Electronic Supplementary Material (ESI) for Dalton Transactions.

Neutral and Cationic Enantiopure Group 13 Iminophosphonamide Complexes

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Supporting Information

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1. NMR Spectra

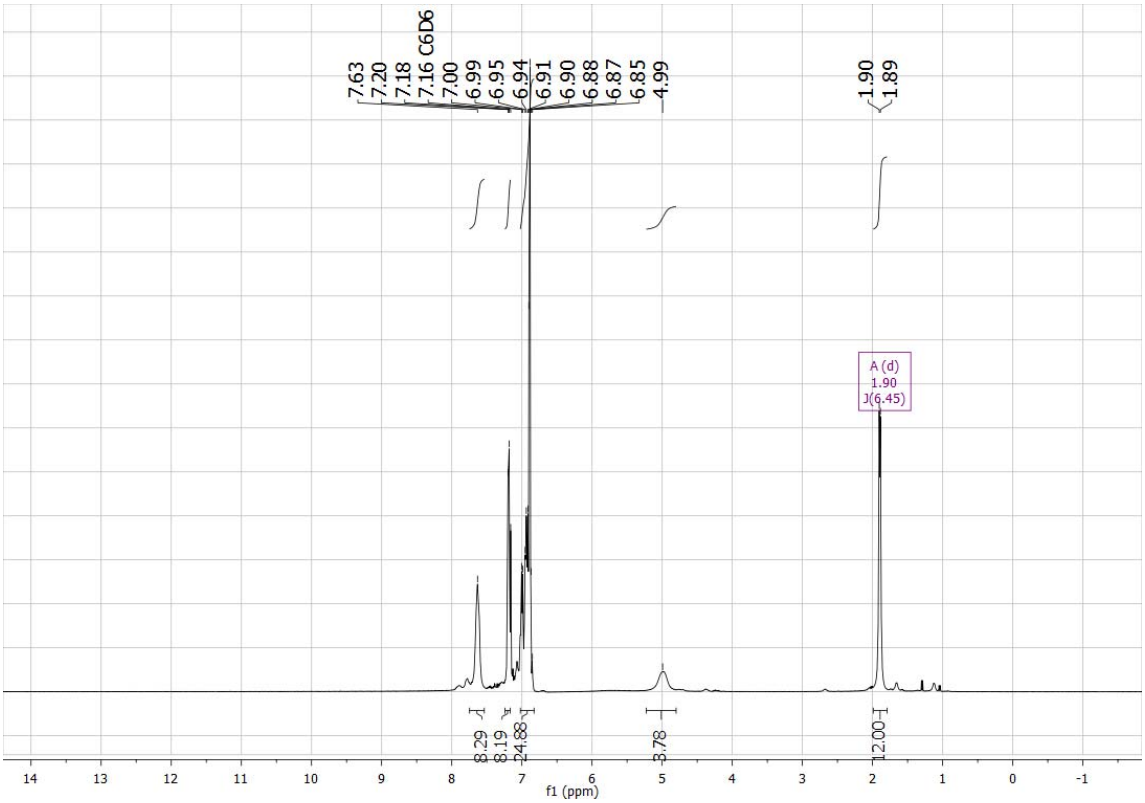

Figure S1: ^{1}H (400 MHz, C_6D_6, 298 K) NMR spectrum of complex **1**.

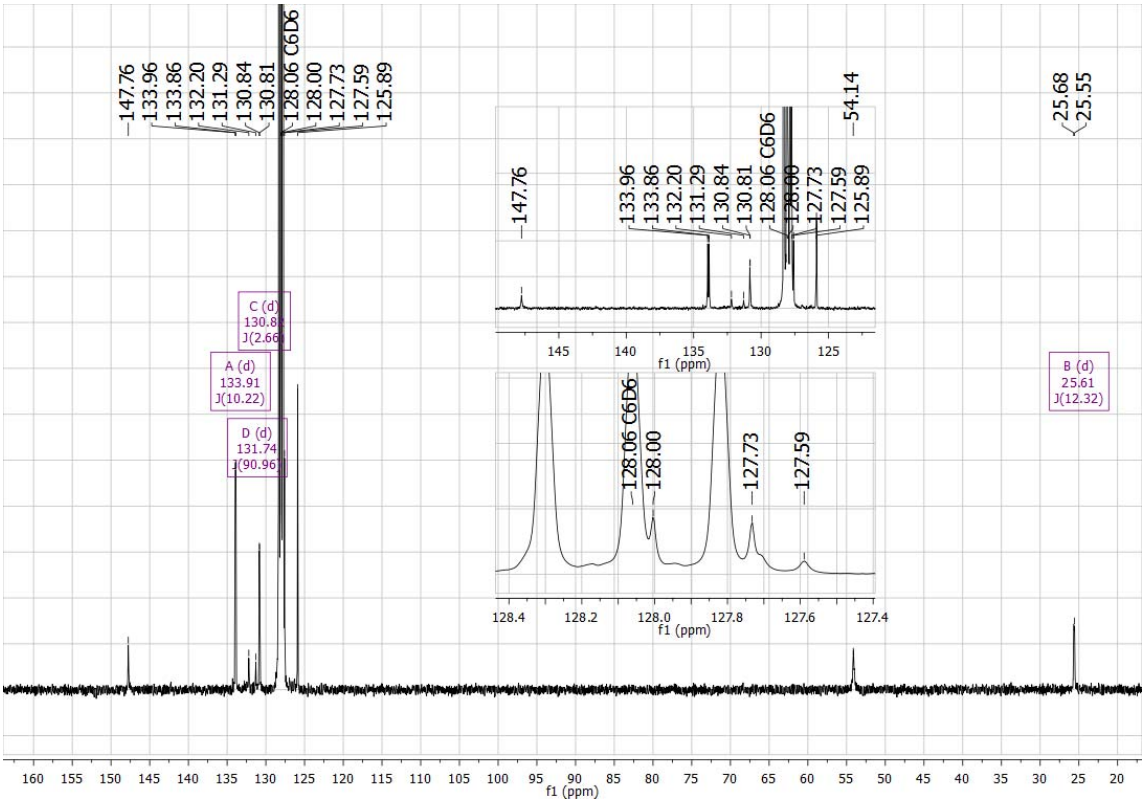

Figure S2: $^{13}C\{^{1}H\}$ (100 MHz, C_6D_6, 298 K) NMR spectrum of complex **1**.

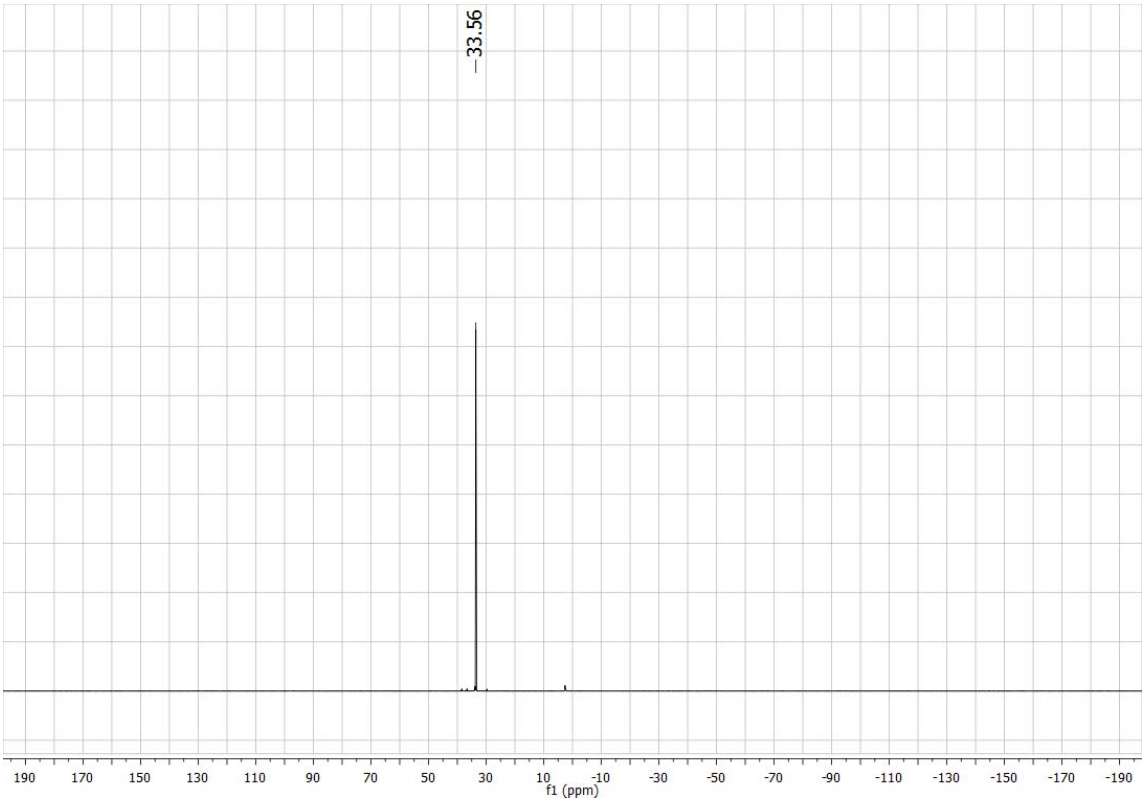

Figure S3: $^{31}P\{^{1}H\}$ (162 MHz, C_6D_6, 298 K) NMR spectrum of complex **1**.

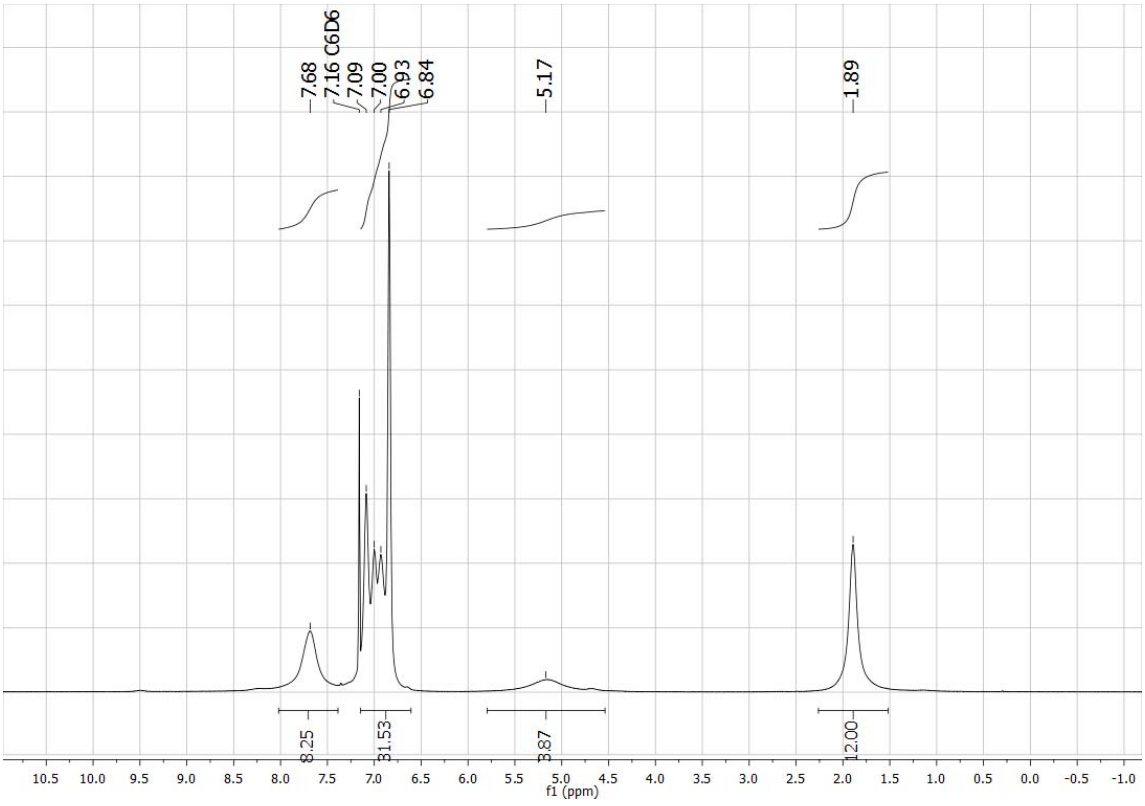

Figure S4: ^{1}H (400 MHz, C_6D_6, 298 K) NMR spectrum of complex **2**.

