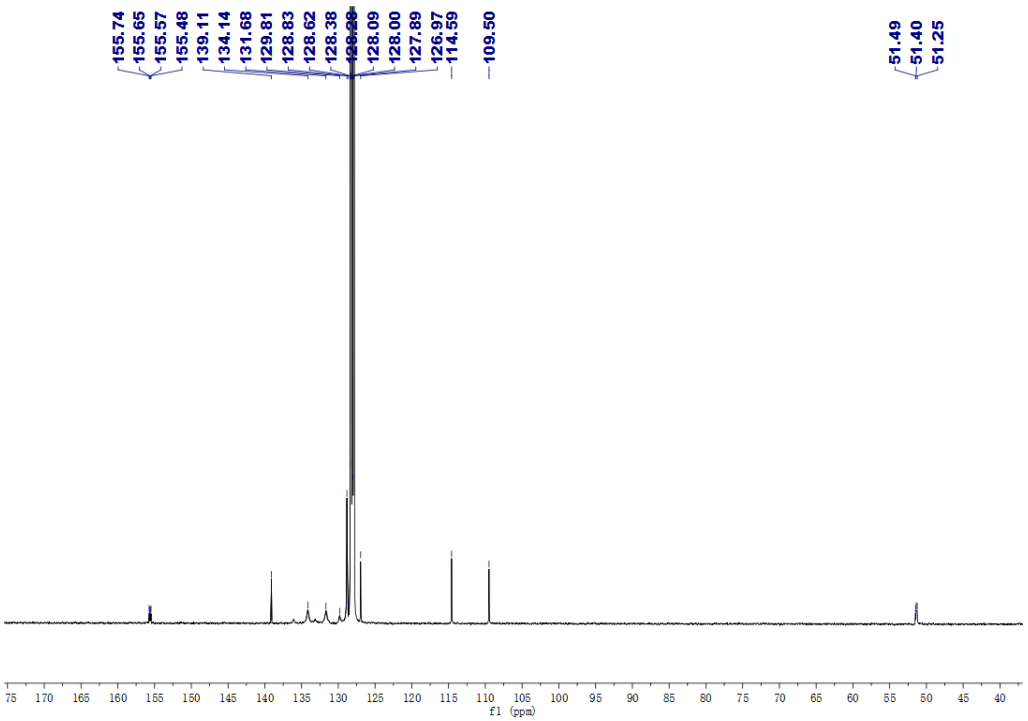


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6 at 25 °C.

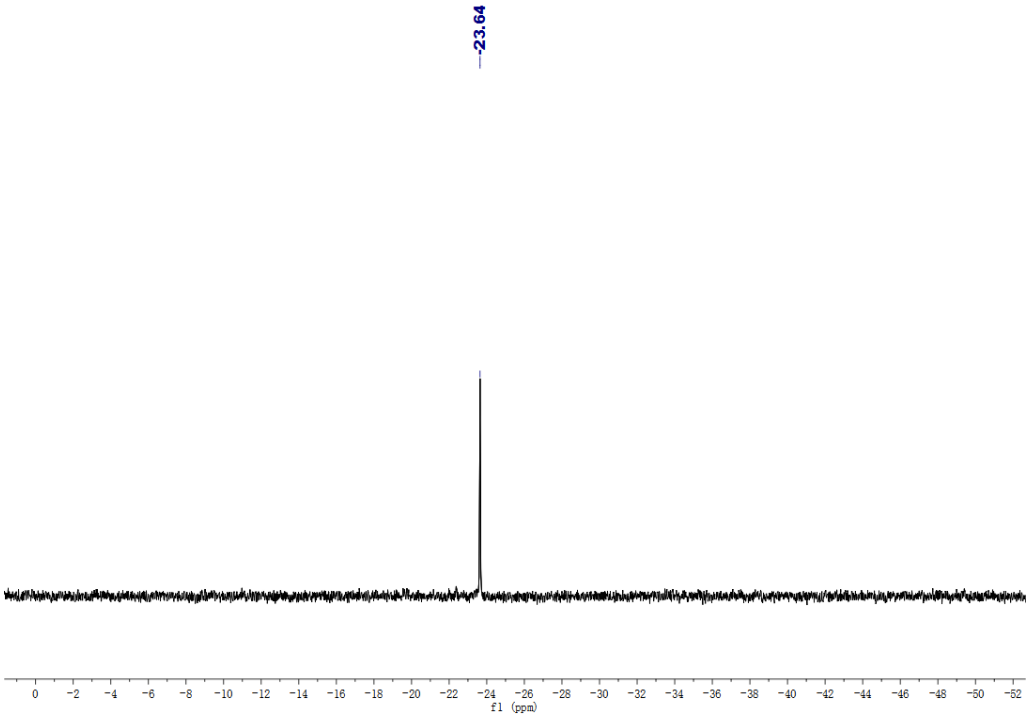


Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in C_6D_6 at 25 °C.

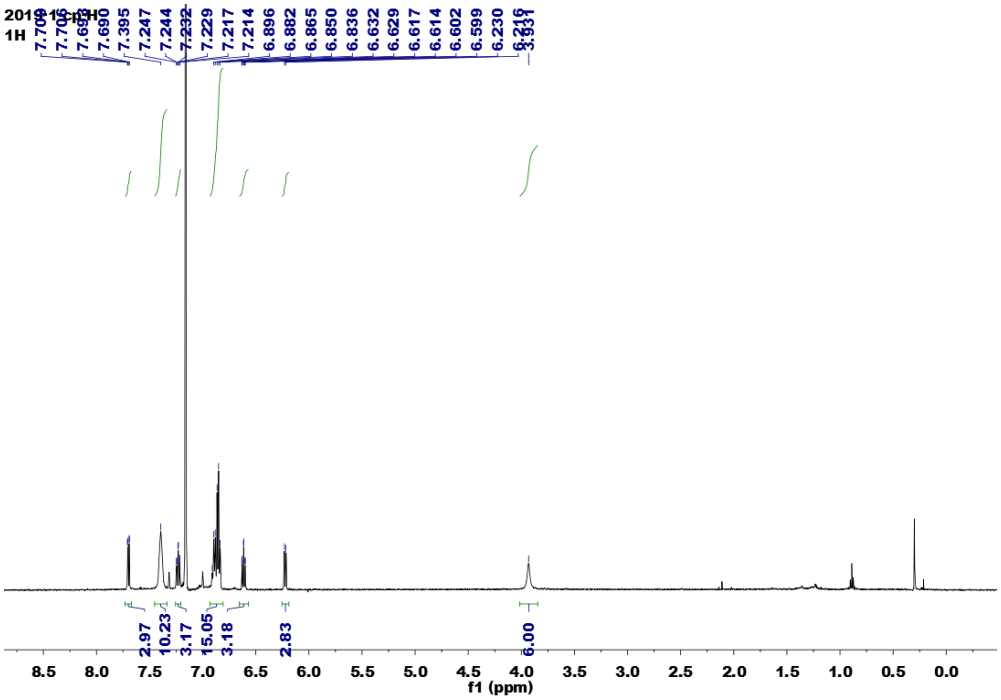


Figure S7. ^{1}H NMR spectrum of **2** in C_6D_6 at 25 °C.

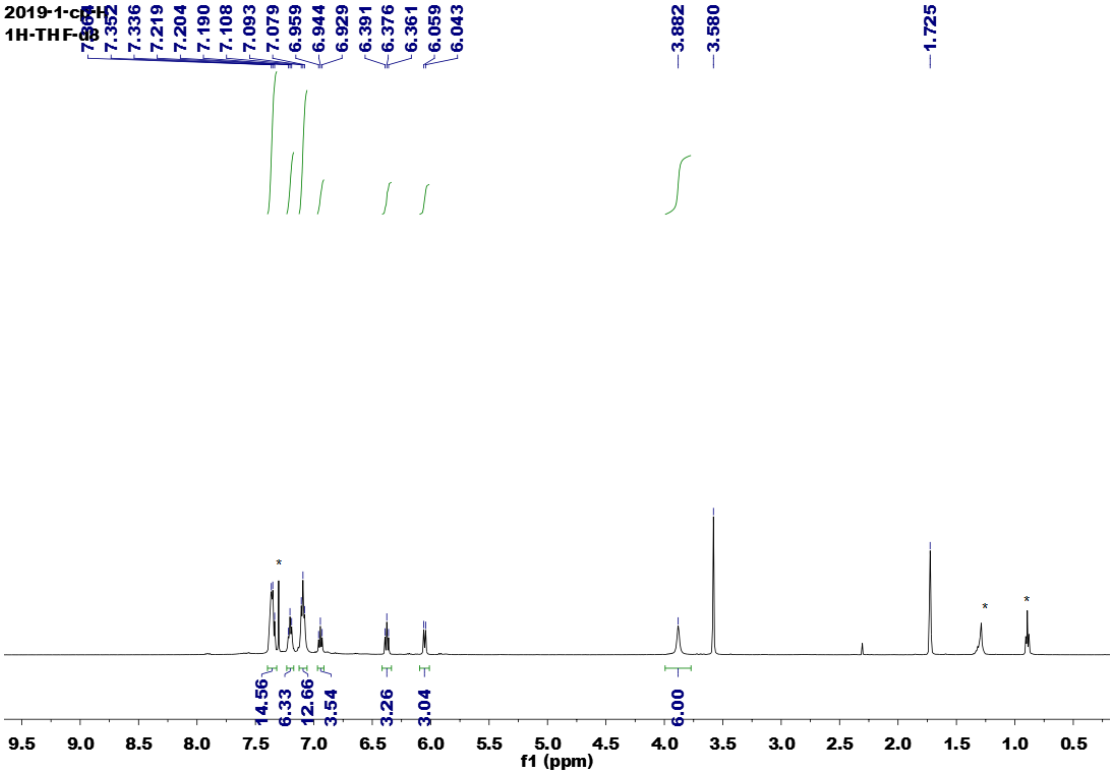


Figure S8. ^{1}H NMR spectrum of **2** in THF-d_8 at 25 °C. (* denotes co-crystallized benzene and small amount of hexane)

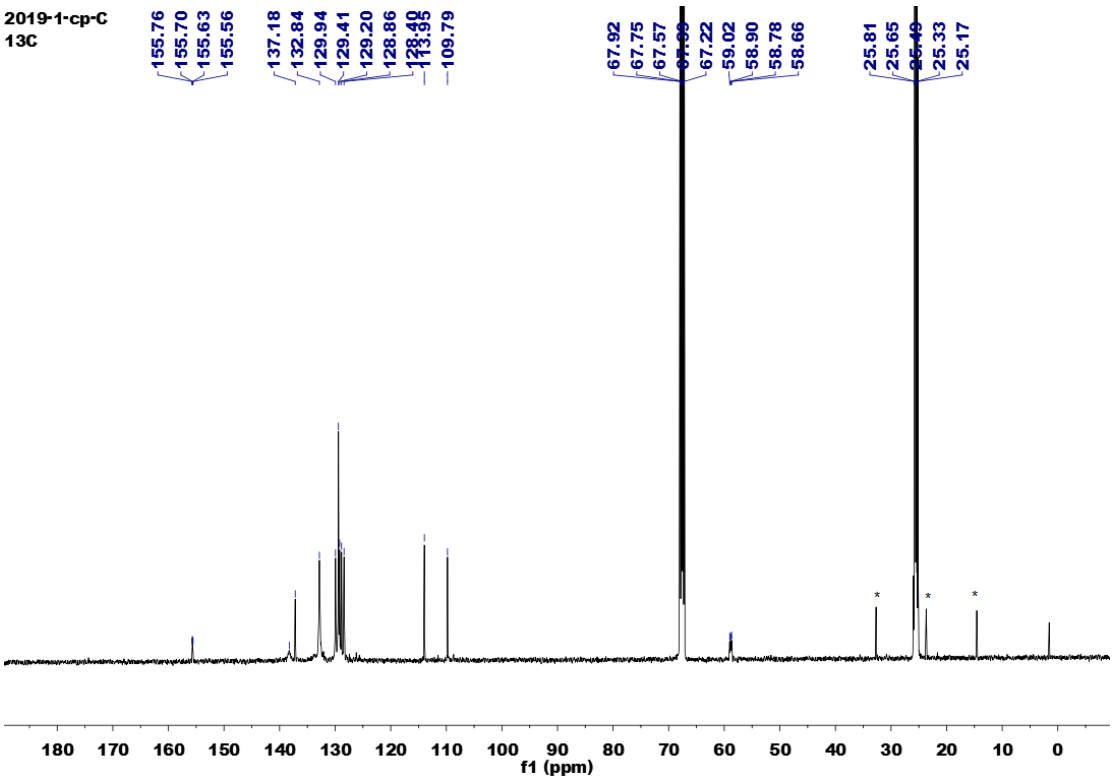


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in THF-d_8 at 25 °C. (* denotes small amount of hexane)

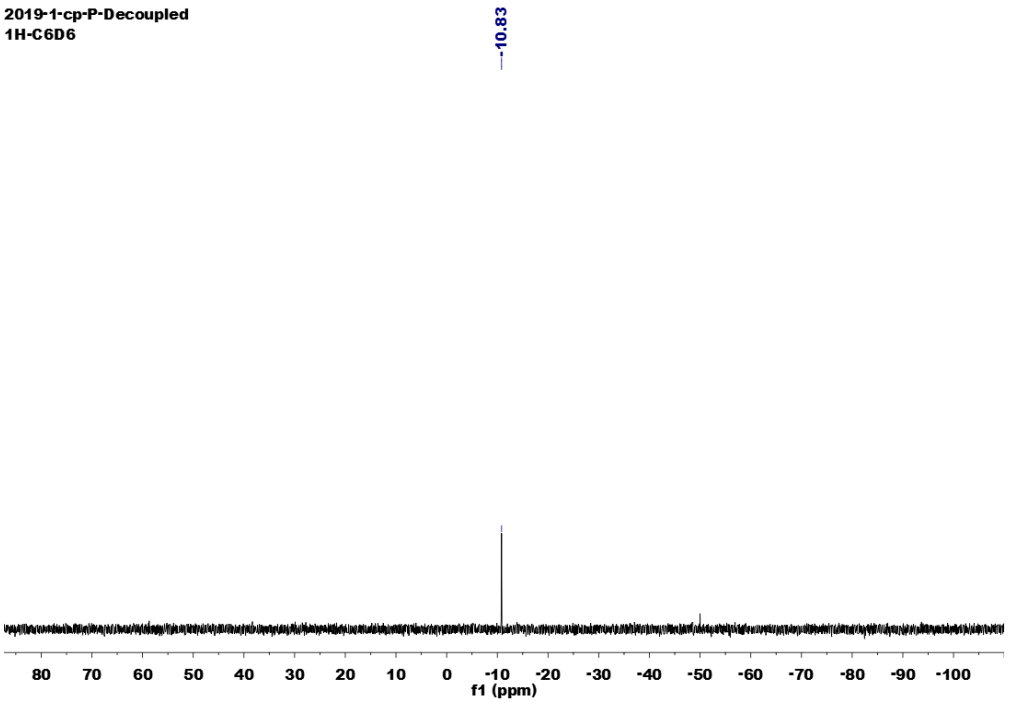


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 25 °C.