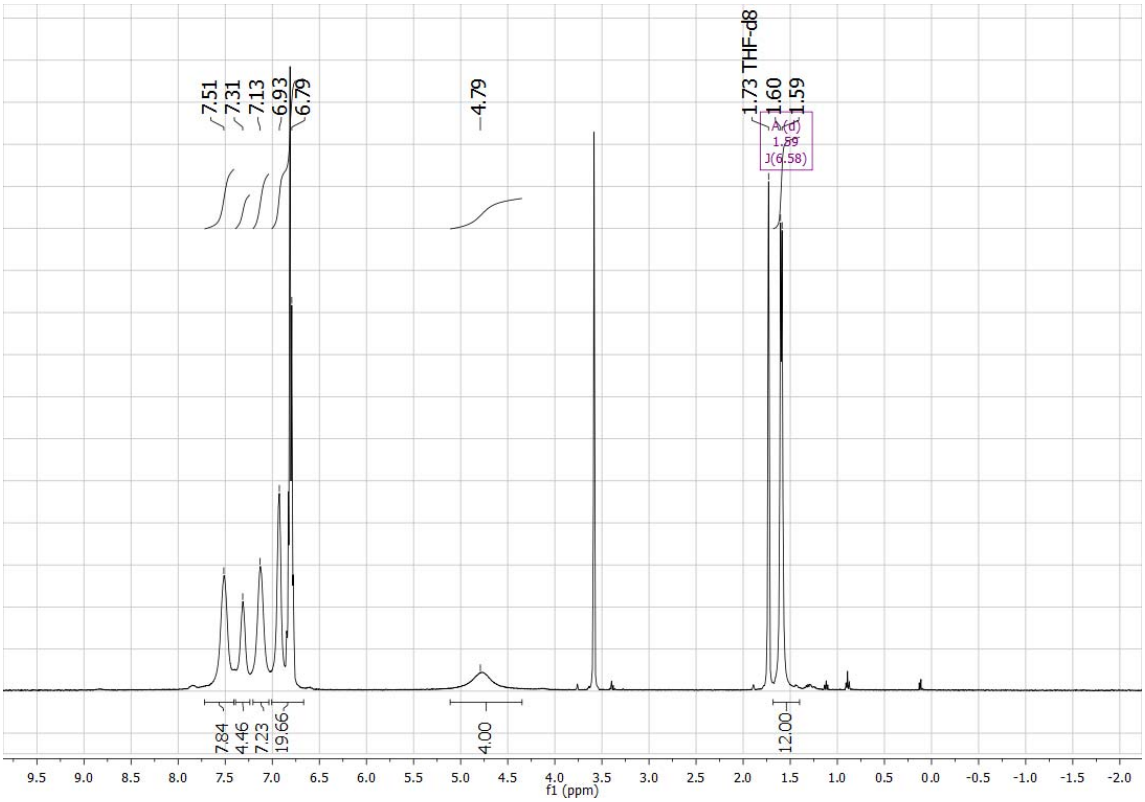

Figure S5: ^{1}H (400 MHz, thf-d_8, 298 K) NMR spectrum of complex **2**.

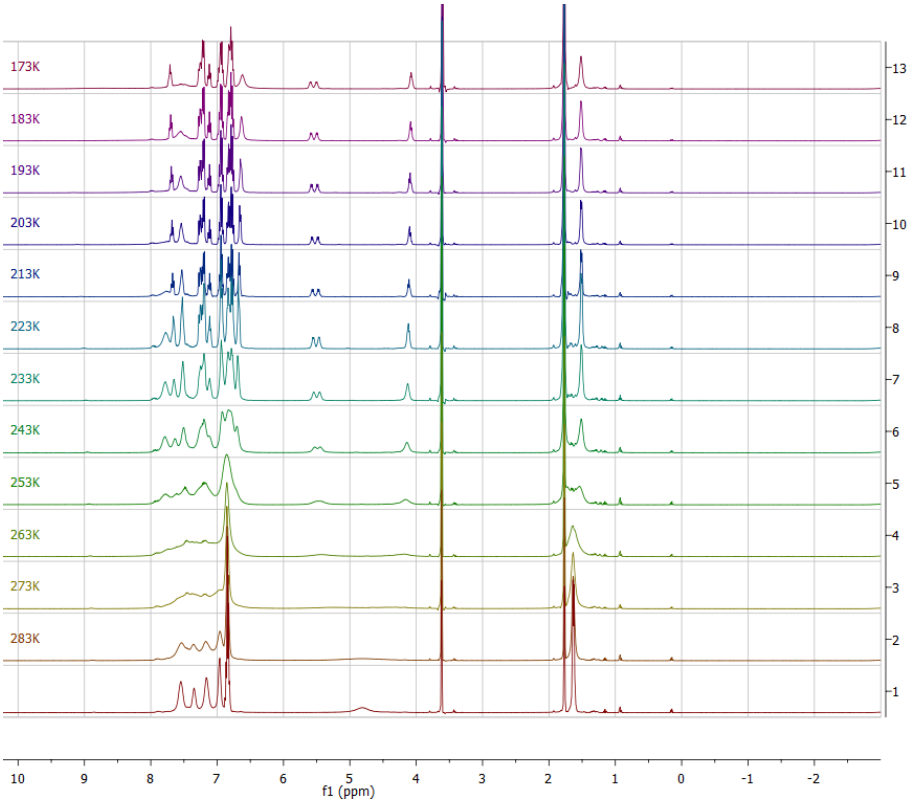

Figure S6: Variable temperature ^{1}H (300 MHz, thf-d_8, 298 K-173 K) NMR spectrum of complex **2**.

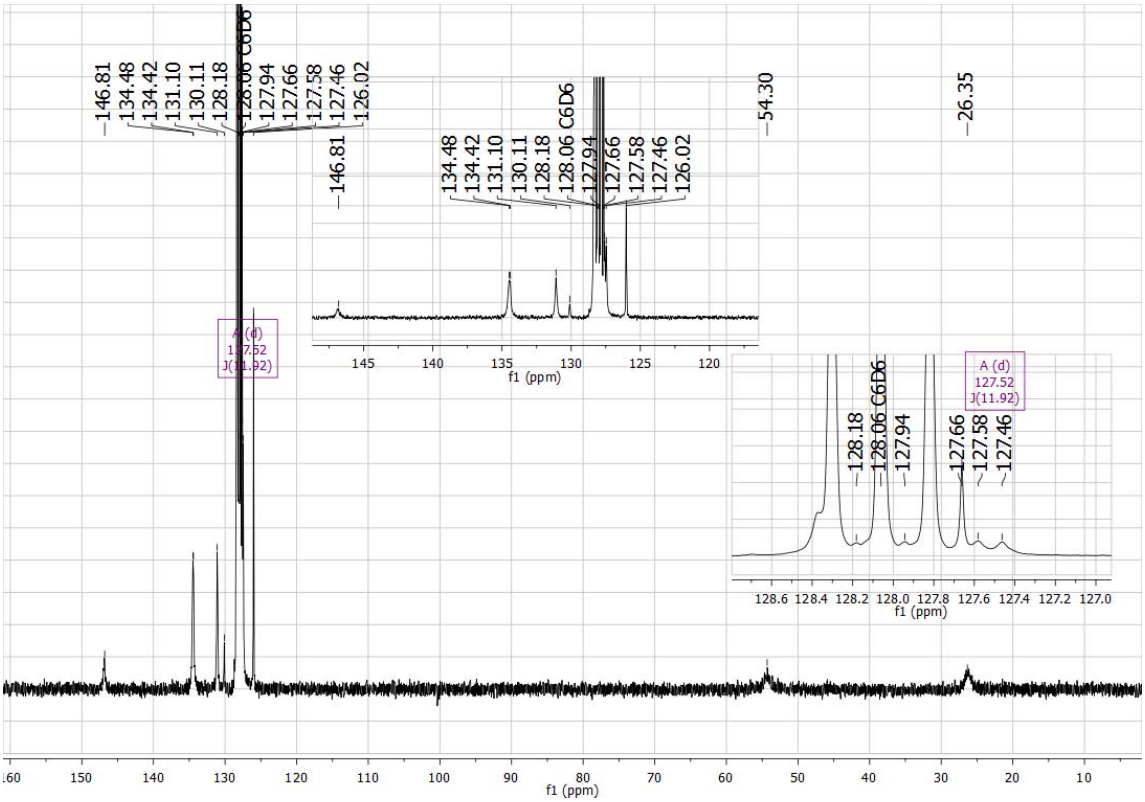

Figure S7: $^{13}C\{^{1}H\}$ (100 MHz, C_6D_6, 298 K) NMR spectrum of complex **2**.

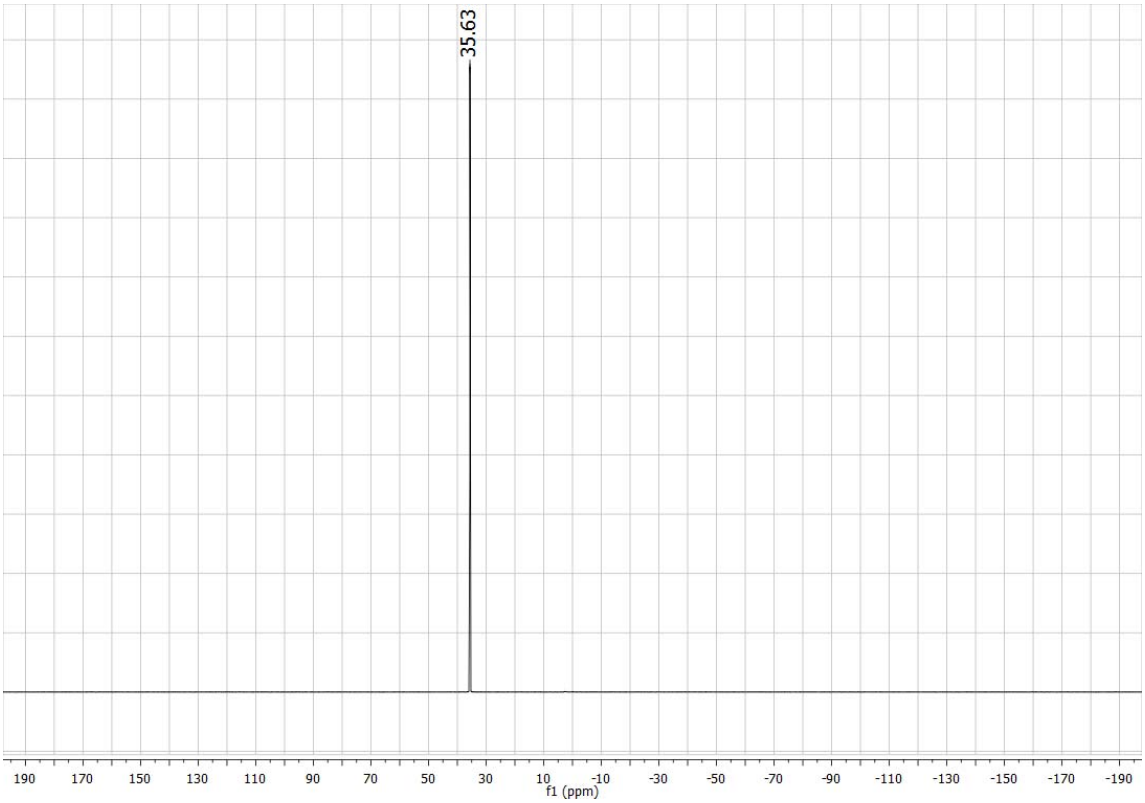

Figure S8: $^{31}P\{^{1}H\}$ (162 MHz, C_6D_6, 298 K) NMR spectrum of complex **2**.