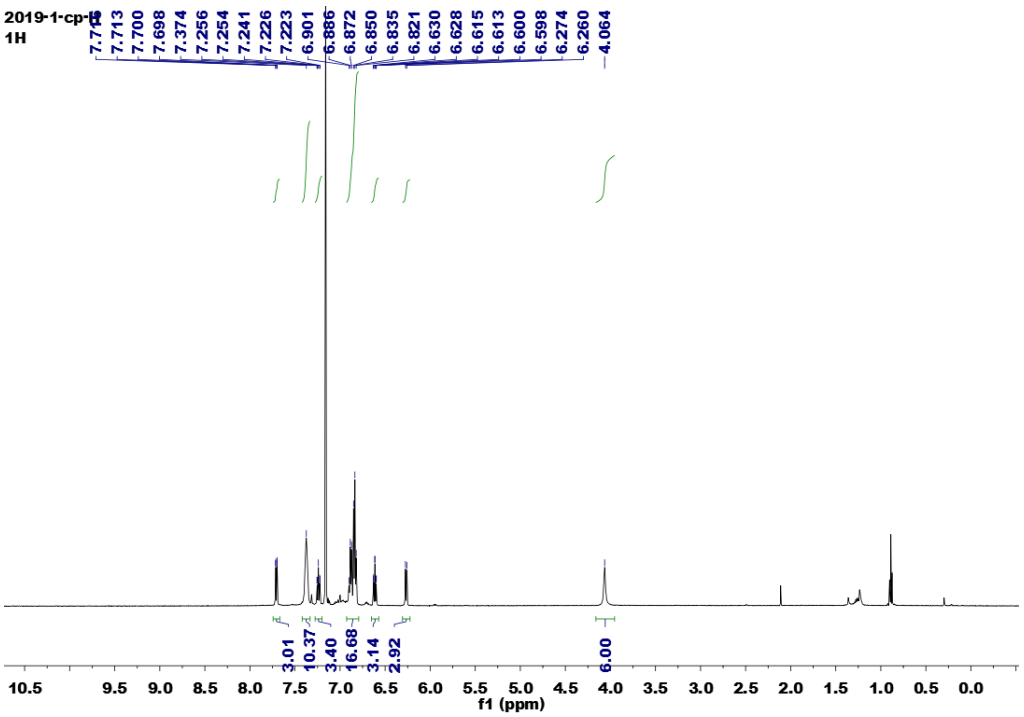


Figure S11. ^{1}H NMR spectrum of **3** in C_6D_6 at 25 °C.

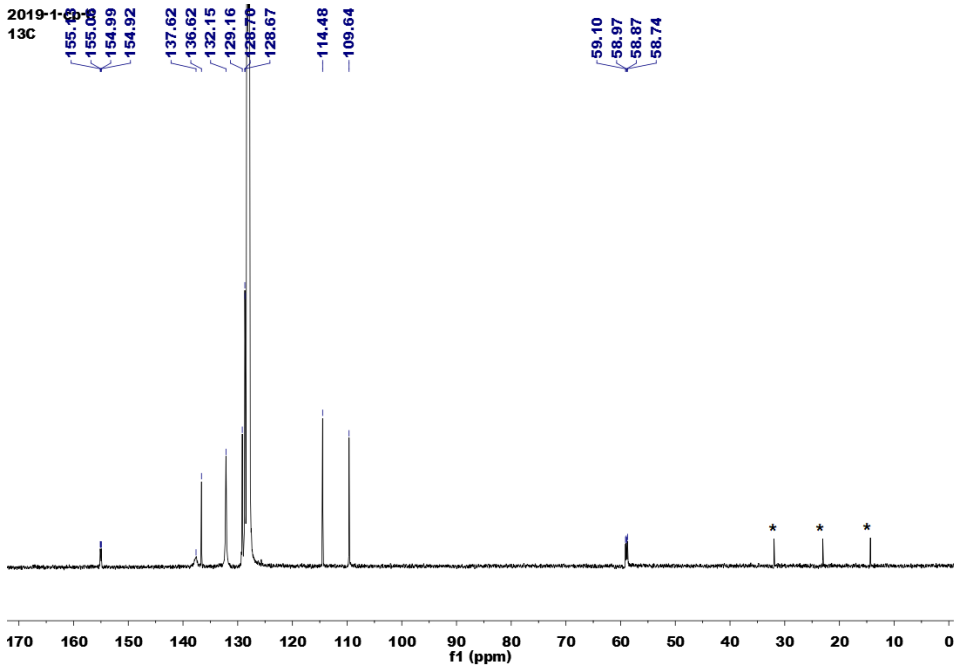


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at 25 °C. (* denotes small amount of hexane)

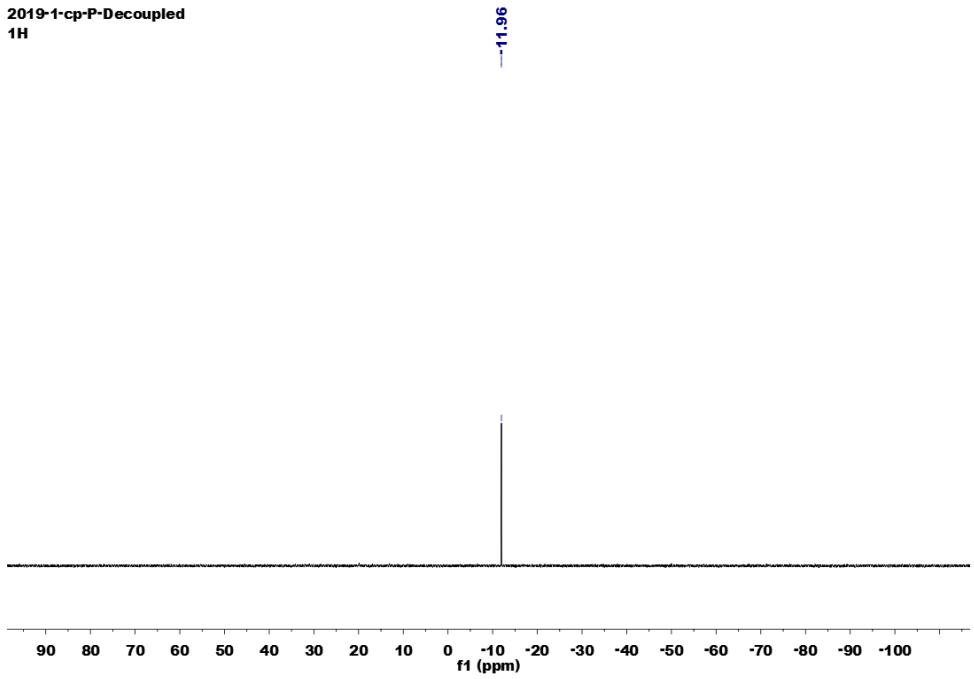


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at 25 °C.

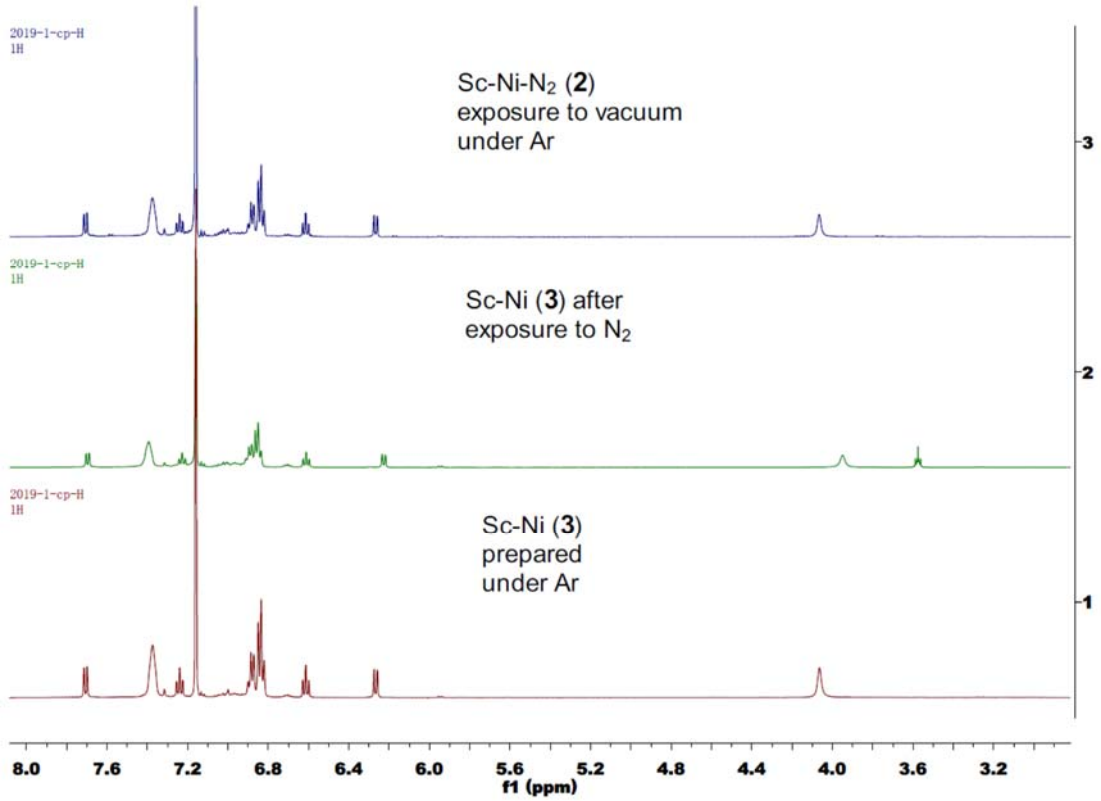


Figure S14. ^{1}H NMR spectra recorded in C_6D_6 at 25 °C showing the reversible transformation between **2** and **3**.

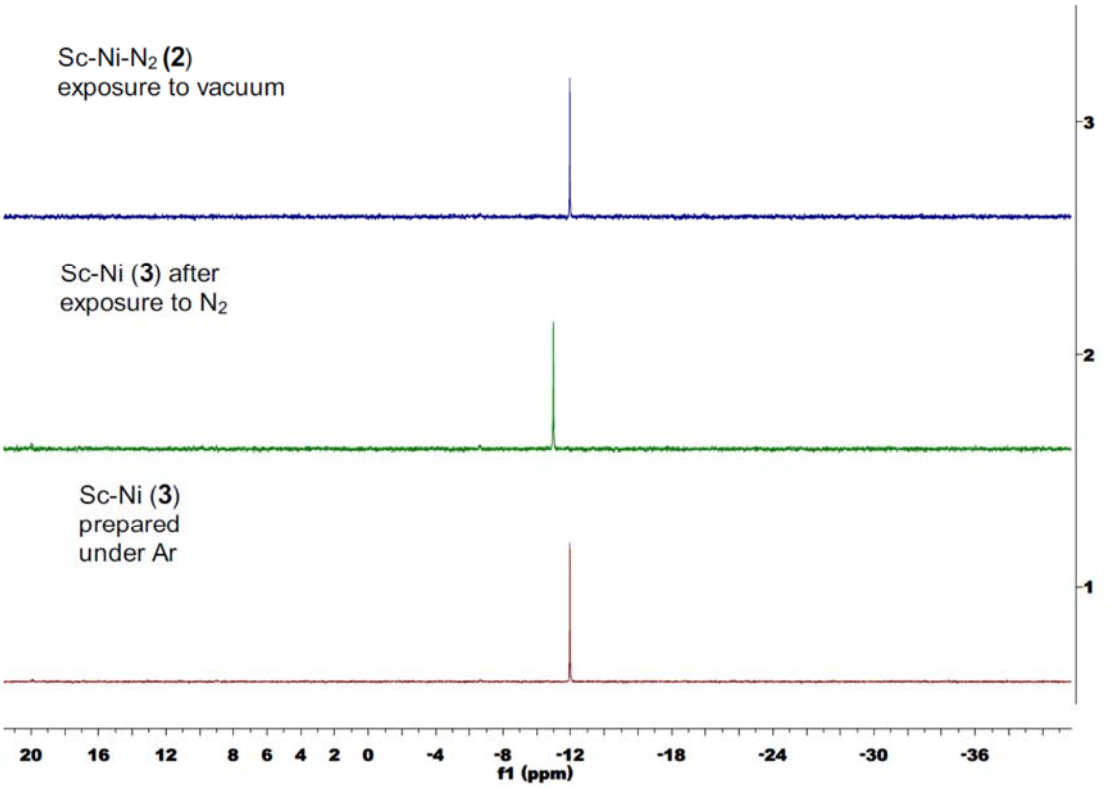


Figure S15. $^{31}P\{^{1}H\}$ NMR spectra recorded in C_6D_6 at 25 °C showing the reversible transformation between **2** and **3**.