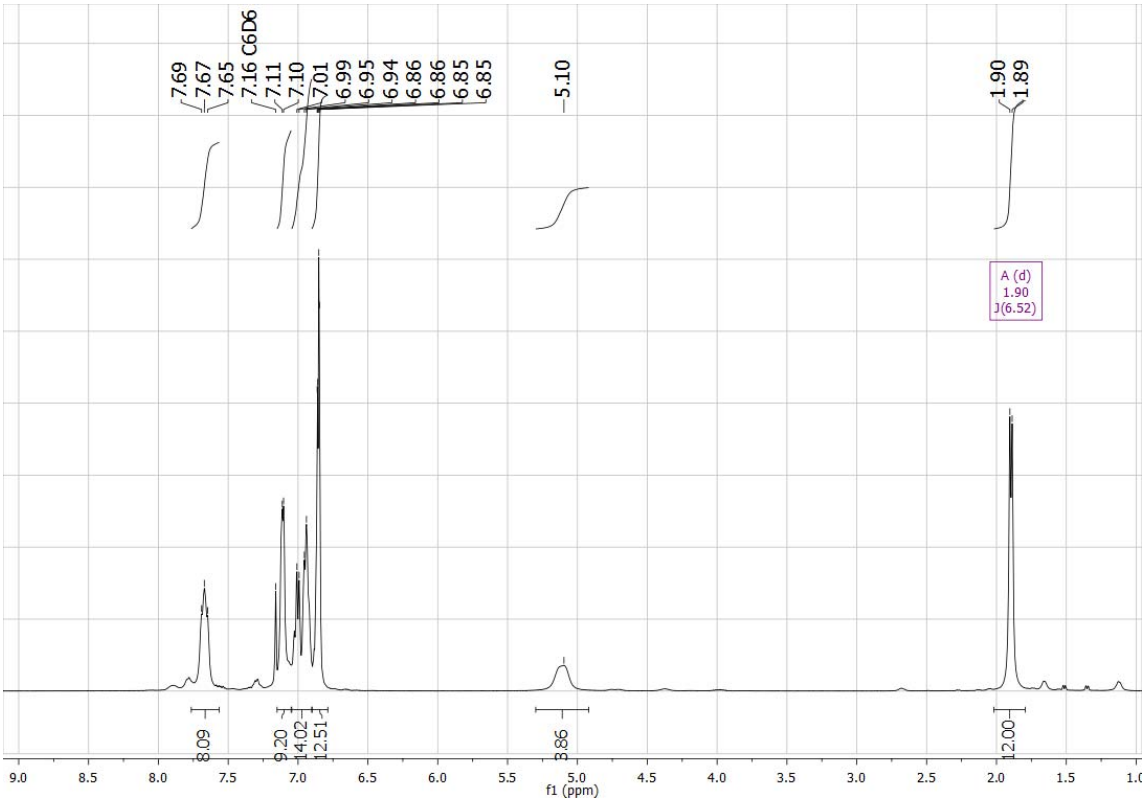

Figure S9: ^{1}H (400 MHz, C_6D_6, 298 K) NMR spectrum of complex **3**.

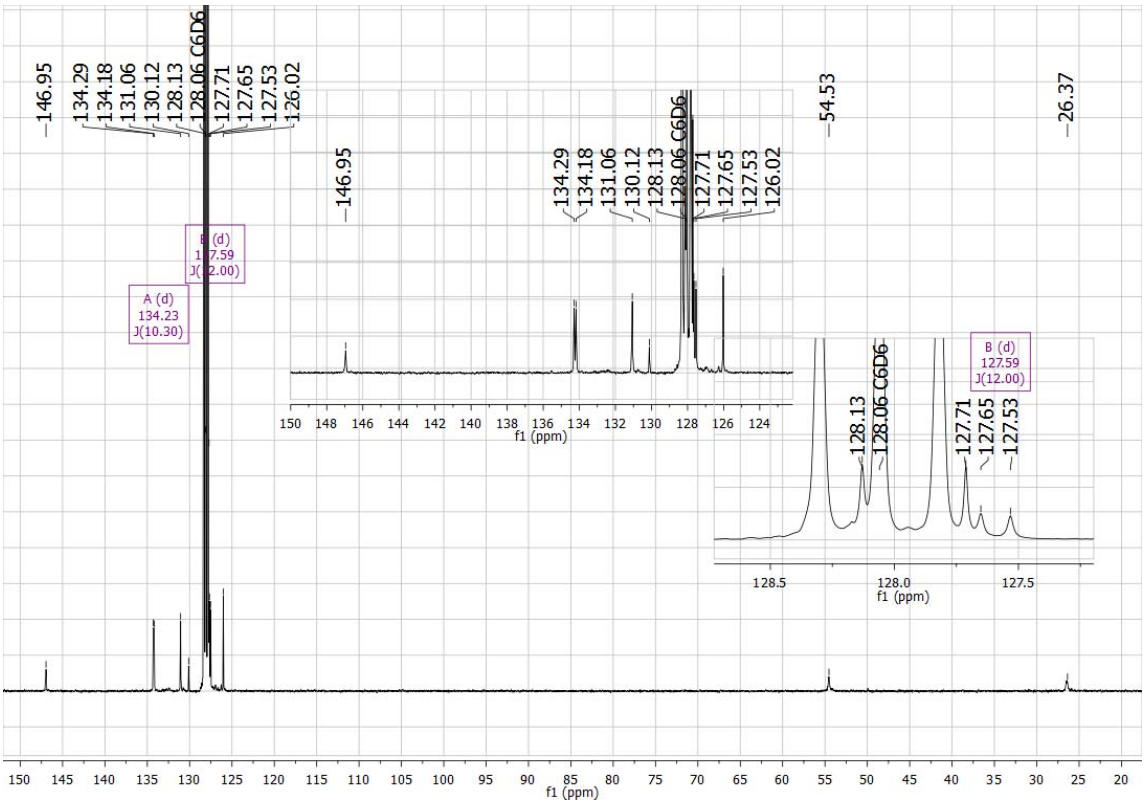

Figure S10: $^{13}C\{^{1}H\}$ (100 MHz, C_6D_6, 298 K) NMR spectrum of complex **3**.

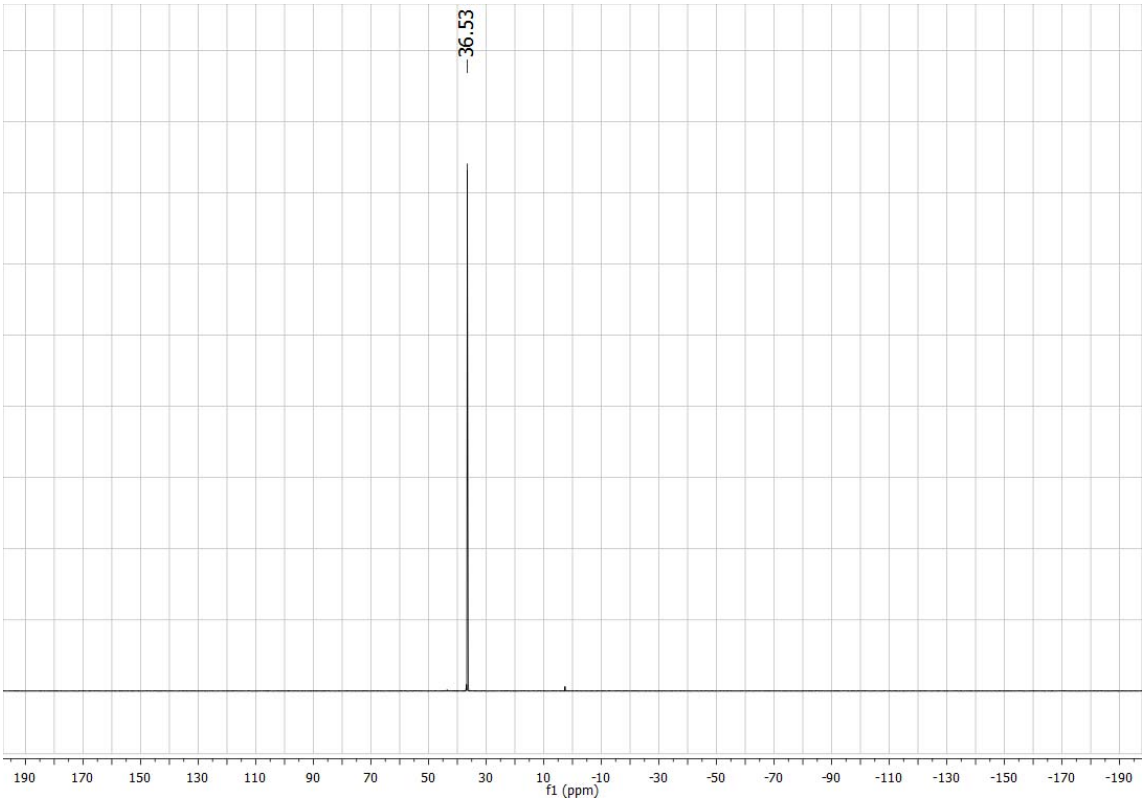

Figure S11: $^{31}P\{^{1}H\}$ (162 MHz, C_6D_6, 298 K) NMR spectrum of complex **3**.

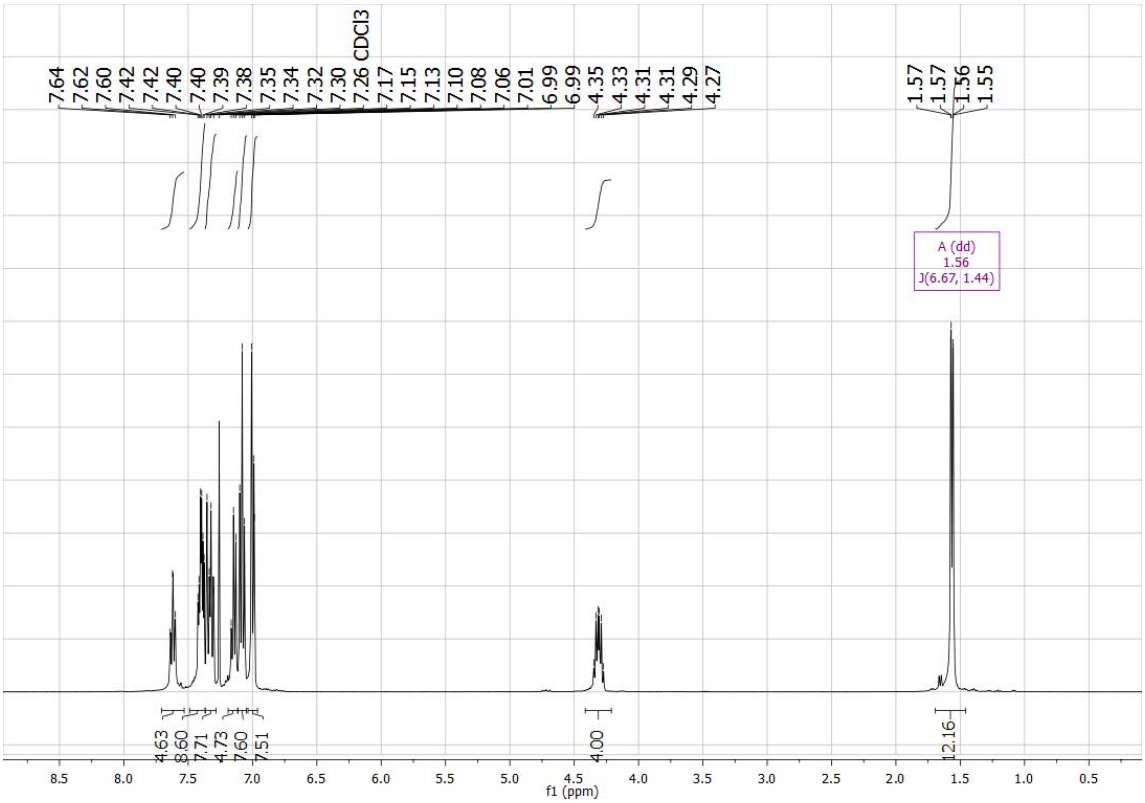

Figure S12: ^{1}H (400 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **4**.

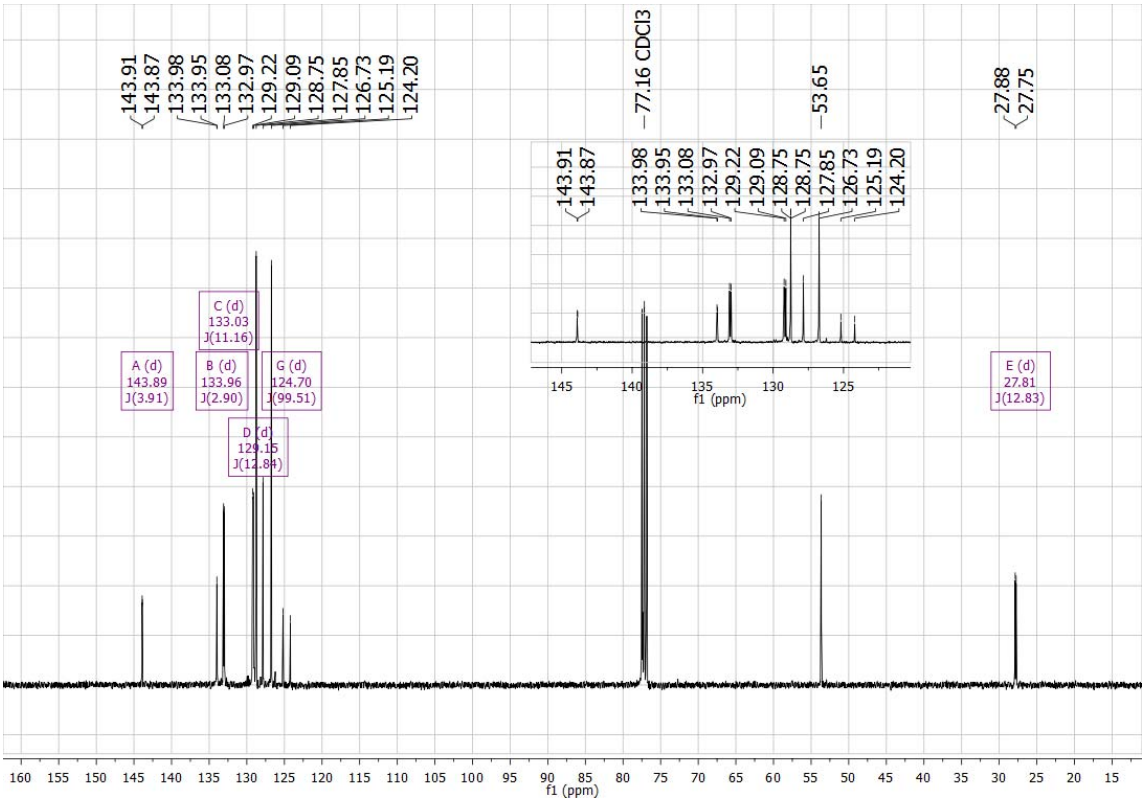

Figure S13: $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **4**.

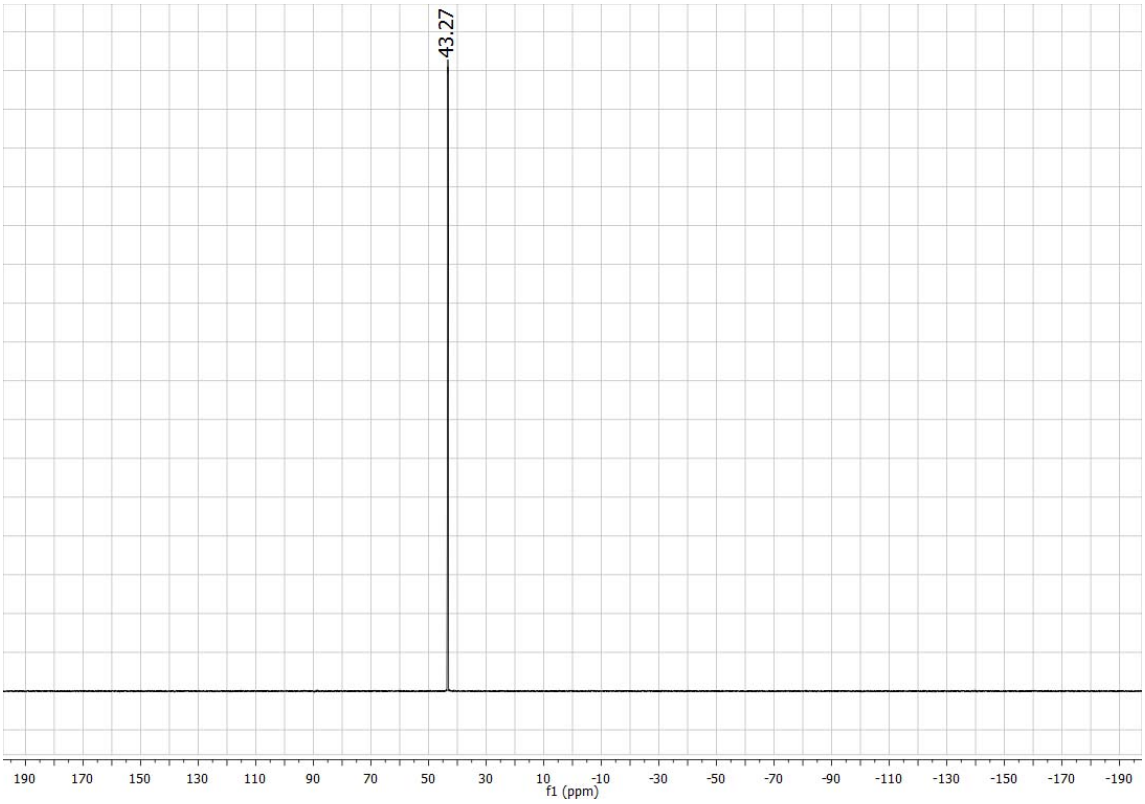

Figure S14: $^{31}P\{^{1}H\}$ (162 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **4**.

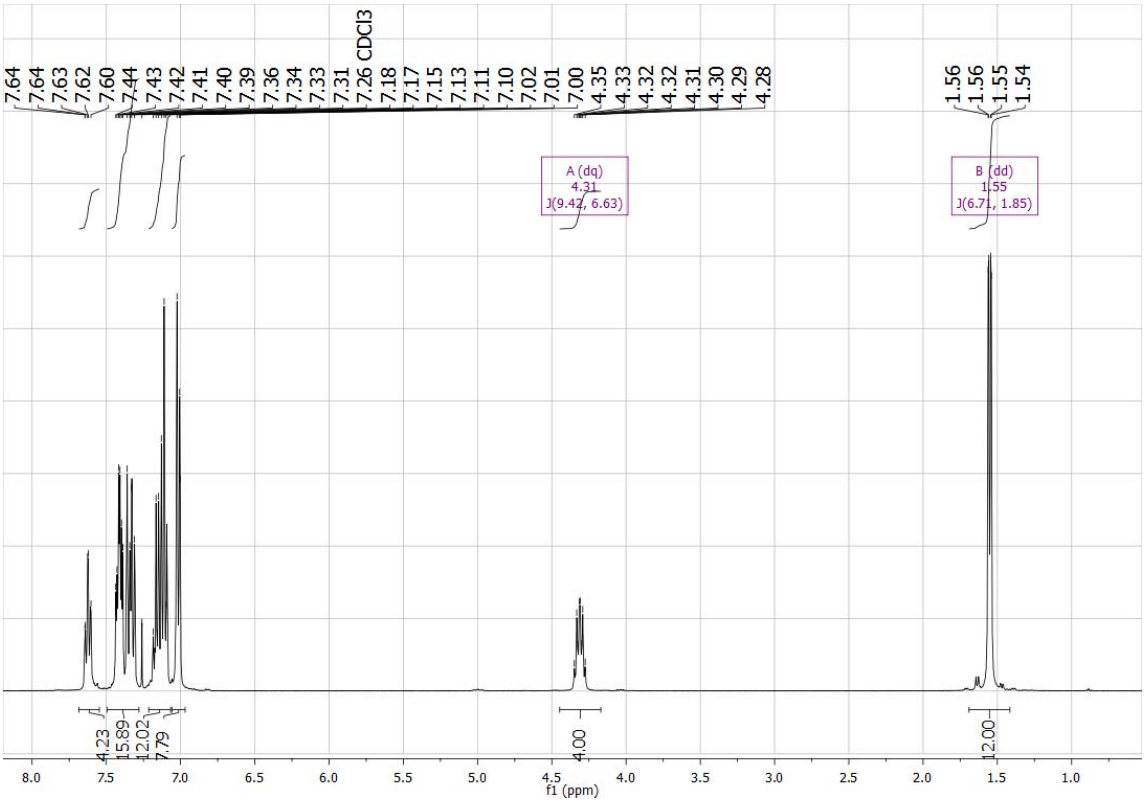

Figure S15: ^{1}H (400 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **5**.