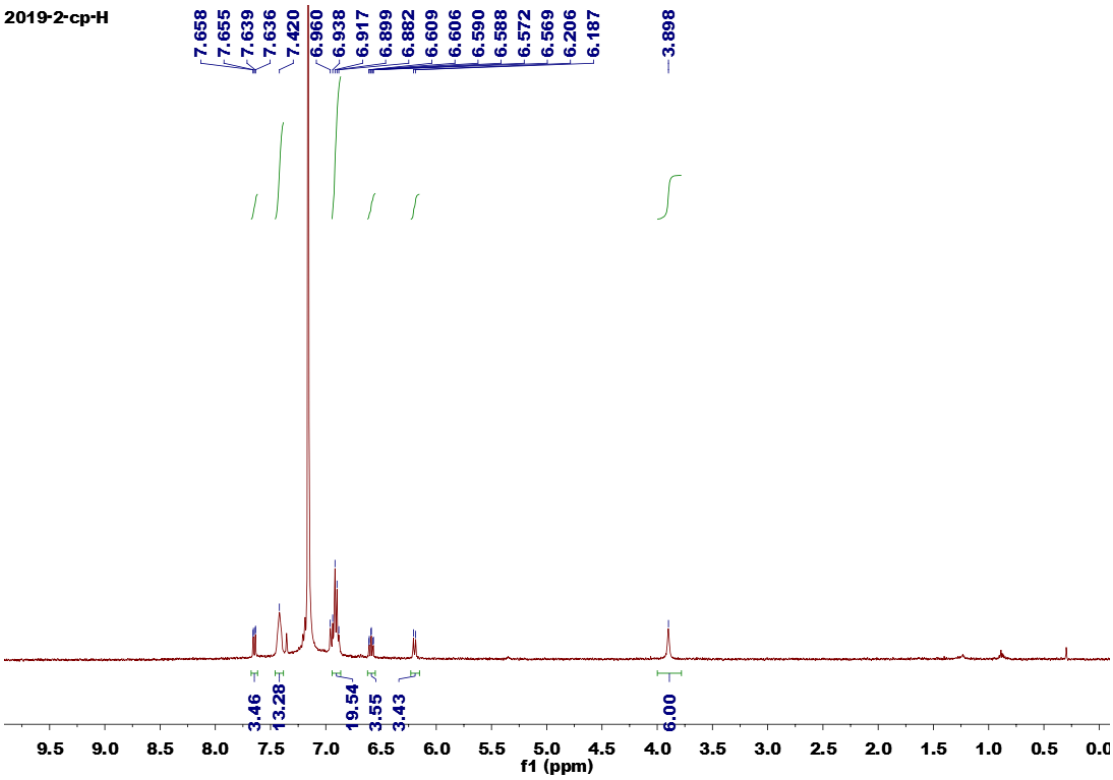


Figure S16. ^{1}H NMR spectrum of **4** in C_6D_6 at 25 °C.

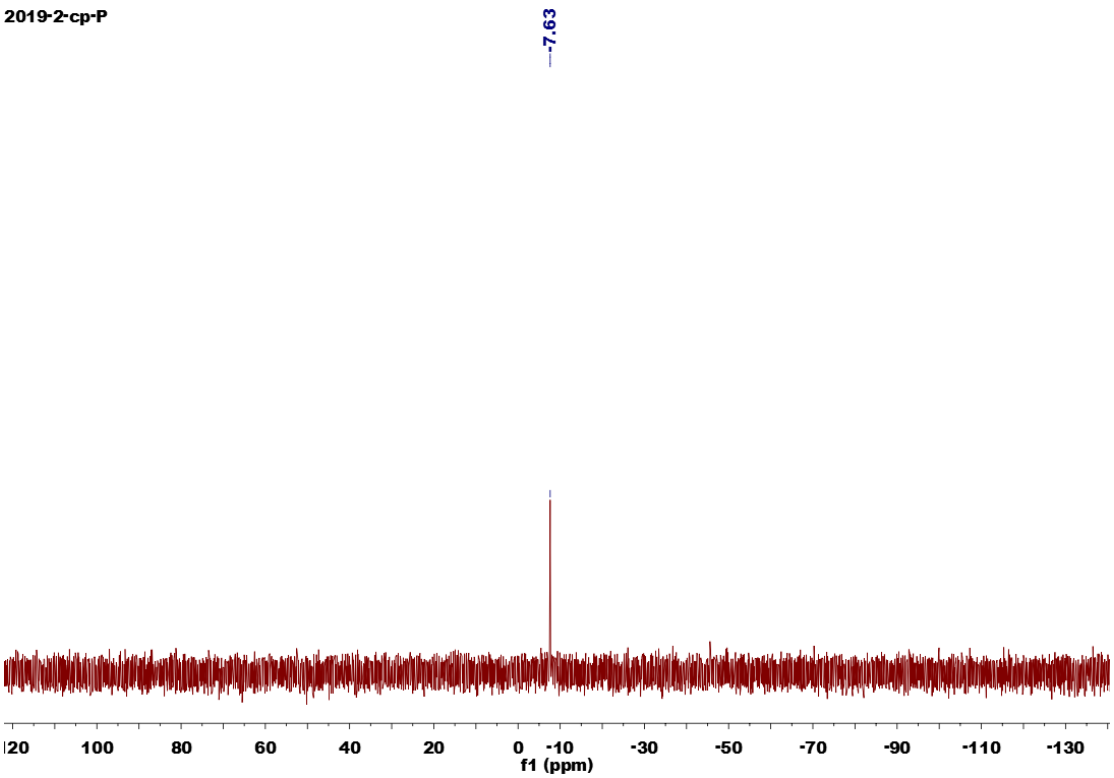


Figure S17. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 25 °C.

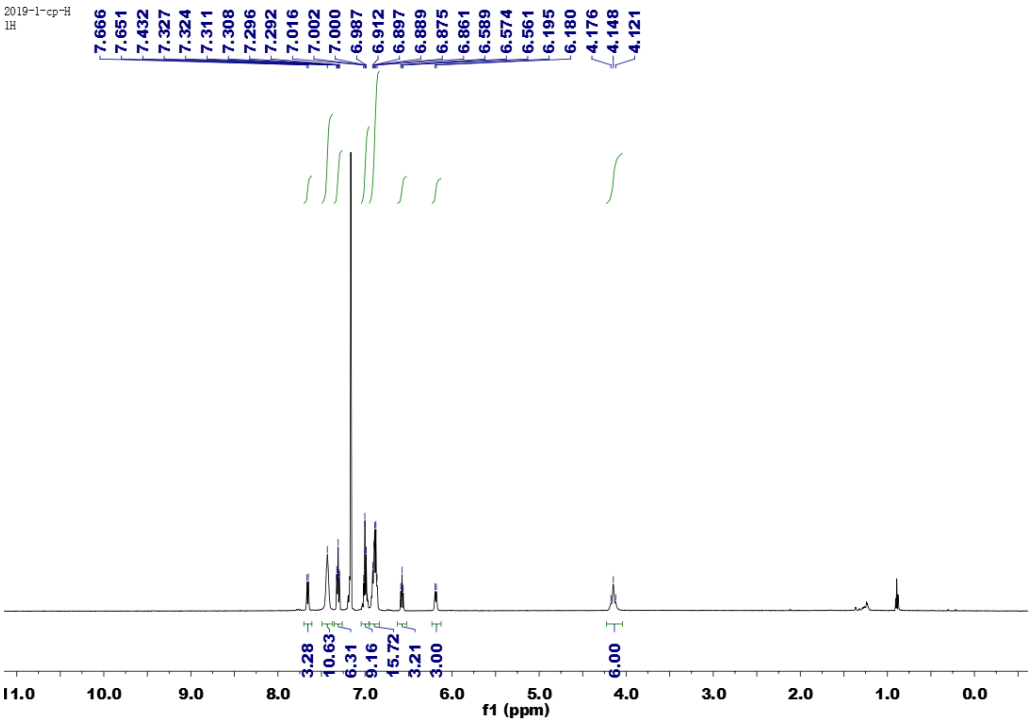


Figure S18. ^{1}H NMR spectrum of **5** in C_6D_6 at 25 °C.

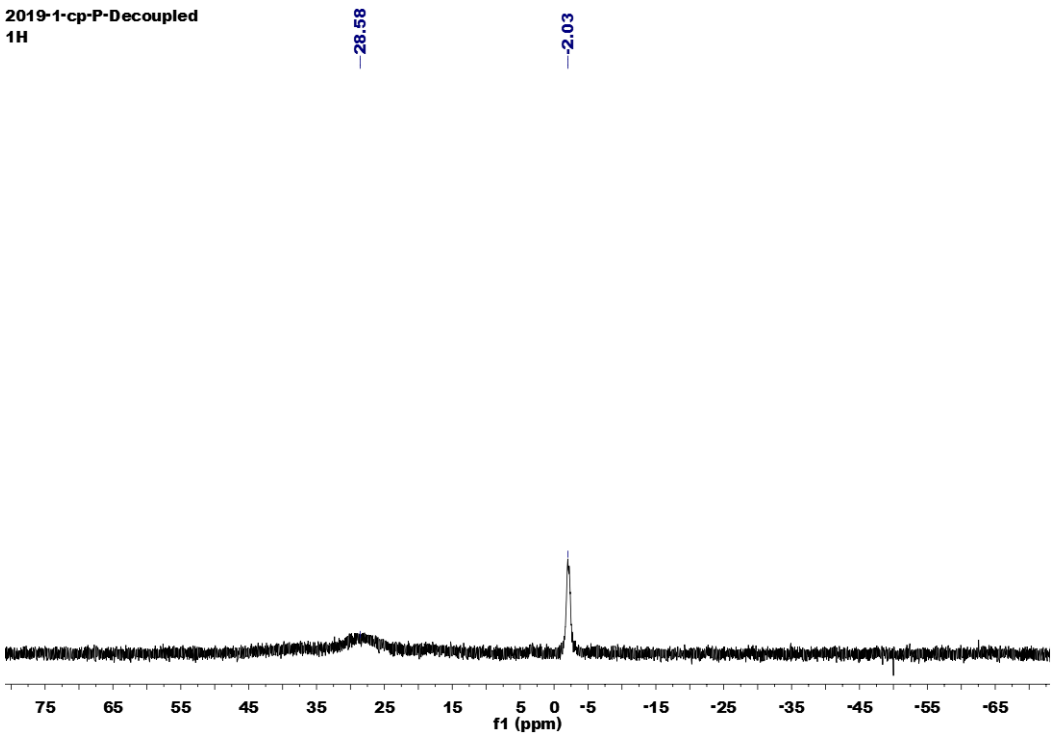


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 25 °C.

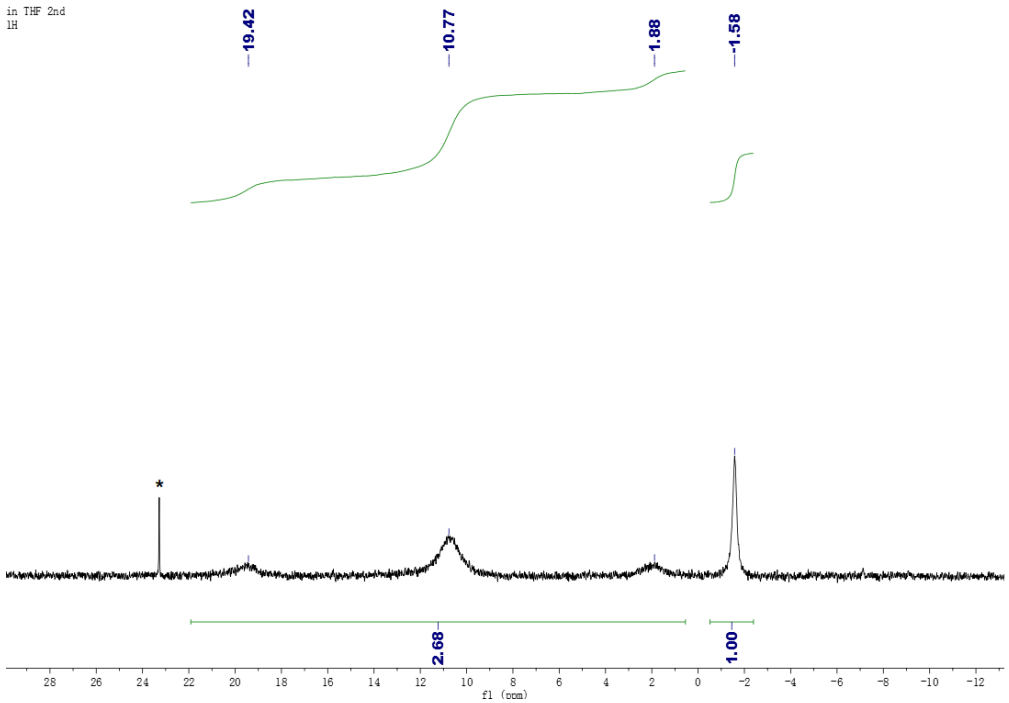


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in THF-d_8 at 25 °C. (* denotes small amount of $Pt(PPh_3)_4$)

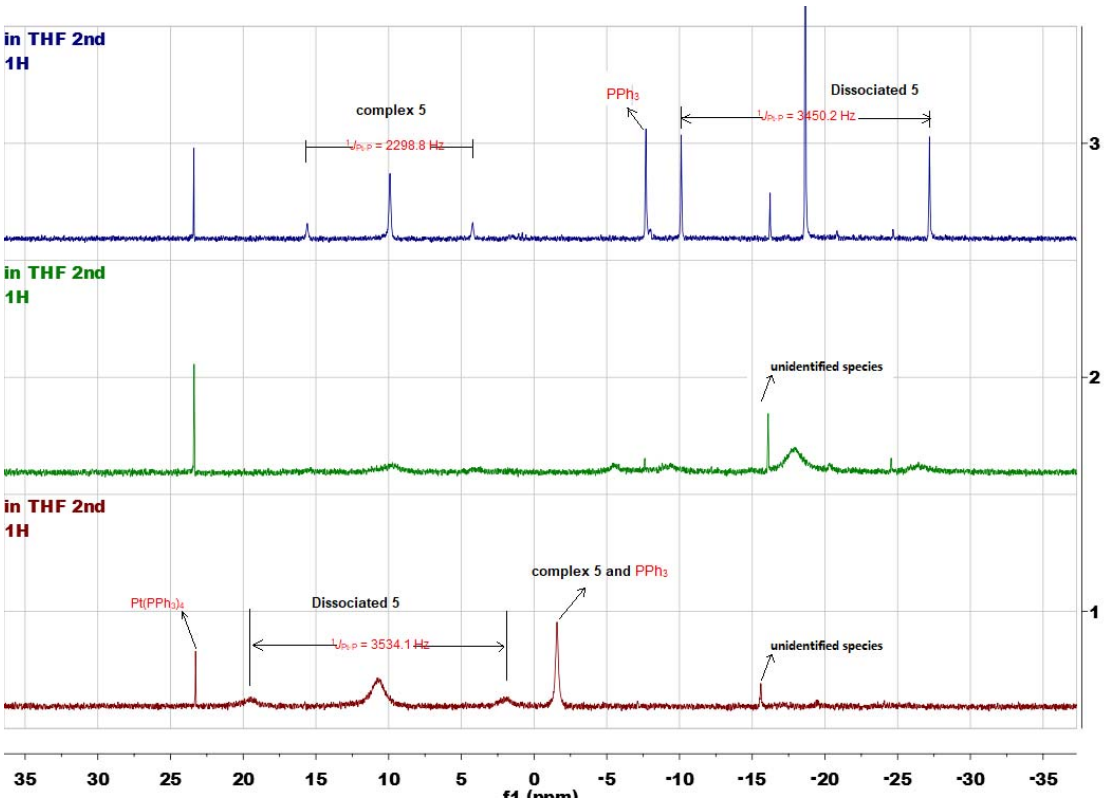


Figure S21. VT-$^{31}P\{^{1}H\}$ NMR spectra of **5** in THF-d_8.

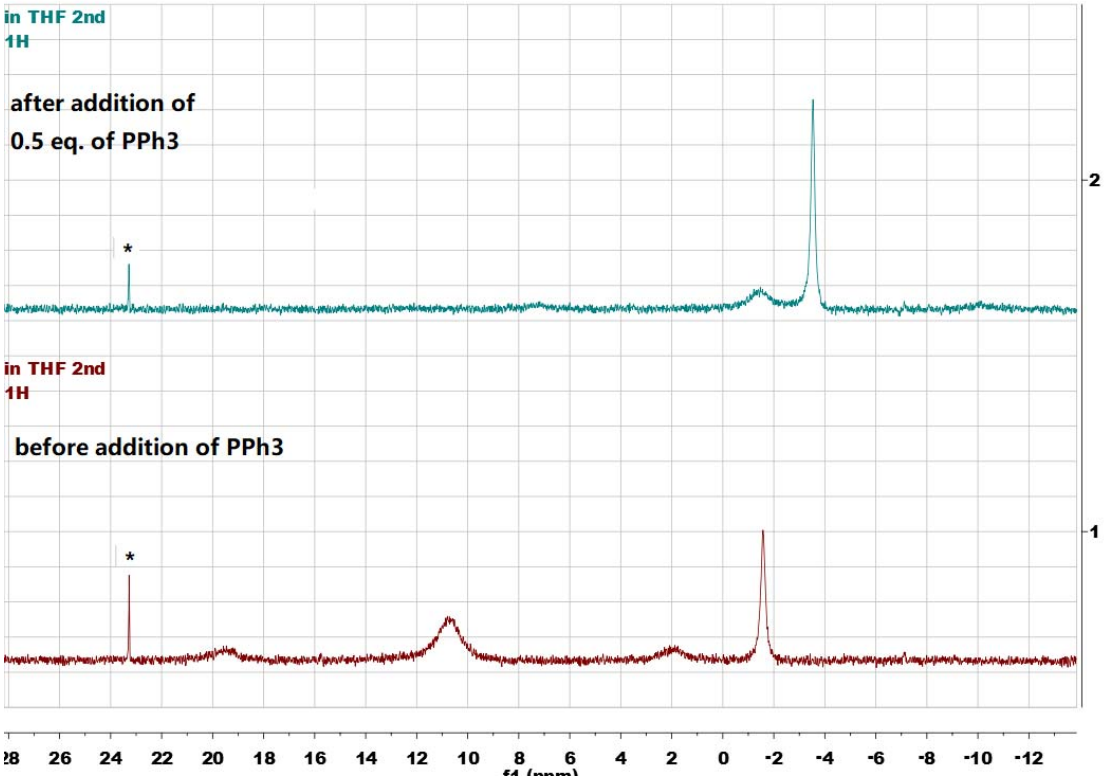


Figure S22. $^{31}P\{^{1}H\}$ NMR spectra of **5** in THF-d_8 before and after addition of PPh_3.
(* denotes to small amount of $Pt(PPh_3)_4$)

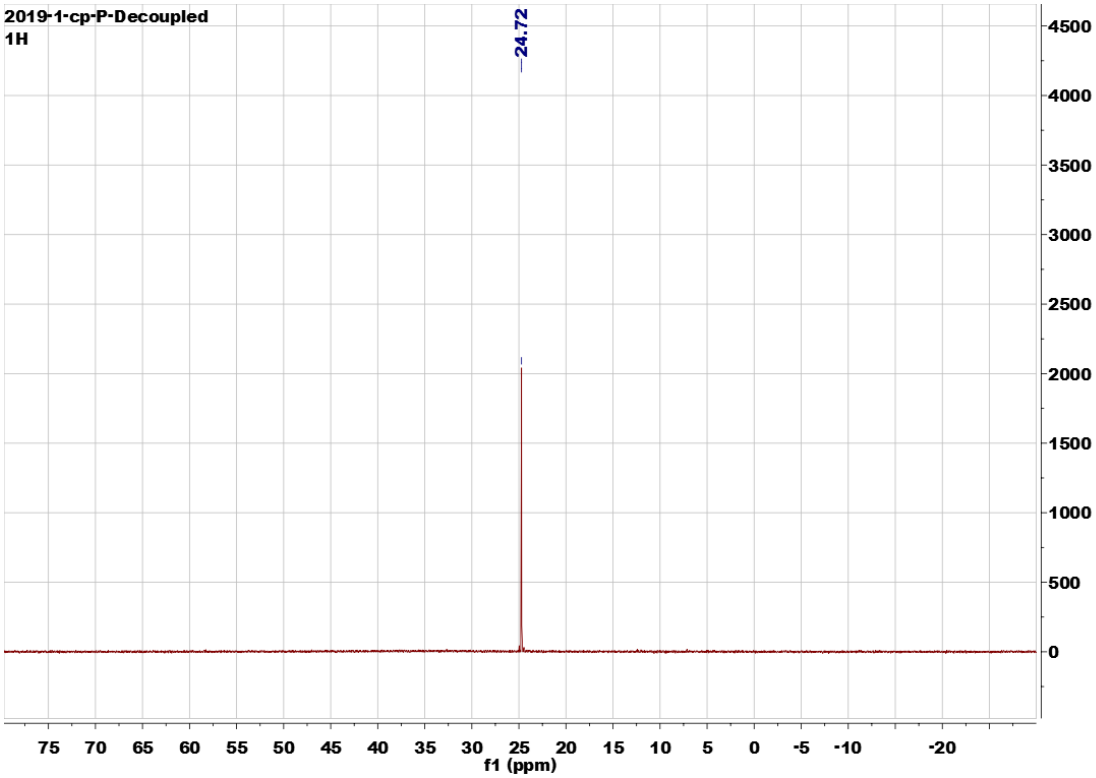
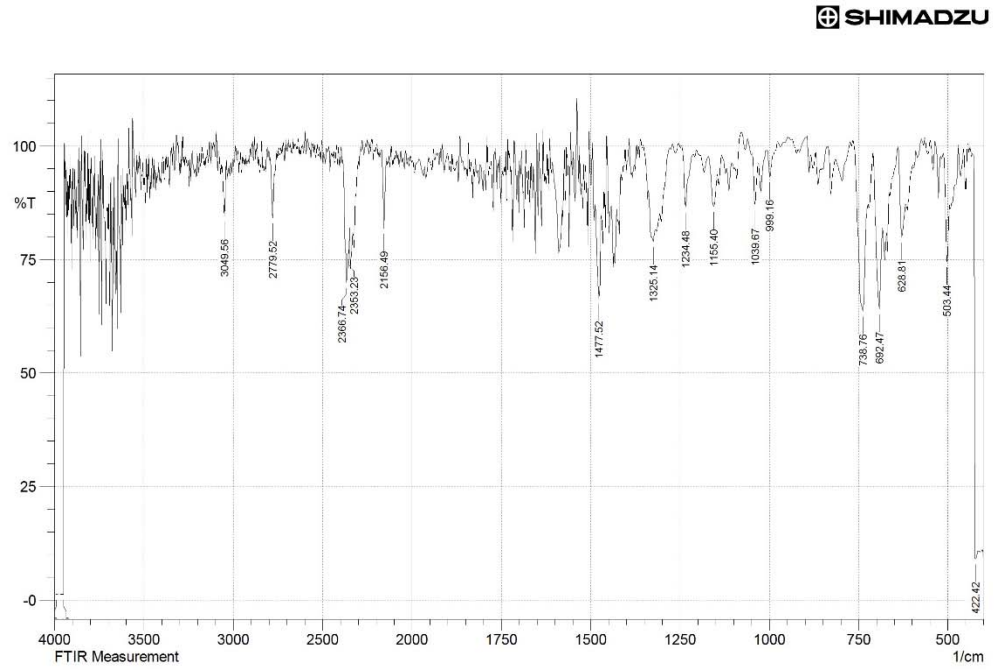


Figure S23. $^{31}P\{^{1}H\}$ NMR spectra of $Pt(PPh_3)_4$ in C_6D_6

IR spectrum



	Peak	Height	Corr. Height	Base (H)	Base (L)	Area	Corr. Area	
1	422.42	90.957	50.481	426.28	416.64	9.772	4.047	
2	503.44	25.522	17.532	513.08	495.72	1.285	0.694	
3	628.81	20.033	13.032	640.39	619.17	1.307	0.674	
4	692.47	35.858	23.801	709.83	682.82	3.042	1.801	
5	738.76	36.325	28.659	765.77	723.33	4.324	3.185	
6	999.16	6.735	5.85	1006.88	983.73	0.331	0.241	
7	1039.67	13.017	10.364	1047.38	1031.95	0.55	0.369	
8	1155.4	13.225	8.463	1170.83	1145.75	1	0.518	
9	1234.48	13.542	12.876	1246.06	1215.19	0.851	0.728	
10	1325.14	21.074	5.775	1338.64	1317.43	1.826	0.411	
11	1477.52	33.527	19.447	1487.17	1469.81	2.196	1.062	
12	2156.49	18.124	16.414	2169.99	2142.99	1.118	0.915	
13	2353.23	23.744	2.506	2355.16	2349.38	0.61	0.035	
14	2366.74	30.052	13.795	2389.88	2355.16	3.251	1.061	
15	2779.52	15.862	11.106	2793.02	2771.8	0.957	0.553	
16	3049.56	15.384	11.57	3063.06	3037.99	1.074	0.645	
17	3950.35	98.795	74.326	3958.06	3948.42	14.812	7.35	
18	3990.85	98.767	0.087	3998.57	3986.99	21.873	0.13	

Comment;
FTIR Measurement

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No. of Scans;
Resolution;
Apodization;
User; dujun

Figure S24. IR spectrum of **2**

2. X-ray Crystallography

X-ray Crystallography. Diffraction was performed on a Bruker SMART APEX II CCD area detector diffractometer using graphite-monochromated Mo *Kα* radiation (λ = 0.71073 Å) at 293(2) K, φ and ω scan technique. An empirical absorption correction was applied using the SADABS program.[1a] All structures were solved by direct methods, completed by subsequent difference Fourier syntheses, and refined anisotropically for all nonhydrogen atoms by full-matrix least-squares calculations based on F^2 using the SHELXTL program package.[1b] The hydrogen atom coordinates were calculated with SHELXTL by using an appropriate riding model with varied thermal parameters. The residual electron densities of solvent were squeezed by using PLATON.[1c] Crystal parameters and refinement results are given in Table S1.