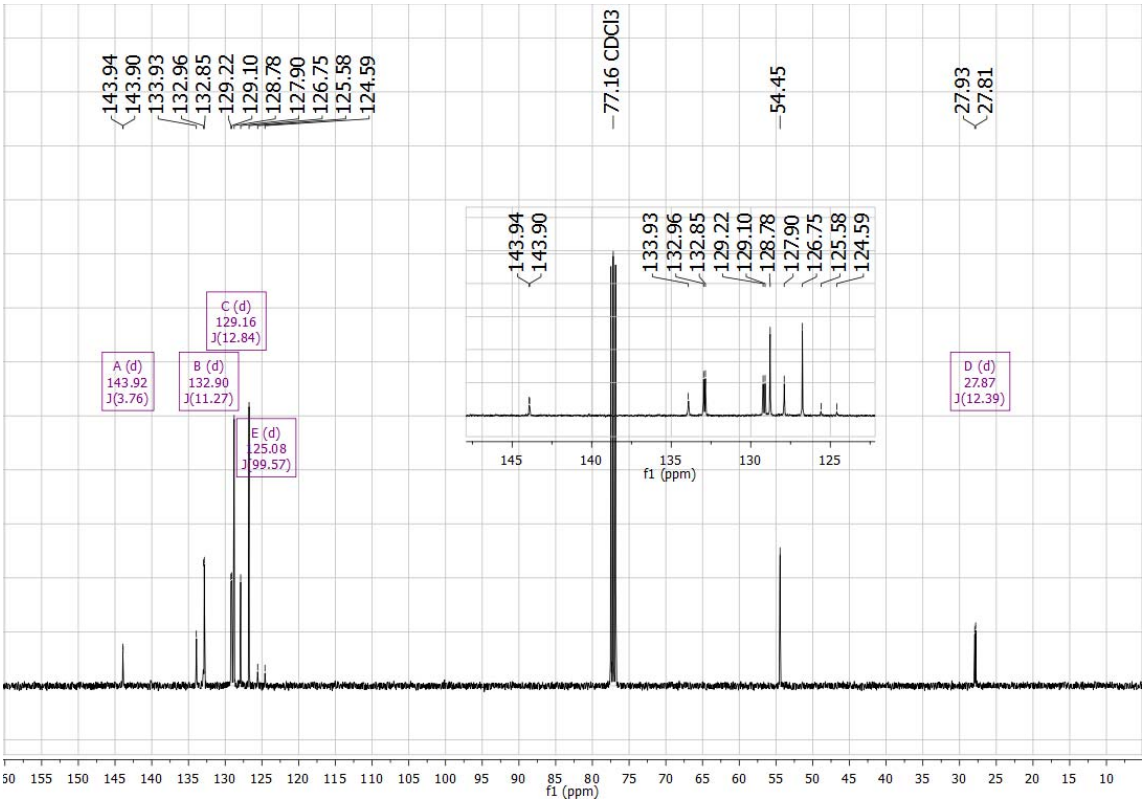

Figure S16: $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **5**.

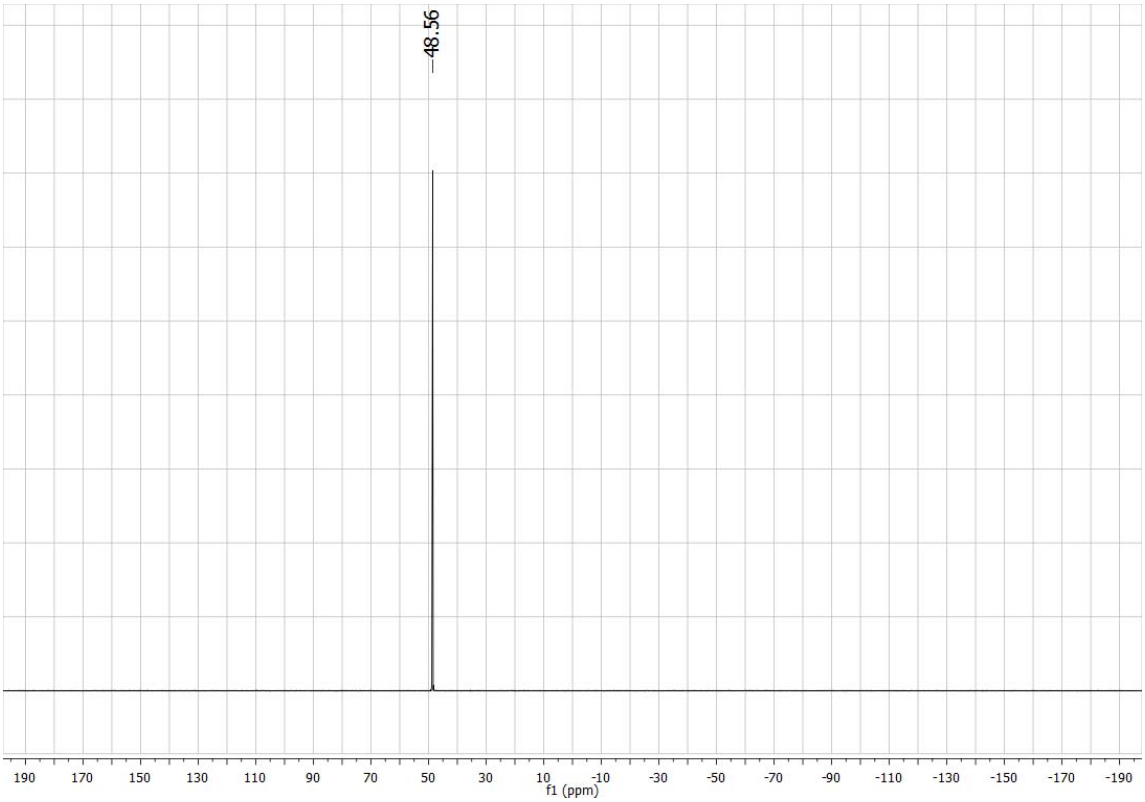

Figure S17: $^{31}P\{^{1}H\}$ (162 MHz, $CDCl_3$, 298 K) NMR spectrum of complex **5**.

2 IR Spectra

The predicted Al-H stretching vibration is found as a broad signal at about 1693 cm^{-1} (**1_H**). By harmonic correction according to the method of Becher[1] using the anharmonicity constant of the diatomic AlH and AlD[2] the harmonic value determined to be 1764 cm^{-1} is in excellent agreement with the value obtained from an orientational DFT calculation (1740 cm^{-1}). In the experimentally deduced IR spectrum of **1_D** a signal at 1203 cm^{-1} is attributed to the Al-D stretching vibration (after harmonic correction 1234 cm^{-1}). The harmonic isotopic splitting of 530 cm^{-1} fits fairly with the splitting determined by the DFT calculation (486 cm^{-1}). The low symmetry of the molecule give rise to a variety of coupling possibilities (which are difficult to model by theoretical methods), so that a better match is not expected. (In the IR spectrum of H_2GaCl there are even vibrations of the D-isotopomer with a higher energy compared to those of its H-isotopomer.[3] The Al-H stretching mode in compound $[Ph_2P(NSiMe_3)_2]_2AlH$[4], is found at 1853 cm^{-1}. Due to this unexpectedly high value compared to **1_H** we investigated this molecule by theoretical methods as well (see below section 4). We calculated the Al-H valence vibration to be at 1784 cm^{-1}. We suppose that the band found in the experimental IR spectrum results in an overtone or combination mode of this likewise less symmetric molecule, amplified by Fermi resonance coupling to a (weak) AlH valence vibration. Another method for the reliable detection of Al-H (D) bonding in **1_H** and **1_D** is provided by the investigation of the two usually very intense Al-H(D) deformation modes in the IR spectrum. They are found at 636 and 606 cm^{-1} (**1_H**) as well as close to 482 cm^{-1} (**1_D**). A second Al-D-deformation mode is presumably overlapped by the signals of the AlN_4 framework at 537 and 508 cm^{-1} (both **1_H** and **1_D**).

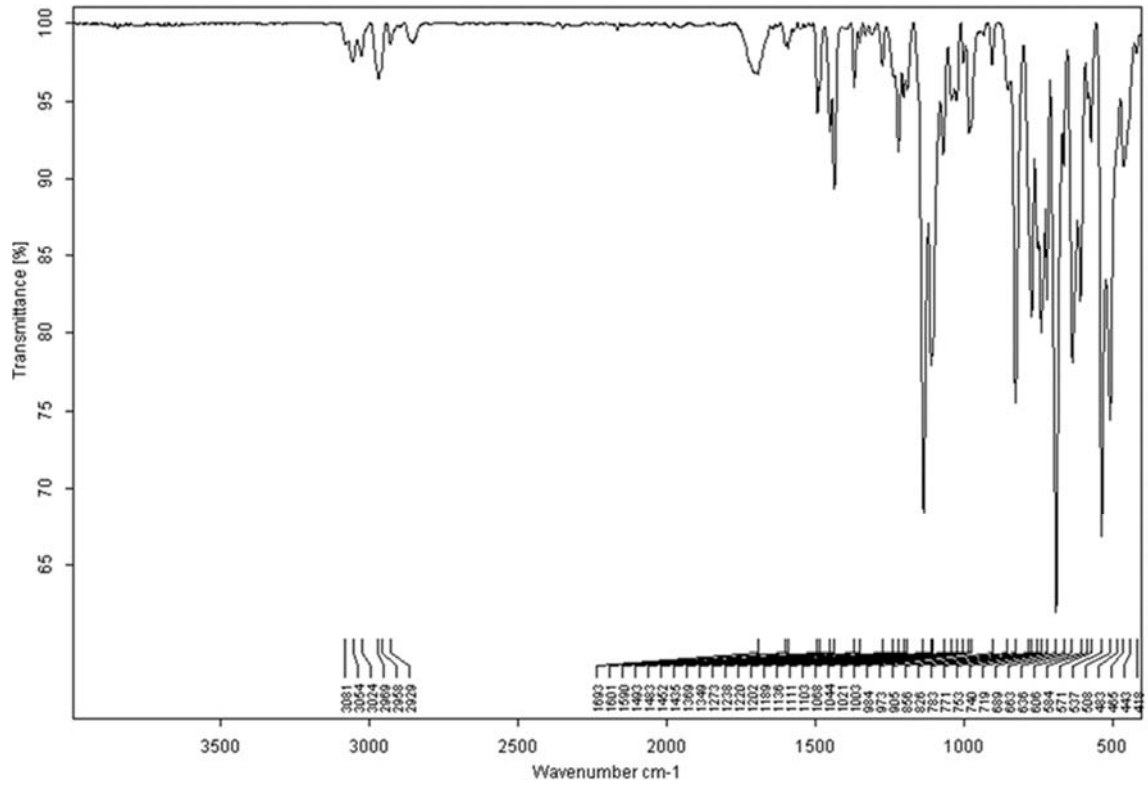

Figure S18: IR spectrum of complex **1**.

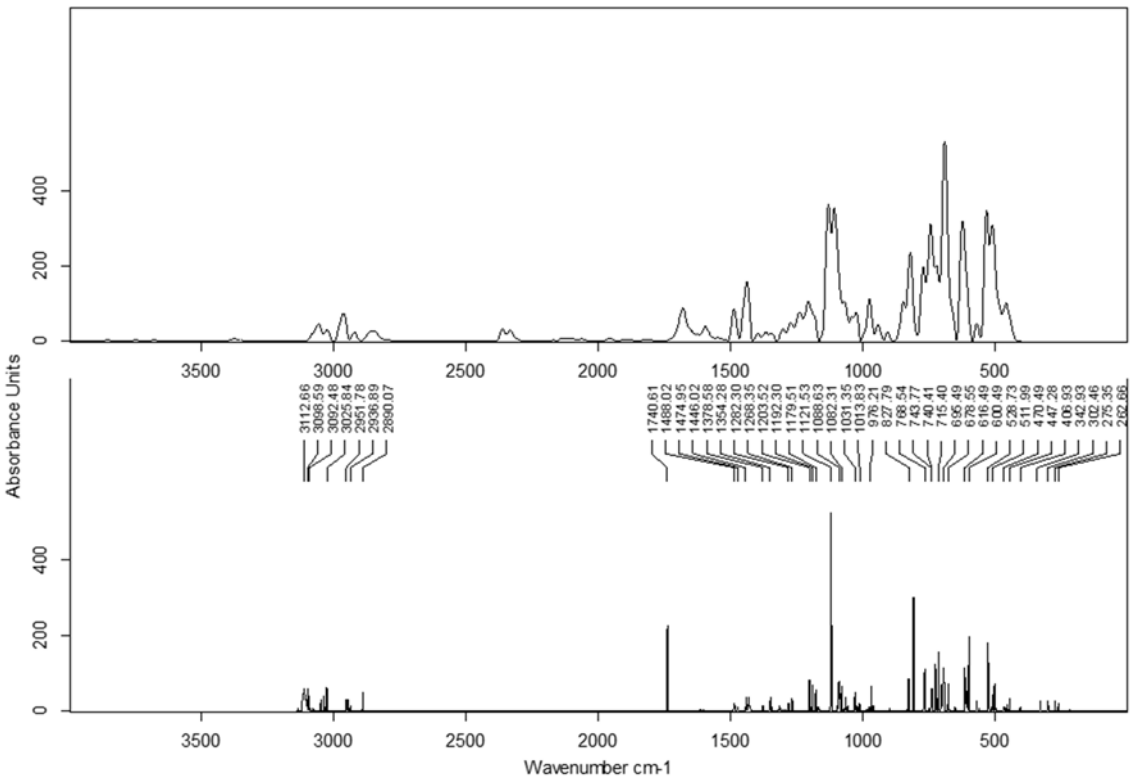

Figure S19 Experimental (above) and calculated (below) spectra for $\mathbf{1_H}$.

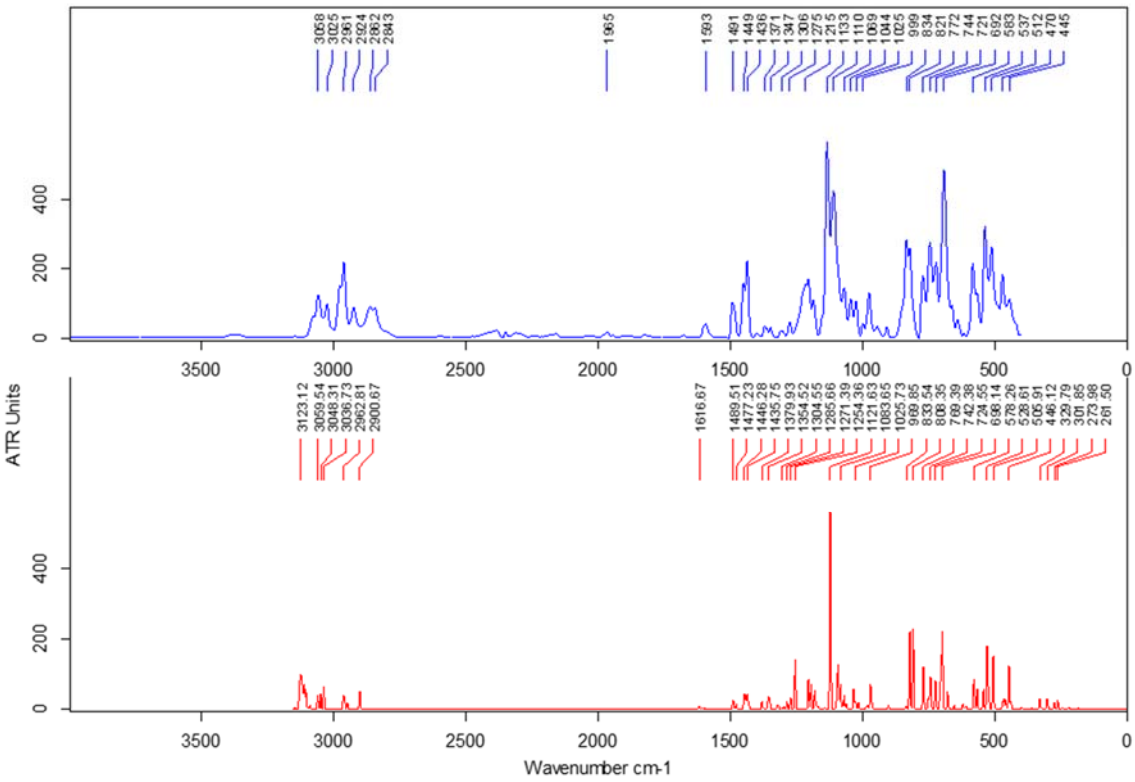

Figure S20 Experimental (above) and calculated (below) spectra for $\mathbf{1_D}$

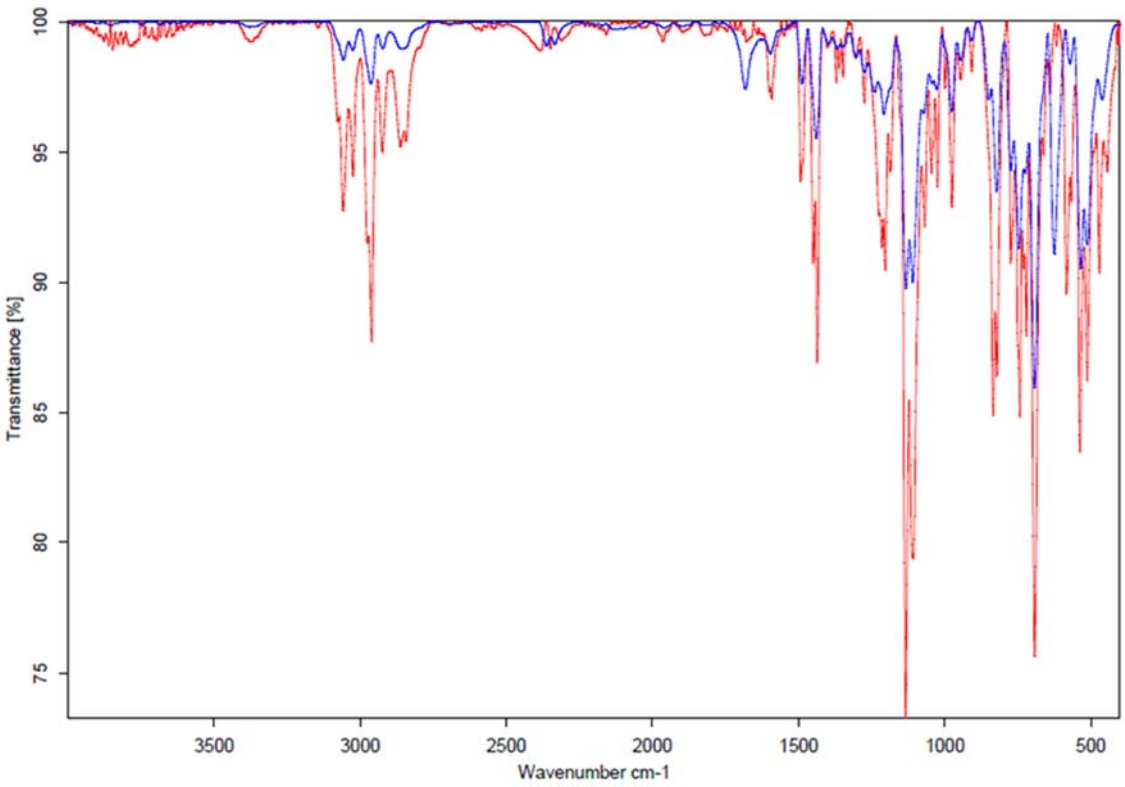

Figure S21 Comparison of experimental spectra for $\mathbf{1_H}$ (blue) and $\mathbf{1_D}$ (red).

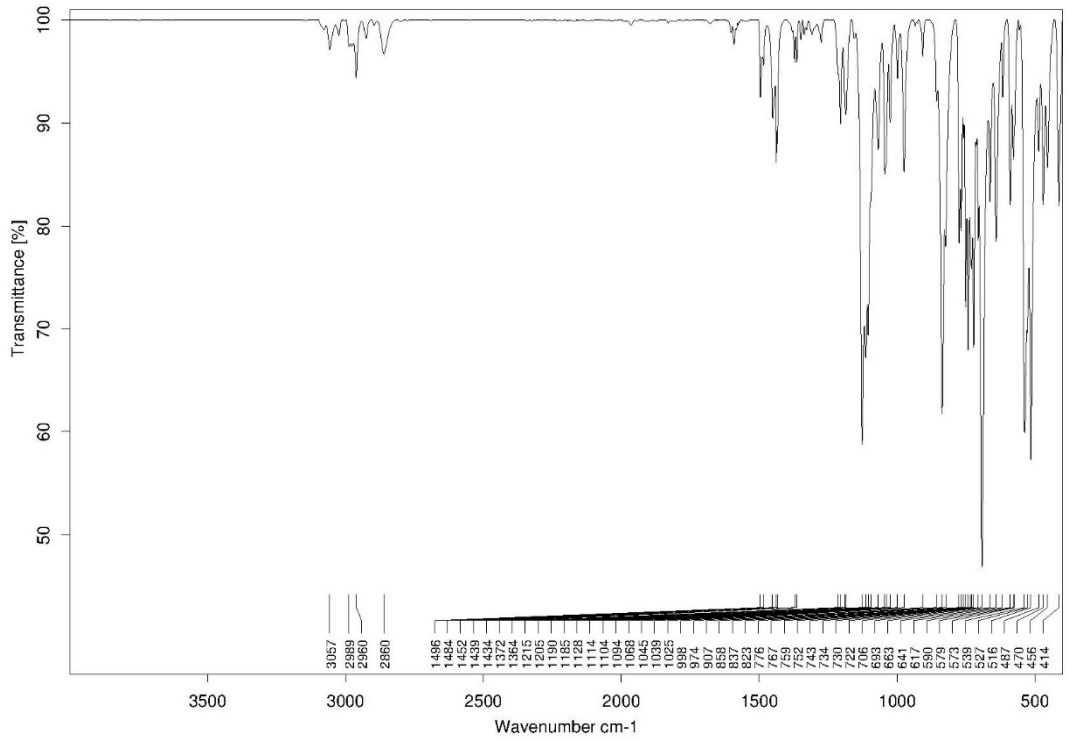

Figure S22: IR spectrum of complex **2**.

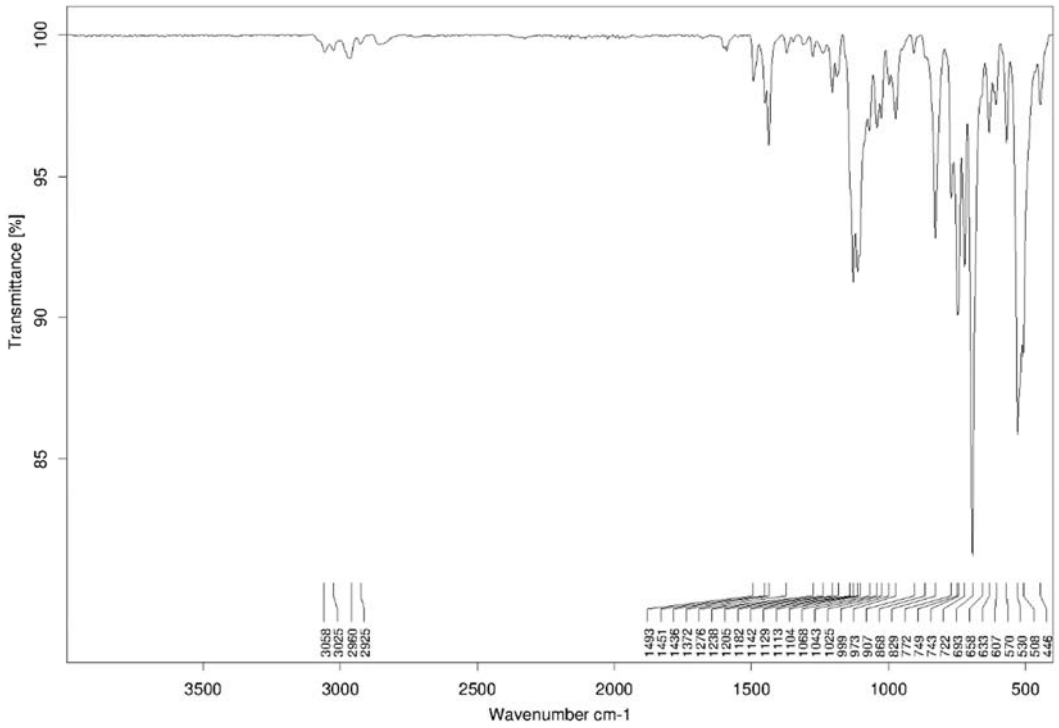

Figure S23: IR spectrum of complex **3**.