Table S1. Crystallographic and Refinement Data[a,b] for **1-5**

	1	**2**	**3**	**4**	**5**
formula	$C_{57}H_{48}N_4P_3Sc$	$C_{57}H_{48}N_6NiP_3Sc$ ·C_6H_6	$C_{57}H_{48}N_4NiP_3Sc$ ·0.5C_6H_6	$C_{57}H_{48}N_4P_3PdSc$· 2C_6H_6	2($C_{75}H_{63}N_4P_4PtSc$)
Fw, g·mol^{-1}	926.86	1091.71	1024.62	1189.48	2768.47
cryst size, mm	0.24 x 0.21 x 0.20	0.13 x 0.12 x 0.1	0.24 x 0.22 x 0.2	0.21 x 0.19 x 0.18	0.22 x 0.21 x 0.20
cryst. syst.	monoclinic	trigonal	triclinic	monoclinic	trigonal
space group	P 1 21/n 1	R -3	P-1	P 1 21/c 1	P 3 1 c
T, K	273.15	273.15	273.15	273.15	273.15
a, Å	14.0508(5)	17.0935(4)	13.4558(7)	12.7713(7)	17.5350(8)
b, Å	21.3065(7)	17.0935(4)	14.5244(8)	13.5609(7)	17.5350(8)
c, Å	16.4830(5)	33.2789(11)	14.8808(7)	34.0377(16)	29.2315(12)
α, °	90	90	67.261(2)	90	90
β, °	99.061(2)	90	74.295(2)	96.025(2)	90
γ, °	90	120	85.223(2)	90	120
V, Å^3	4873.0(3)	8421.0(5)	2581.3(2)	5862.4(5)	7783.8(8)
Z	4	6	2	4	2
D_{calcd}, Kg·m^{-3}	1.263	1.292	1.318	1.348	1.181
F(000)	1936	3408	1066	2456	2800
μ, mm^{-1}	0.292	0.587	0.632	0.550	2.003
θ range /°	2.821 –27.557	2.808 - 27.560	2.840 - 27.608	2.949 - 27.595	3.023 - 27.701
refns collected	209048	120124	71672	230850	315796
indep reflns (R_{int})	11199 (0.0519)	4326 (0.0622)	11313 (0.1080)	13516 (0.0575)	11949 (0.0506)
reflns obsd [$I > 2\sigma(I)$]	8692	3438	6775	10935	10715
data/restrnts/params	11199 / 1212 / 586	4326 / 423 / 199	11313 / 24 / 622	13516 / 0 / 679	11949 / 7 / 500
*R*1, *wR*2 ($I > 2\sigma(I)$)	0.0530, 0.0747	0.0806, 0.1000	0.0722, 0.1417	0.0451, 0.0631	0.0424, 0.0532
*R*1, *wR*2 (all data)	0.1307, 0.1525	0.2253, 0.2479	0.1456, 0.1815	0.0901, 0.0962	0.0855, 0.0954
GOF on F2	1.086	1.057	1.034	1.197	1.128
$\Delta\rho_{max,\ min}$, e·Å^{-3}	0.560, -0.478	0.888, -0.996	0.892, -0.717	0.399, -0.798	0.874, -0.941

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

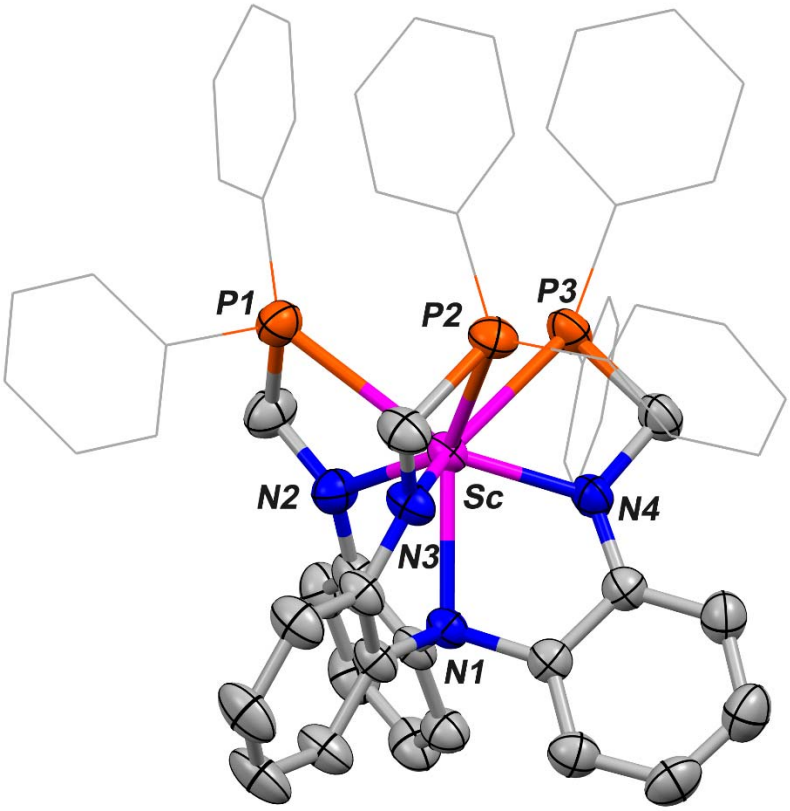

Figure S25. Molecular structure of complex **1**.

3. Computational Details

All calculations were performed with the ORCA program package.[2] For geometry optimizations, the hybrid B3LYP[3] density functional and the GGA-type BP86[4] density functional was used. The all-electron triple-ζ quality Def2-TZVP basis[5] sets were assigned for Ni, Sc metal centers and the coordinated atoms (such as N, P in the ligand, N in N_2 axial ligand), Def2-ECP pseudopotentials[6] with Def2-TZVP valence basis sets were used for heavier metal element Pd (28 core electrons) and Pt (60 core electrons), and Def2-SV(P) bases sets[5] were applied for the remaining elements in these compounds. The RI plus chain of spheres (RIJCOSX for B3LYP) approximation[7] was used to accelerate the calculations with the Weigend's "universal" Coulomb fitting auxiliary basis set def2/J[8] We had included the atom-pairwise dispersion correction with Becke-Johnson damping (D3BJ) to account for the van der Waals interaction.[8] All the geometries were fully optimized without symmetry constraints. The natural bond orbitals (NBO) analysis was done using NBO 6.0 program.[9]

Data based on B3LYP functional:

Calculated structures:

2:

N	-0.23034980139697	10.25627276945342	5.13381062459122
N	-0.13155097550762	10.13538386037523	4.03977206090800
Ni	-0.01688071988974	9.96976366281961	2.18658567962341
Sc	-0.00742573757397	9.90673407420410	-0.41902993870930
P	-1.84219076424606	8.71388459761186	1.68887712368500
N	0.04287744146237	9.86536359177495	-2.75688200102000
N	-1.24228520917076	8.33065425285143	-0.90414352328784
C	-1.87325319796535	7.61598882881388	0.17422511876504
H	-2.92744749372743	7.33714575624669	-0.03308170596464
H	-1.33246643377081	6.68933300556192	0.45430520370653
C	-0.23057271078937	6.54223083227593	-4.57404560362895
H	0.10085088270629	6.08101494584828	-5.50834733406048
C	0.14113964343288	7.86309123225298	-4.27247964727242
H	0.76238939270944	8.42749772950626	-4.97069226114562
C	-0.26858943844922	8.46401425438716	-3.08858061780777
C	-1.01572777798071	7.72601531772051	-2.11848126700811
C	-1.41167225548174	6.41447541704988	-2.45461546591366
H	-1.99876102476749	5.83436888969933	-1.73838154513845
C	-1.02848951331788	5.83768511978144	-3.67150871827979
H	-1.34987910989673	4.81738066250412	-3.90579579806905
C	-5.38800824995504	11.64915919754071	1.11333281901468
H	-6.19249732603657	12.38013835059020	0.98552045350345
C	-5.07932750749223	11.15594923966170	2.38592114709787
H	-5.64371200876481	11.50014587968404	3.25817339168325
C	-4.04713733326453	10.22761716004079	2.54797764613320

H	-3.81090976101144	9.84619310043322	3.54540042188458
C	-3.30806475224503	9.77997974332206	1.43901407423974
C	-3.63263880961397	10.27088007732062	0.16176493950961
H	-3.06628621989628	9.94117441810209	-0.71190661091441
C	-4.66433663391920	11.20058073907651	0.00321747213946
H	-4.89129364033271	11.58134525250287	-0.99678397348577
C	-3.30350493445369	5.58801553704639	4.79764560846047
H	-3.64607008836690	4.83682812411826	5.51663824130078
C	-2.05428428478899	6.19404655450217	4.95558987866090
H	-1.41163113505424	5.91922972988232	5.79740229707550
C	-1.61856355169327	7.15351062566715	4.03447644462242
H	-0.64022247105955	7.61735919973241	4.15563187173437
C	-2.42634175562939	7.52129770891366	2.95076421092051
C	-3.68642829696988	6.91271719020013	2.80511203727587
H	-4.33654765894100	7.19969521593693	1.97426348080511
C	-4.11946402613730	5.95062510996761	3.71871103035186
H	-5.09910014842646	5.48086069548850	3.58875770734695
P	1.94280311135583	8.96464330568447	1.69748835868503
N	2.00110983669926	9.72304795466110	-0.86013837555391
C	2.93038420085365	9.54673280334566	0.22652317586753
H	3.72033173487004	8.79580966332494	0.01945416475968
H	3.43474786672636	10.48605867638029	0.53066596426200
C	3.06061851920366	11.10920004298312	-4.68989638395041
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C	3.18570856783998	7.14582154825212	19.36795489639761
H	2.95361931812155	6.79731848972649	20.37628886376125
C	2.37920335321297	6.76338140738430	18.29148690023234
H	1.52073891108374	6.10685897968973	18.46344254962143
C	2.68021495856792	7.21098950813081	17.00227084728635
H	2.06072845572838	6.89993533719214	16.15558304949730
C	3.77539088747725	8.06049931832042	16.79857434809140
H	4.01317192617712	8.42556940514175	15.79444103790878
C	4.57658149024695	8.44088853561053	17.87660126049182
H	5.42608448817116	9.10626331331393	17.70077007861260
C	5.22739341060340	10.18199180090746	20.79807258806143
C	6.11240240072485	10.81702519871864	21.69020831691351
H	6.90301038291571	10.24164485557800	22.17762192188964
C	5.96657097214008	12.17278180906252	21.98404830265804
H	6.66492318270939	12.65032727295619	22.67844726217723

C	4.92233792548634	12.90856335051771	21.40743420620873
H	4.78965918535512	13.96550820691452	21.65969000871990
C	4.04105355384231	12.28508309477080	20.51922919949769
H	3.22714928713460	12.85594961469983	20.06133933586602
C	4.19417203011483	10.92894246477757	20.21031057822490
H	3.50070322969448	10.44844023506218	19.51589827555615
N	7.86784070567263	4.01443785998236	20.50830267047328
N	7.70587632485211	5.01559057532450	23.10421514296292
N	5.15058818923842	4.02963514525858	20.97922151426565
N	7.38666005372293	6.71335586232715	20.07113259412377
P	6.65910724306397	7.18725809232063	24.31600642872685
P	3.59222991820362	5.27553194448952	22.75443384065690
P	5.36697396170276	8.37772653066192	20.60277550927147
Pd	4.98349937600015	7.21539969893197	22.63596547069556
Sc	6.47003054353167	5.54255331716155	21.51873020721895

5:

Pt	-8.76902336799131	15.16748678976565	12.28401301408518
Sc	-8.71374888782785	15.21772237891154	15.03992116172369
P	-6.70266882401875	14.13208279659253	12.96188984699062
P	-8.68386202240861	15.24664917361602	9.85762849875986
C	-5.29217286900159	13.95585955936861	11.80352313366992
C	-6.31736260522864	15.68330594806226	16.66483207894198
N	-8.65772953015455	15.27383392094744	17.36182838508294
C	-7.32816798463528	15.83473162202413	17.66710632382344
N	-6.70233366193502	15.13598466903957	15.46475489149913
C	-7.01321082528211	12.41932693133144	13.53219151326141
C	-5.01793071747143	16.14305260449532	16.96725712664542
H	-4.22935538193335	16.03752620817665	16.21773596841600
C	-7.04478007710527	16.48444824848587	18.86310983886579
H	-7.84366383749353	16.63454001402032	19.59182587712140
C	-12.58700499257554	15.77895173400356	8.74755642959390
H	-13.53774659274587	15.30793088840182	9.01663355224058
C	-5.77109964667011	14.87014481614621	14.40629645541403
H	-4.96703899878676	14.15895918171196	14.68859516468362
H	-5.27559043330842	15.77867048549598	14.01382379993480
C	-10.13811408500904	16.95170638142780	8.07989868286432
H	-9.18897562975925	17.41932048126280	7.81240391258718
C	-7.91520397167071	10.21380001206339	13.02015983099733
H	-8.35039649011377	9.52032016982874	12.29466447818686
C	-4.64218461304758	12.73298989942863	11.56297712848314
H	-4.96451917912816	11.83264633163829	12.08855168611797
C	-11.40693975877225	15.32688764354218	9.33843951878119
H	-11.43799638689084	14.50086004152355	10.05222421072062