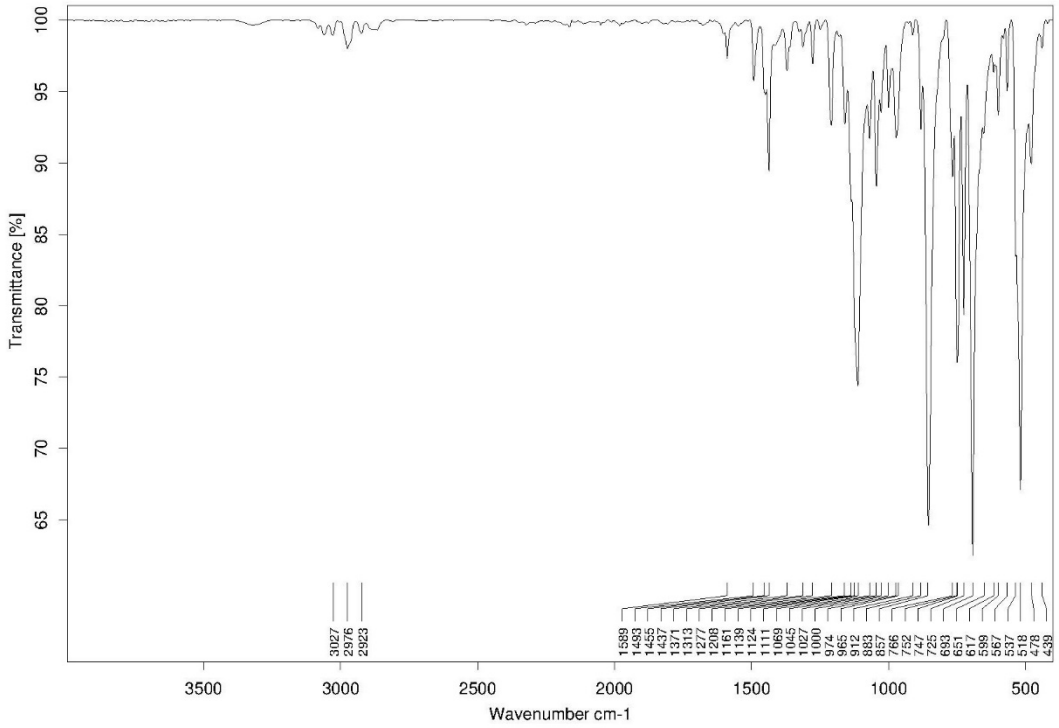

Figure S24: IR spectrum of complex **4**.

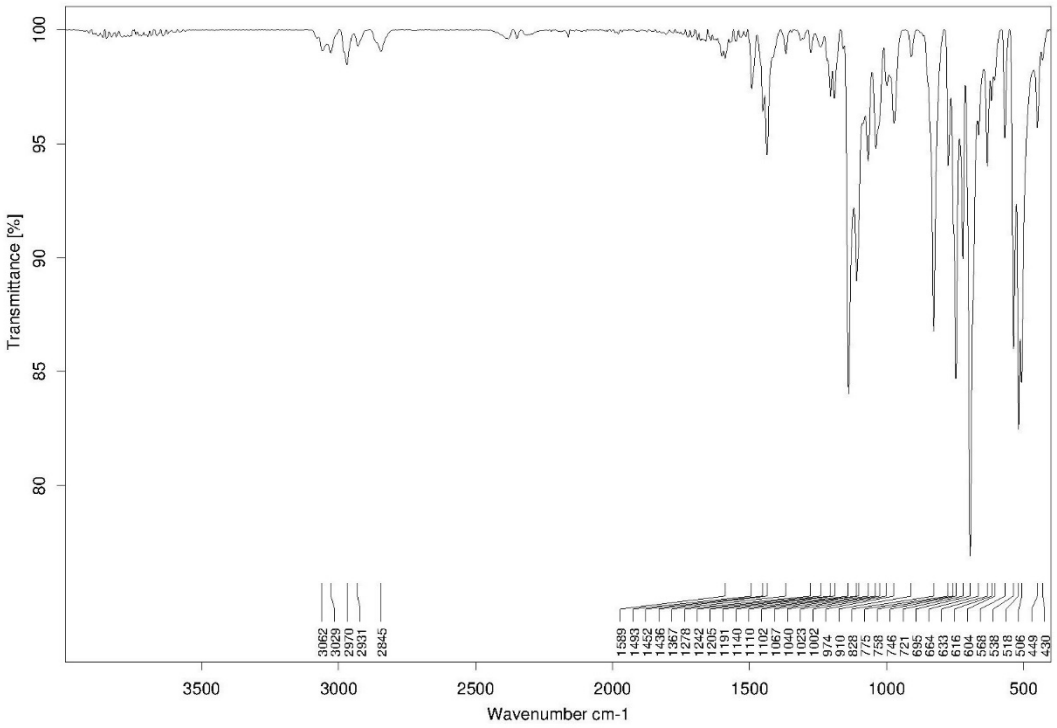

Figure S25: IR spectrum of complex **5**.

3 Crystallographic data

Single crystal X-ray diffraction

A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber. The crystal was transferred directly to the cold stream of a STOE IPDS 2 or a STOE StadiVari diffractometer. All structures were solved by using the program SHELXS/T[5] and Olex2[6]. The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F^2 by using the program SHELXL.[5] In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. 1959904-1959908. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Refinement Details

The crystal structure of complex **1** contains a half molecule of Et_2O in the asymmetric unit. This could not be modeled satisfactorily and was therefore removed from the electron density map using the OLEX2 solvent mask.[6]

Table S1 Crystal data, data collection and refinement for complexes **1-5**.

Compound	**1**	**2*(0.5 Et_2)O**	**3*(0.5 Et_2O)**	**4**	**5**
Formula	$C_{56}H_{57}AlN_4P_2$	$C_{58}H_{61}AlClN_4OP_2$	$C_{58}H_{61}ClGaN_4O_{0.5}P_2$	$C_{56}H_{56}AlCl_4GaN_4P_2$	$C_{56}H_{56}AlCl_4GaN_4P_2$
$D_{calc.}$**/ g cm^{-3}**	1.108	1.160	1.188	1.341	1.331
m**/mm^{-1}**	0.138	0.186	0.644	0.827	0.821
Formula Weight	874.97	954.47	989.21	1085.48	1085.48
Colour	clear colourless	clear colourless	clear colourless	clear colourless	clear colourless
Shape	rhombohedral	prism	plate	irregular	prism
Size/mm^3	0.28×0.23×0.19	0.29×0.22×0.18	0.43×0.28×0.09	0.52×0.32×0.18	0.26×0.16×0.08
T**/K**	150	150	240	150	150
Crystal System	orthorhombic	orthorhombic	orthorhombic	trigonal	trigonal
Flack Parameter	-0.06(3)	0.05(3)	-0.012(15)	-0.024(8)	0.024(15)
Hooft Parameter	-0.02(2)	0.01(2)	-0.047(8)	0.003(7)	0.019(10)
Space Group	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P3_121$	$P3_121$
a**/Å**	18.1730(2)	18.3994(4)	18.4844(4)	12.6047(3)	12.6494(2)
b**/Å**	14.6537(5)	14.4577(5)	14.5247(8)	12.6047(3)	12.6494(2)
c**/Å**	9.8443(6)	10.2758(7)	10.2958(8)	58.597(2)	58.6453(12)
α**/°**					
β**/°**					
γ**/°**				120	120
V/Å^3	2621.55(19)	2733.5(2)	2764.2(3)	8062.5(5)	8126.5(3)
Z	2	2	2	6	6
Z'	0.5	0.5	0.5	1	1
Wavelength/Å	0.71073	0.71073	0.71073	0.71073	0.71073
Radiation type	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α
Θ_{min}**/°**	1.785	1.791	1.783	1.866	1.859
Θ_{max}**/°**	29.546	27.134	29.493	25.553	25.606
Measured Refl.	35079	16111	19503	20530	28278
Independent Refl.	7327	6036	7672	9628	10102
Reflections with I > 2(I)	5686	4707	3984	6842	6721
R_{int}	0.0424	0.0261	0.0639	0.0597	0.1149
Largest Peak	0.317	0.727	0.685	0.569	0.423
Deepest Hole	-0.184	-0.586	-0.287	-0.431	-0.402
GooF	0.947	1.058	0.983	0.942	1.034
wR_2 **(all data)**	0.0862	0.1697	0.1979	0.0813	0.1306
wR_2	0.0819	0.1546	0.1590	0.0767	0.1145
R_1 **(all data)**	0.0554	0.0787	0.1388	0.0771	0.1150
R_1	0.0384	0.0575	0.0635	0.0485	0.0654

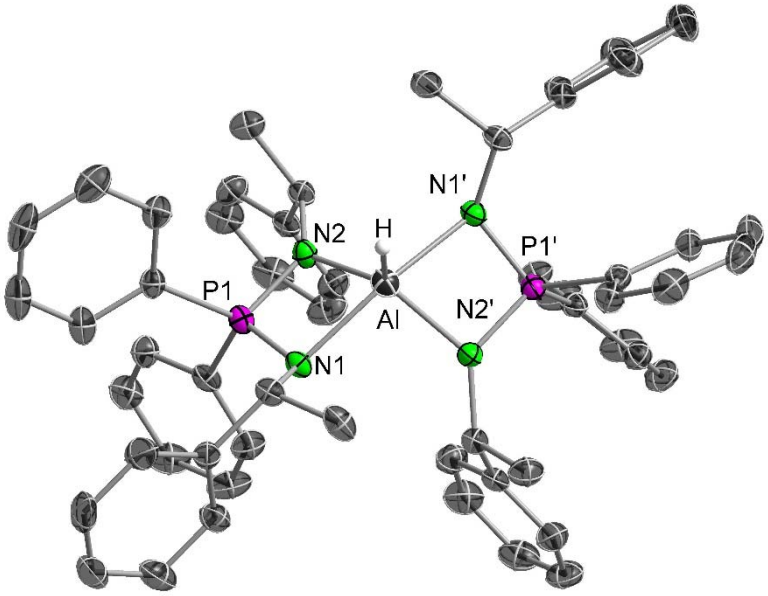

Figure S26: Molecular structure of **1** in the solid state with ellipsoids drawn at 40 % probability. All the hydrogen atoms except the hydride are omitted for clarity. Selected bond lengths (Å) and bond angles [°]: Al-N1 2.040(2), Al-N2 1.932(2), Al-H 1.48(4), P1-N1 1.621(2), P1-N2 1.622(2); N1-Al-N1' 165.03(9), N2-Al-N1 97.68(7), N2-Al-N2' 121.99(11), N1-Al-H 97.49(5), N2-Al-H 119.01(5), P1-Al-P1' 139.94(4), N2-P1-N1 96.46(9).