C	-4.74322587379002	16.76593961550901	18.18970751639558
H	-3.73035423732146	17.12933662458207	18.39478793880050
C	-4.85322489887228	15.09903105350501	11.11668760248966
H	-5.36278604096816	16.05032679137066	11.26555820986837
C	-3.16718964070895	13.80403424939857	9.96005882855769
H	-2.34790831145041	13.74081998391320	9.23711619080524
C	-6.82644353431405	12.01388061440468	14.86379848179410
H	-6.44731691505867	12.71634703741192	15.60635420945093
C	-7.56579810353639	11.50359789760399	12.61875178496946
H	-7.73647095039046	11.80918474454062	11.58546844157648
C	-5.75056125348274	16.95510201363705	19.13704874311299
H	-5.53971318070307	17.46354343564407	20.08188323109299
C	-3.59960352853835	12.65736855511123	10.63428116953642
H	-3.11671571746370	11.69491957536775	10.43761247102354
C	-3.79169035465793	15.02919424636929	10.21288859636482
H	-3.47162456379917	15.93273276567844	9.68859279880097
C	-11.32060570348037	17.40875719107756	7.48816852586056
H	-11.27974148187151	18.23293392197835	6.76910386520000
C	-12.54777881823617	16.82960856001141	7.82151073403986
H	-13.47035483672871	17.19817897044027	7.36247791678902
C	-7.19733743573649	10.72742087130466	15.27111693618180
H	-7.07515296634753	10.44166167755625	16.31862526640859
C	-7.73893413267514	9.82390738893787	14.35345676442540
H	-8.04307143234294	8.82512149835610	14.68117217974630
C	-10.17047309668834	15.91289592732360	9.01957142106770
P	-9.09499564688917	17.43775568689360	12.99381103728667
C	-9.74776344524153	18.64567632983715	11.79275421109869
C	-10.33054326413516	17.00445991569243	16.75703073601984
C	-9.78948062232535	16.13255784672813	17.75599833720103
N	-9.83256976703818	16.89284306521528	15.48623460850729
C	-7.58769243934735	18.22203606096297	13.69917398650081
C	-11.36697477025346	17.88168362230559	17.14894386179434
H	-11.81121344441803	18.54642348007860	16.40510671790950
C	-10.32105918803396	16.10980147170190	19.03993146480047
H	-9.92557993364190	15.39546222481597	19.76611070026422
C	-10.29807584600768	17.70288875957073	14.39343517114098
H	-10.33718897652070	18.78771838045572	14.61852480613788
H	-11.29929669710698	17.41800972900549	14.02036397025890
C	-5.17010978046621	18.52829934260217	13.56566133352837
H	-4.23103152408203	18.34541454347574	13.03323499258918
C	-9.08968387916486	19.83692853742788	11.45084247595630
H	-8.13396859113970	20.08441279466935	11.91852974530511
C	-11.86418100148861	17.87169738521853	18.45657486957416
H	-12.67597915785240	18.55580509293224	18.72709181177621

C	-10.98119048286919	18.34917163195190	11.18927643142566
H	-11.49047904737314	17.41625067053490	11.43256433069018
C	-10.88208982105625	20.40798430874533	9.91938000781873
H	-11.32031497217357	21.09201710667444	9.18581231804865
C	-7.58466532635086	18.93953195082031	14.90848423027744
H	-8.50645314503985	19.10199611127628	15.46430745482786
C	-6.36225434019263	18.02199768688507	13.04601024667705
H	-6.34548499495101	17.43665245095231	12.12819407946321
C	-11.35994850335702	16.98043495830105	19.40621343764209
H	-11.76957212434278	16.95279885982736	20.41952650241093
C	-9.64832724473104	20.70467507276184	10.50644198190847
H	-9.11841544860304	21.62236963264882	10.23244660943097
C	-11.55184293054937	19.23155462802733	10.27286604416702
H	-12.51322449242668	18.98360506848309	9.81657384364749
C	-6.39015929359769	19.42359467077075	15.44669724456670
H	-6.40678840362663	19.94503854910887	16.40761510638758
C	-5.17921861975841	19.22505458134065	14.77773441688793
H	-4.24729860772749	19.59770178670251	15.21325526217523
P	-10.64239756325037	13.84320460359337	13.02405557819948
C	-11.42940376700950	12.61994599977150	11.91178382162042
C	-9.47856249808162	12.99980836888418	16.78772022026421
C	-8.81985747442790	13.85377487755414	17.73128852712420
N	-9.74710742214536	13.51457620938108	15.54365446558835
C	-12.08330838041420	14.83983174957384	13.58158728019345
C	-9.75476305168824	11.67532786113689	17.18856607952159
H	-10.27405176987796	11.00918295234107	16.49576266515577
C	-8.35221915218541	13.34534373105254	18.93636608721339
H	-7.79592740557227	14.00294712509711	19.60834662321195
C	-10.38386319391565	12.73967909852113	14.51302594251849
H	-11.37833914810332	12.34382626709825	14.80695141848515
H	-9.77647633679126	11.88067228393962	14.16949856806530
C	-13.88431840372350	16.37804530135067	12.99769431189351
H	-14.45482056101653	16.90976100715700	12.22987944229699
C	-12.74906162962935	12.18491314737060	12.12676767546711
H	-13.33832620756119	12.61555810978173	12.94054424703744
C	-9.32005778161840	11.19293799733030	18.42810954089911
H	-9.54301008030426	10.15783590419883	18.70825688761248
C	-10.68959349132563	12.05309011260034	10.86678762648877
H	-9.66857993623784	12.39161629397076	10.69758148077756
C	-12.56773968330249	10.65686518611420	10.25123385900084
H	-13.01526229473598	9.89817856656271	9.60112416746435
C	-12.41603006666135	15.00376706366183	14.93763814444510
H	-11.83231483888218	14.50328848788172	15.71075171427416
C	-12.83706730374247	15.53626393791787	12.62064610279356

H	-12.60082992719132	15.42167354693026	11.56286440614797
C	-8.58979430767336	12.00753921515844	19.29512984920047
H	-8.21515804774814	11.61960090254991	20.24618777502711
C	-13.31145297478765	11.20742221194699	11.30291013741045
H	-14.33574645156954	10.86839989698849	11.48706760212731
C	-11.25312845060279	11.08031802036598	10.03526313997157
H	-10.65946221829591	10.66289340099267	9.21770903302525
C	-13.45491532183726	15.86198198863254	15.31690347626541
H	-13.67447647104879	15.99804826167390	16.37936406993489
C	-14.19163038433203	16.55331339479020	14.35221008879065
H	-15.00057002197538	17.22590324965551	14.65428386595547
C	-7.00559966608556	11.72814627193820	8.60775696630843
H	-6.12217393390959	11.15397094490449	8.90390410384598
C	-9.24464780876538	13.23859820434673	7.87849247047215
H	-10.11644424479799	13.82153011143506	7.57666345514597
C	-7.30457101808666	12.91355231816788	9.27677033706688
H	-6.64433220147939	13.25792790732834	10.07003839572247
C	-8.94987281892429	12.04467999597046	7.20743225024570
H	-9.60093367049301	11.70921377284907	6.39391962879699
C	-7.83275349748059	11.28530003055337	7.56824251755314
H	-7.60128740520378	10.35641170756212	7.03809369922545
C	-8.42499807843645	13.68308410583845	8.92590226836600
C	-6.02921182843339	18.31909825690324	9.22958200917170
H	-5.83418007204705	19.28595087894133	9.70394953639713
C	-6.54586164829032	15.84313064015070	8.04476769444651
H	-6.73239022571036	14.88038194724520	7.56859178380630
C	-7.07710657633336	17.52120026100570	9.69112195153825
H	-7.70466023987276	17.87566349470538	10.50535812356175
C	-5.49751484838490	16.64047306256601	7.57569844152639
H	-4.88236057444429	16.28525132130075	6.74292039105740
C	-5.22597808605644	17.87487393917728	8.17311177123466
H	-4.39731768878598	18.49281876195059	7.81352291065566
C	-7.33815369470354	16.26532259388300	9.12381665243123

Table S2. Calculated bond lengths for selected bonds in **2**, **3**, **4**, **5**

	Sc-M (M = Ni, Pd, Pt) (Å)	Sc-N (Å)	M-P (M = Ni, Pd, Pt) (Å)	Ni-N (Å)
2	2.606	2.061; 2.060; 2.065; 2.339 (axial)	2.275; 2.256; 2.271	1.864
3	2.369	2.073; 2.076; 2.076 2.307 (axial)	2.225; 2.224; 2.218	-
4	2.501	2.078; 2.075; 2.079; 2.304 (axial)	2.373; 2.390; 2.373	-
5	2.757	2.055; 2.063; 2.057; 2.323 (axial)	2.411; 2.401; 2.409; 2.429 (axial)	-

Table S3. Calculated atomic charges

	Mülliken Charges		Löewdin Charges		Natural Charges	
	Sc	M (M = Ni, Pd, Pt)	Sc	M (M = Ni, Pd, Pt)	Sc	M (M = Ni, Pd, Pt)
2	0.472	-0.360	-0.536	-1.000	1.700	0.160
3	0.639	-0.379	-0.525	-0.872	1.611	0.020
4	0.999	-0.606	-0.404	-0.854	1.693	-0.061
5	0.441	-0.184	-0.571	-0.682	1.738	-0.011

Table S4. Calculated Wieberg and Mayer bond orders for selected bonds in **2**, **3**, **4**, **5**

	Wieberg Bond Orders	Mayer Bond Orders
2	0.612	0.416
3	0.873	0.488
4	0.869	0.430
5	0.649	0.446

Table S5. Calculated natural electron configurations for metal centers in **2**, **3**, **4**, **5**

Compound	Electron Configuration
2	Ni [core]4s(0.34)3d(9.45)4p(0.02)5s(0.01)4d(0.02)
	Sc [core]4s(0.18)3d(0.89)4p(0.01)4d(0.21)5d(0.01)
3	Ni [core]4s(0.37)3d(9.57)4p(0.02)4d(0.01)
	Sc [core]4s(0.17)3d(1.04)4p(0.01)4d(0.16)5d(0.01)
4	Pd [core]5s(0.41)4d(9.62)5p(0.02)6p(0.01)
	Sc [core]4s(0.18)3d(0.95)4p(0.01)4d(0.16)5d(0.01)
5	Pt [core]6s(0.47)5d(9.49)6p(0.02)6d(0.02)7p(0.01)
	Sc [core]4s(0.16)3d(0.81)4p(0.01)4d(0.26)5d(0.01)

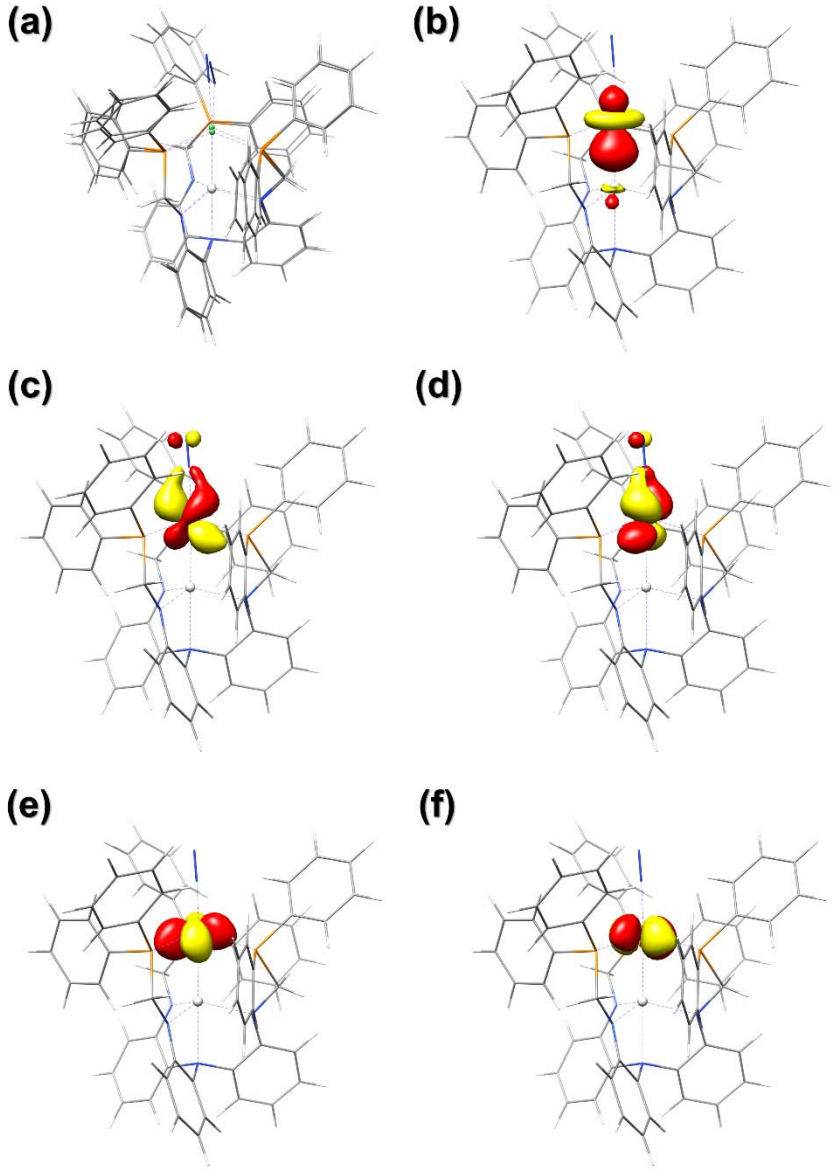

Figure S26. Superimposing of the calculated structure and solid state structure of **2** (a), localized orbitals representing the dative Ni-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **2** (isovalue = 0.05).

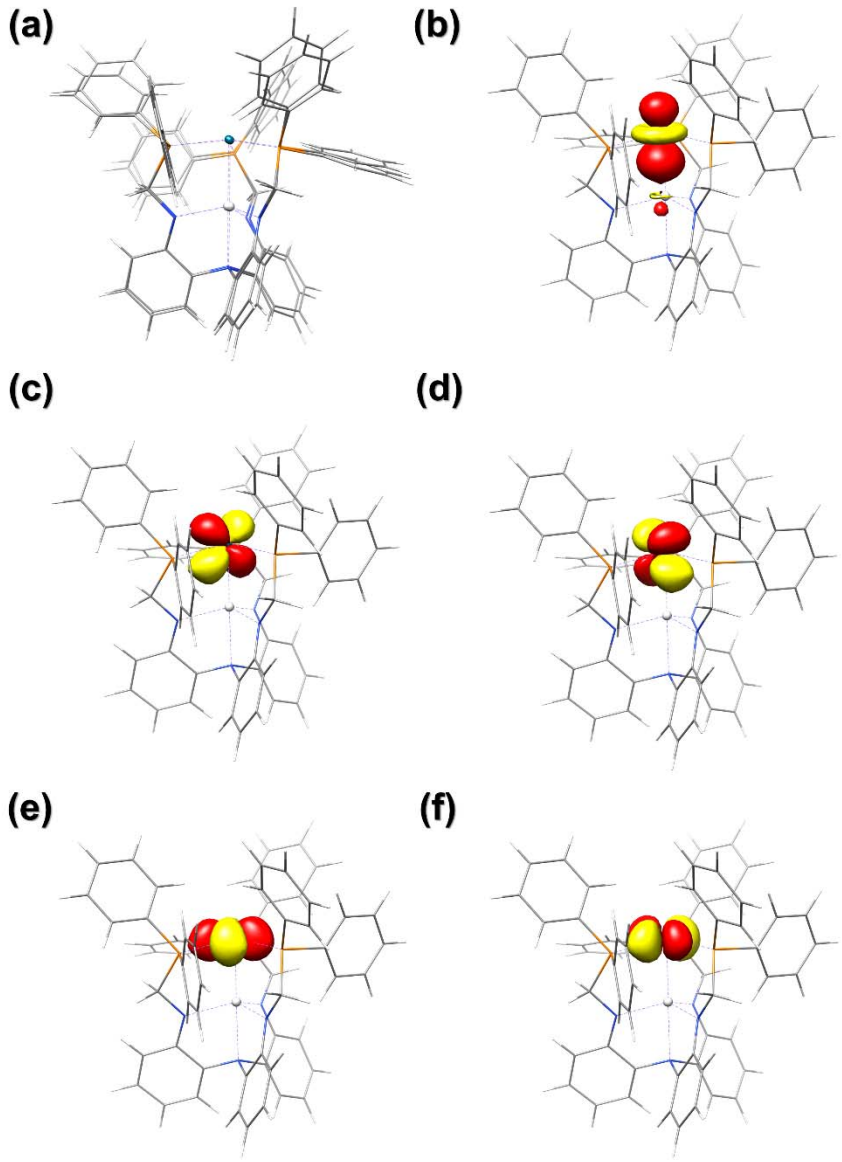

Figure S27. Superimposing of the calculated structure and solid state structure of **4** (a), localized orbitals representing the dative Ni-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **4** (isovalue = 0.05).

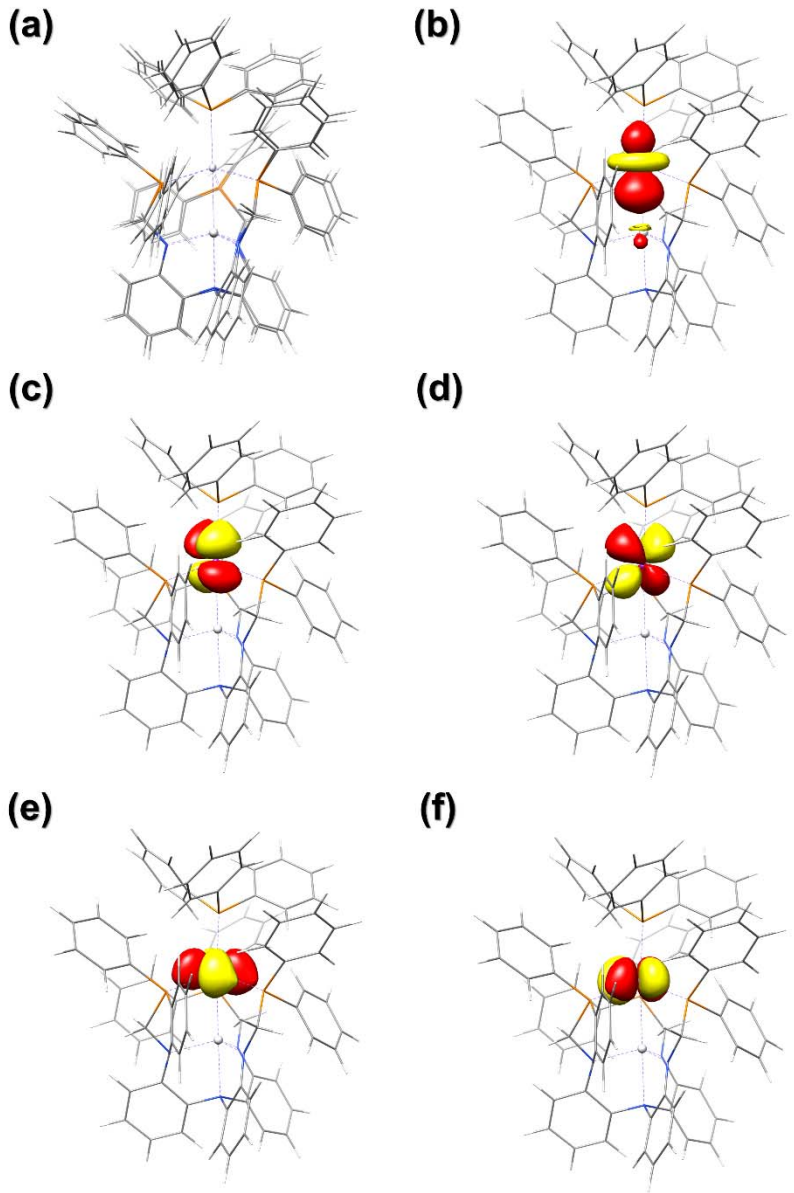

Figure S28. Superimposing of the calculated and solid state structure of **5** (a), localized orbitals representing the 4 doubly occupied *d* atomic orbitals of Ni metal center (b-e) in **5**.

Data based on BP86 functional:

Calculated structures:

2:

N	-0.40404603391517	10.39442195342852	5.11712708307927
N	-0.22715937146876	10.18263014804910	4.02798340262188
Ni	-0.04738530611833	9.96012198406046	2.22438937667926
Sc	-0.03097598095388	9.90105462906554	-0.39416402921180
P	-1.80970493151695	8.69195696850887	1.67789306178692
N	0.01193549134774	9.88100410169229	-2.73014076826989
N	-1.19831186345264	8.27856673491874	-0.90287549650472
C	-1.80548700477861	7.55410360428885	0.18577824030904
H	-2.86232131154230	7.24095683940917	-0.01212719234164
H	-1.23247444133255	6.64289221287362	0.49011522226633
C	-0.00878594120503	6.54670721778931	-4.56401053277156
H	0.36055282750345	6.10762948913649	-5.50414661412589
C	0.26010737039540	7.89993107570834	-4.26335100304254
H	0.84398894267435	8.52267973892226	-4.95965852955508
C	-0.20341742798011	8.46544547768517	-3.07472160257526
C	-0.91272477763819	7.67505320530431	-2.10847515532258
C	-1.20493863745689	6.32942568925662	-2.44336961112759
H	-1.75734363865224	5.70470327753621	-1.72385420182025
C	-0.75781224695721	5.77916964474219	-3.65820702971688
H	-0.98727542728603	4.72478074397673	-3.88762956905506
C	-5.30290224728411	11.67024425119819	0.98144846966745
H	-6.09101821715192	12.42575918385300	0.82584394091698
C	-4.98717184907941	11.23678887017841	2.28202399200230
H	-5.53237500912305	11.64503397787568	3.14906640008342
C	-3.97189876591694	10.28793976569774	2.48196205814463
H	-3.72491362975715	9.95210262555589	3.50273805407966
C	-3.26740506390951	9.75355626564461	1.37966672998243
C	-3.60701533824307	10.17203898172155	0.07369050497010
H	-3.06752588375577	9.76139777202130	-0.79508008978632
C	-4.61639199791812	11.12935097732091	-0.11988232234827
H	-4.85540325968383	11.45380323981995	-1.14517124578394
C	-3.26330738707393	5.65084239694011	4.87710587259808
H	-3.60323548329785	4.91513470738926	5.62528413042055
C	-2.00305800462589	6.25709887871134	5.00904345252887
H	-1.35011537386490	6.00367925209792	5.86053096475845
C	-1.57241693421358	7.19575468134804	4.05681425344922
H	-0.59055093844726	7.67787890450118	4.15582451557972
C	-2.39454253134172	7.53315682911204	2.96569696215221
C	-3.66552729685546	6.92858636537969	2.84357327753219
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H	9.48751389305961	8.06749056660288	18.93903408612972
C	8.62886998550043	6.21947338888729	19.71797132695642
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H	5.15022611145752	14.05925523074774	21.41107807664173
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H	3.58946317241533	10.52363528052793	19.42179064468856
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P	6.56742693192771	7.19608778575939	24.24021634518385
P	3.59138038006372	5.26358461989189	22.75112829604913
P	5.35543754793990	8.37879394984714	20.58082107447893
Pd	4.90350545408476	7.21428796754590	22.57351839014422
Sc	6.42459644796576	5.55514904951484	21.51712615613317

5:

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P	-6.72055782491490	14.24595212095434	12.99003784823366
P	-8.77059842064103	15.19451362513197	9.89380292237657
C	-5.28182494080386	14.09756091556929	11.86571961506562
C	-6.42170295950946	15.70103475979798	16.74313067095907
N	-8.75962679894656	15.18953402804554	17.37498995565478
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N	-6.76630042274230	15.16083480150991	15.52542441673433
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H	-9.02824299753094	21.96115995977859	10.84960839108809
C	-11.19507585090607	19.38661766568895	10.16165828302562
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C	-4.78595067251259	18.92484384613886	14.37724566655474
H	-3.77819451812460	19.24418394691461	14.69015778617572
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C	-8.60401953640889	11.89137839974919	19.26801881978066
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H	-10.60713081393505	10.38335990408528	9.49169544182248
C	-13.39645074759783	15.89441819872130	15.34873881192437
H	-13.69712618399029	15.92494496990203	16.40748303352546
C	-13.98668192688950	16.76227165020370	14.41522651380063
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C	-9.32678121672597	13.03442377140474	8.08274280999942
H	-10.23772593304152	13.57184190138445	7.78092480948833
C	-7.29229268311472	12.87963610639466	9.39621874164915

H	-6.59056117237833	13.31331944372808	10.12285268572099
C	-9.03694228532122	11.78895850123881	7.49965446203259
H	-9.73011105433173	11.36789188520228	6.75204067643901
C	-7.87848298448743	11.08331185387267	7.86357687520932
H	-7.65643121899932	10.10492815701627	7.40684595825448
C	-8.46385166328960	13.58743523937589	9.05030588909644
C	-6.54998866135773	18.50002123780030	8.85671909151381
H	-6.54172816837797	19.55931909403408	9.16221691763830
C	-6.61974485258374	15.79810830558531	8.08783619588206
H	-6.64246853414821	14.74568366766524	7.76938306586920
C	-7.48522816502030	17.62660870977433	9.42945051987798
H	-8.20698489865004	18.01301734298131	10.16235779103981
C	-5.67614806208784	16.67123915422033	7.51971353177745
H	-4.96838560990599	16.28646576741205	6.76595829772662
C	-5.63015586090425	18.02111500412121	7.90571916175703
H	-4.88701499747344	18.70210068512162	7.45824042567432
C	-7.52404191607685	16.26324139943103	9.06377072763532

Table S6. Calculated bond lengths for selected bonds in **2**, **3**, **4**, **5**

	Sc-M (M = Ni, Pd, Pt) (Å)	Sc-N (Å)	M-P (M = Ni, Pd, Pt) (Å)	Ni-N (Å)
2	2.619	2.063; 2.063; 2.067; 2.336 (axial)	2.235; 2.239; 2.248	1.826
3	2.371	2.078; 2.078; 2.080 2.296 (axial)	2.203; 2.207; 2.209	-
4	2.486	2.078; 2.079; 2.083; 2.287 (axial)	2.352; 2.355; 2.358	-
5	2.776	2.056; 2.056; 2.058; 2.331 (axial)	2.368; 2.370; 2.371; 2.374 (axial)	-

Table S7. Calculated atomic charges

	Mülliken Charges		Löewdin Charges		Natural Charges	
	Sc	M (M = Ni, Pd, Pt)	Sc	M (M = Ni, Pd, Pt)	Sc	M (M = Ni, Pd, Pt)
2	0.268	-0.165	-0.662	-0.954	1.577	0.227
3	0.483	-0.378	-0.648	-0.842	1.505	0.046
4	0.702	-0.533	-0.548	-0.810	1.554	-0.037
5	0.135	-0.195	-0.695	-0.622	1.629	0.022

Table S8. Calculated Wiberg and Mayer bond orders for selected bonds in **2**, **3**, **4**, **5**

	Wieberg Bond Orders	Mayer Bond Orders
2	0.609	0.398
3	0.903	0.527
4	0.909	0.463
5	0.617	0.400

Table S9. Calculated natural electron configurations for metal centers in **2**, **3**, **4**, **5**

Compound	Electron Configuration
2	Ni [core]4s(0.36)3d(9.36)4p(0.02)5s(0.01)4d(0.02)
	Sc [core]4s(0.18)3d(1.00)4p(0.01)4d(0.21)5d(0.01)
3	Ni [core]4s(0.41)3d(9.51)4p(0.02)4d(0.01)
	Sc [core]4s(0.17)3d(1.13)4p(0.01)4d(0.18)5d(0.01)
4	Pd [core]5s(0.44)4d(9.56)5p(0.02)5d(0.01)6p(0.01)
	Sc [core]4s(0.18)3d(1.07)4p(0.01)4d(0.17)5d(0.01)
5	Pt [core]6s(0.50)5d(9.43)6p(0.02)6d(0.02)7p(0.01)
	Sc [core]4s(0.16)3d(0.91)4p(0.01)4d(0.27)5d(0.01)

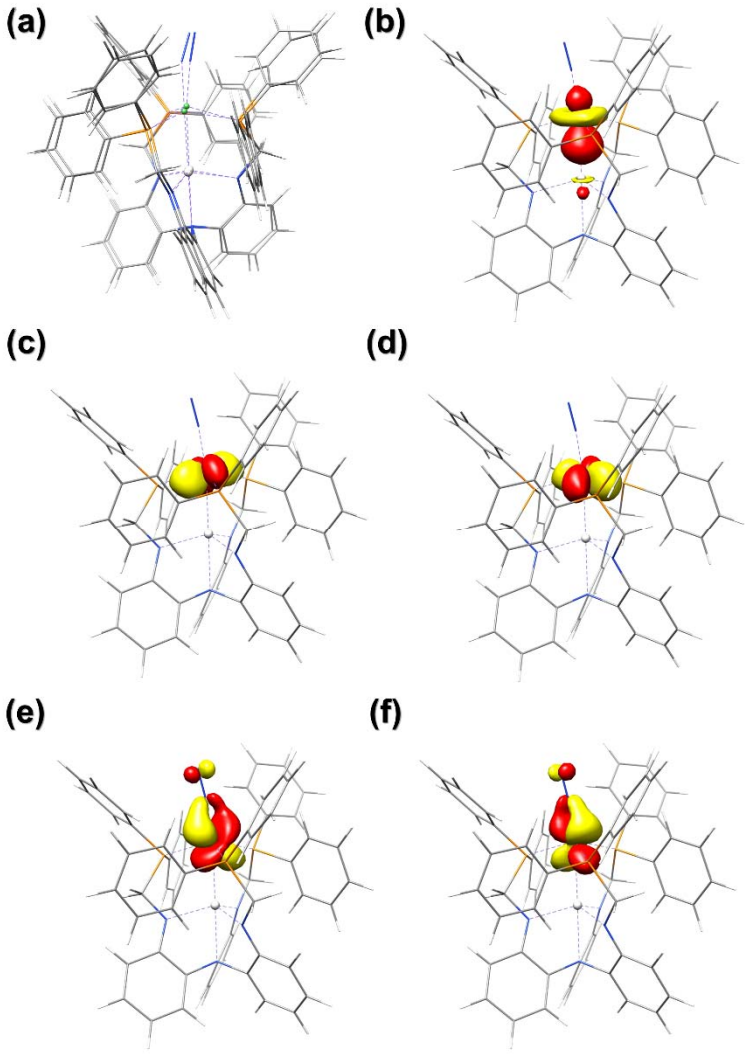

Figure S29. Superimposing of the calculated structure and solid state structure of **2** (a), localized orbitals representing the dative Ni-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **2** (isovalue = 0.05).

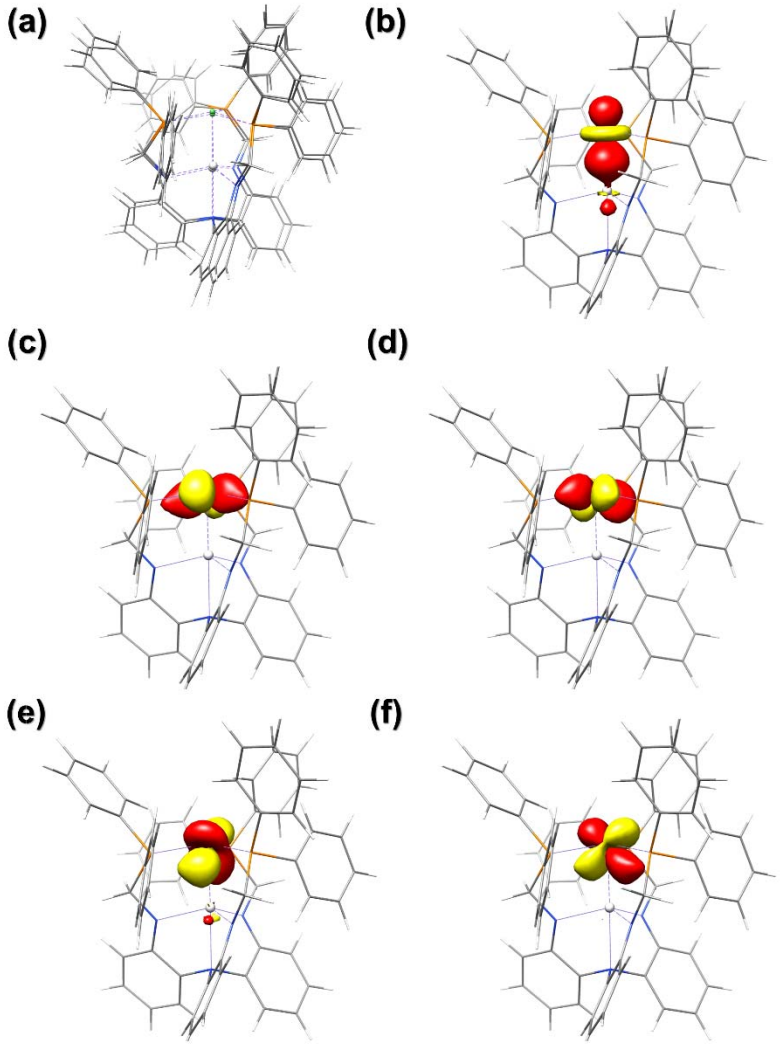

Figure S30. Superimposing of the calculated structure and solid state structure of **3** (a), localized orbitals representing the dative Ni-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **3** (isovalue = 0.05).

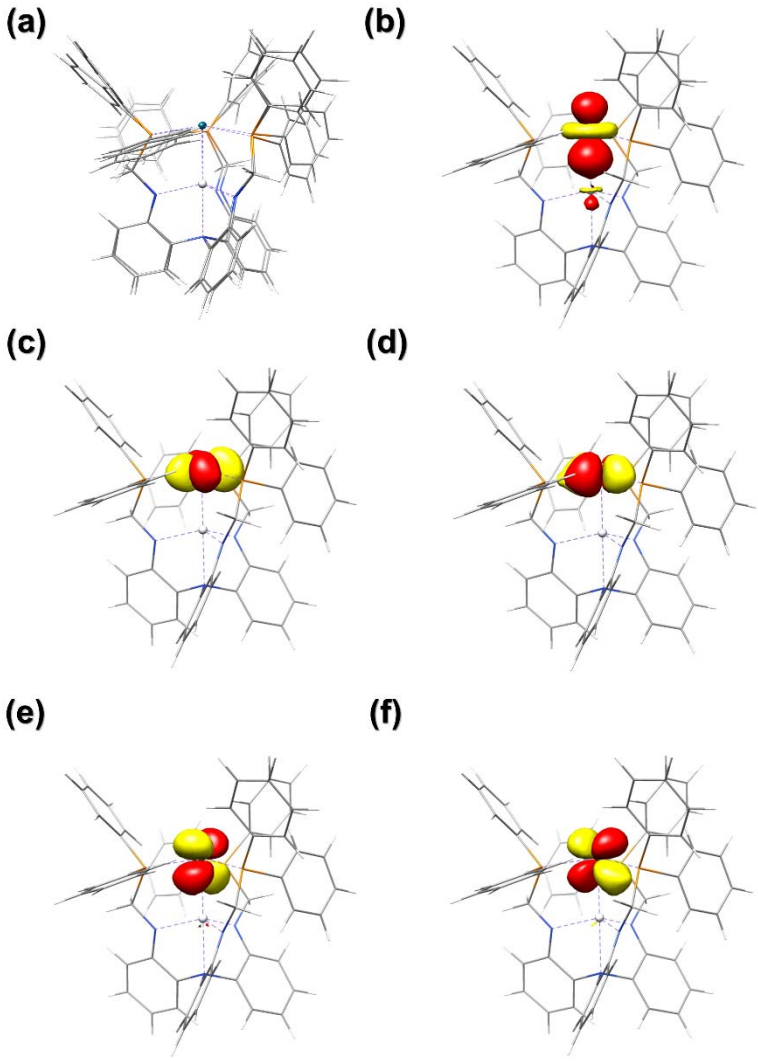

Figure S31. Superimposing of the calculated structure and solid state structure of **4** (a), localized orbitals representing the dative Pd-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **4** (isovalue = 0.05).

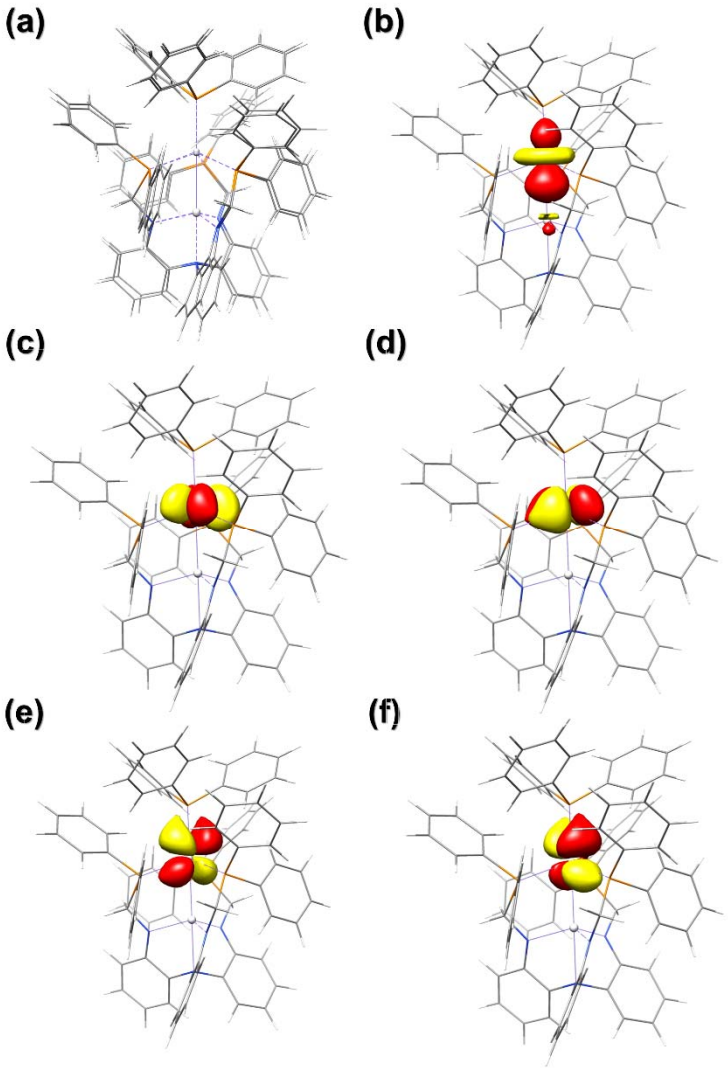

Figure S32. Superimposing of the calculated structure and solid state structure of **5** (a), localized orbitals representing the dative Pt-Sc bond (b) and the other four doubly occupied d orbitals of Ni center in **5** (isovalue = 0.05).

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