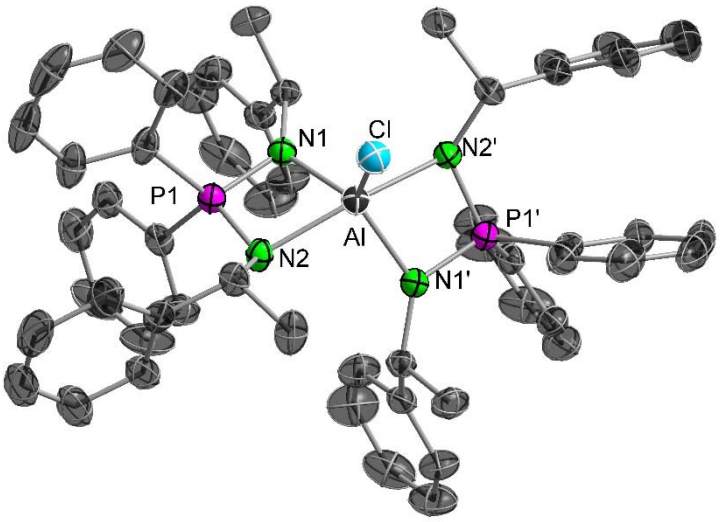

Figure S27: Molecular structure of **2** in the solid state with ellipsoids drawn at 40 % probability. All the hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles: Al-N1 1.909(3), Al-N2 2.040(3), Cl-Al 2.174(2), P1-N1 1.620(3), P1-N2 1.619(3); N1-Al-N1' 126.4(2), N2-Al-N2' 166.6(2), N1-Al-N2 75.13(13), N1'-Al-N2 98.69(14), N1-Al-Cl 116.81(11), N2-Al-Cl 96.72(10), P1-Al-P1' 142.76(8), N2-P1-N1 96.2(2).

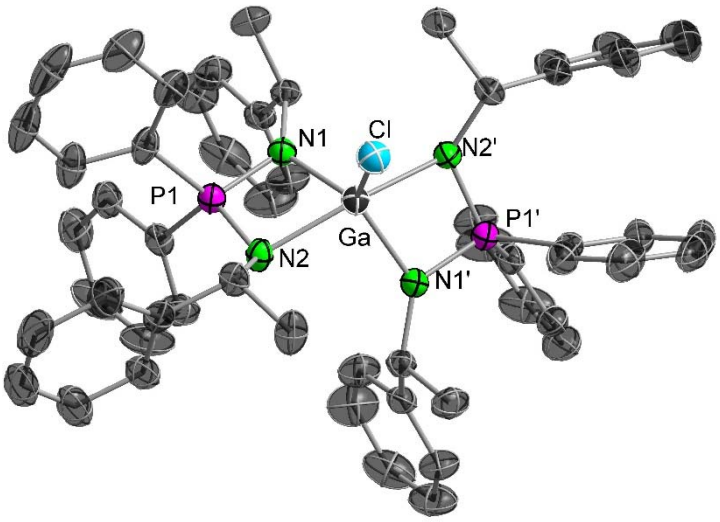

Figure S28: Molecular structure of **3** in the solid state with ellipsoids drawn at 40 % probability. All the hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles: Ga-N1 1.950(6), Ga-N2 2.087(5), Ga-Cl 2.240(2), P1-N1 1.617(6), P1-N2 1.625(7);N1-Ga-Cl 116.2(2), N2-Ga-Cl 96.88(13), N2-Ga-N2' 166.2(3), N1-Ga-N1' 127.7(3), N1-Ga-N2 73.4(2), N1-Ga-N2' 100.4(2), N1-P1-N2 96.4(3).

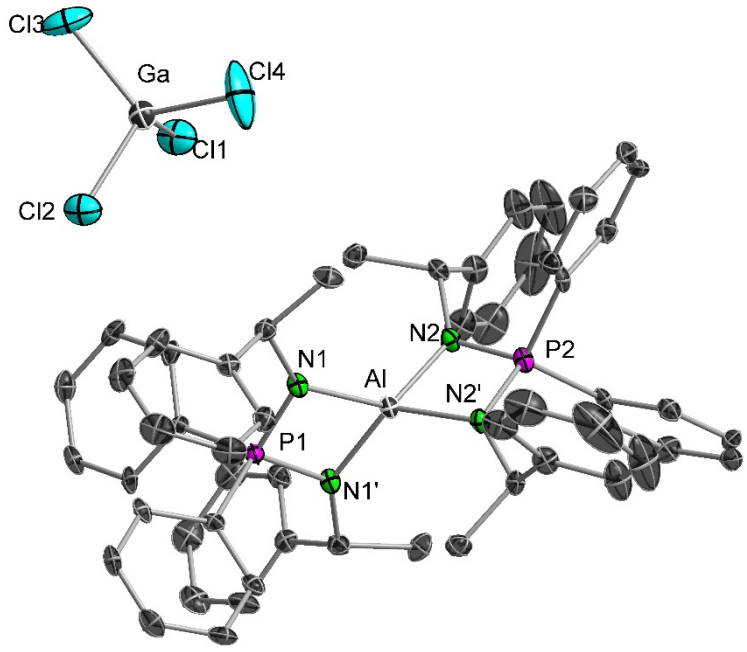

Figure S29: Molecular structure of **4** in the solid state with ellipsoids drawn at 40 % probability. All the hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles [°]: Al-N1 1.857(4), Al-N2 1.871(4), Ga-Cl1 2.166(2), Ga-Cl2 2.171(2), Ga-Cl3 2.158(2), Ga-Cl4 2.15(2), P1-N1 1.631(4), P2-N2 1.629(4); N1-Al-N1' 79.2(2), N1-Al-N2 126.3(2), N1-Al-N2' 126.3(2), N2-Al-N2' 79.7(2), P2-Al-P1 180.0, Cl1-Ga-Cl2 110.89(6), Cl3-Ga-Cl1 109.87(7), Cl3-Ga-Cl2 106.93(7), Cl4-Ga-Cl1 108.97(7), Cl4-Ga-Cl2 108.19(9), Cl4-Ga-Cl3 112.0(9), N1-P1-N1' 93.0(3), N2-P2-N2' 94.7(3).

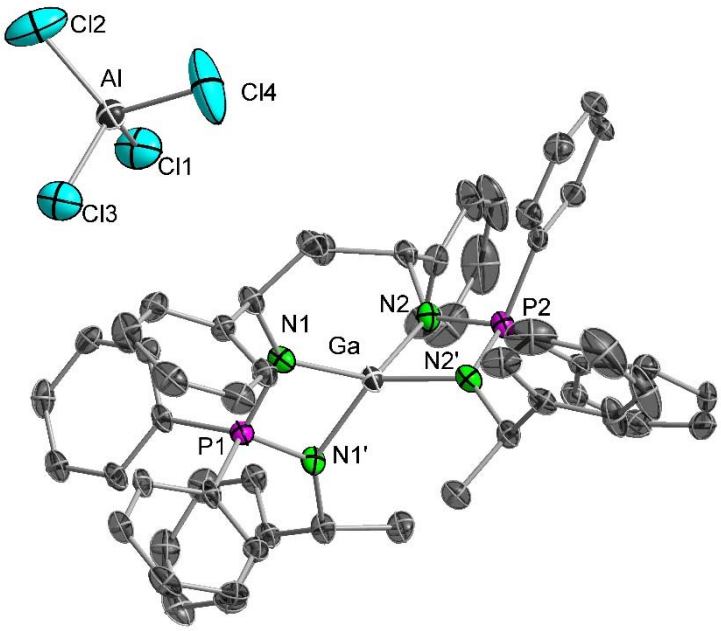

Figure S30: Molecular structure of **5** in the solid state with ellipsoids drawn at 40 % probability. All the hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles [°]: Ga-N1 1.923(6), Ga-N2 1.938(6), Al-Cl1 2.129(3), Al-Cl2 2.119(4), Al-Cl3 2.134(4), Al-Cl4 2.109(4), P1-N1 1.629(6), P2-N2 1.626(6); N1-Ga-N1' 76.9(4), N1-Ga-N2 126.5(3), N2-Ga-N2' 77.2(4), N1-Ga-N2' 129.0(3), Cl1-Al-Cl3 110.7(2), Cl2-Al-Cl1 109.8(2), Cl2-Al-Cl3 107.4(2), Cl4-Al-Cl1 109.2(2), Cl4-Al-Cl2 112.2(2), Cl4-Al-Cl3 107.5(2), N1-P1-N1' 94.4(5), N2-P2-N2' 96.1(5).

4 Theoretical calculations

The geometries of the molecules under discussion were computed with the program system TURBOMOLE 7.3[7] within the framework of Density Functional Theory (DFT) at the RI-BP86 level[8] using a def-SV(P) basis set[9] for each atom without the constraint of symmetry. The theoretical infrared spectra (frequencies and intensities) were calculated using the module AOFORCE.[10] The motions related to the vibrations (eigenvector analysis) were investigated by means of the program TmoleX[11].

Cartesian Coordinates of **1** (given in atomic units (a.u.))

-2.93613909680825	3.88473074135491	-1.01029020552826	p
0.00103807722899	0.00023944662147	-2.63589807954752	al
-0.00865473250568	3.94756282150709	-2.10474278390948	n
-3.16353056632907	0.76041747376893	-0.87154985146691	n
-3.48651934221284	5.46606416396477	2.03253403872687	c
-5.14495963168304	5.36932873632122	-3.26759274917761	c
2.94007531633281	-3.88417960440561	-1.01384013076607	p
0.01221391947129	-3.94684440647514	-2.10731808789015	n
3.16761436702161	-0.76003456344250	-0.87466540765508	n
-0.00060722316645	0.00188556353295	-5.71861634927987	h
0.85920373242740	5.97415974294083	-3.82538453999972	c
-5.22152851873937	-0.84662174160188	0.07497026801889	c
-5.94028462404118	5.76111632290634	3.04536816771354	c
-1.38517766395601	6.29548099133062	3.44475765590195	c
-6.34718497429745	7.71277765312564	-2.84339976990652	c
-5.45839481156891	4.15610643594993	-5.62851689074520	c
3.49132829405871	-5.46683918816969	2.02813981510524	c
5.14728032854033	-5.36867828058910	-3.27277923088350	c
-0.85663074601923	-5.97481288515241	-3.82575862573304	c
5.22483544819413	0.84610299554096	0.07523266981111	c
1.37815945429355	8.50274694712744	-2.50317303525710	c

-0.62483414086502	6.36934824101996	-5.27462658686970	h
3.21396252820119	5.11160132212776	-5.30316820839365	c
-5.60659540835962	-0.75008325977710	2.95728568059524	c
-4.50255062126007	-2.78919615186080	-0.30316156211008	h
-7.68384694135012	-0.55859411312513	-1.44373941348010	c
-7.60738258138762	5.11252929413938	1.97812578962156	h
-6.27781339441292	6.87592379688191	5.42836589163743	c
0.52353417638141	6.07247655890979	2.65157274879776	h
-1.72902005605873	7.41316256181961	5.82775061755902	c
-6.07040970690810	8.71995253966722	-1.04295650544429	h
-7.89123242710610	8.78728159328130	-4.72112872836756	c
-4.46765600326461	2.35897351870847	-6.00046697531311	h
-6.99024752696171	5.23975834684861	-7.50219156846124	c
5.94570422240314	-5.76865610634695	3.03741181724009	c
1.38976300178742	-6.29129631771574	3.44299568407544	c
6.34433389607656	-7.71548743718684	-2.85247747823534	c
5.46382909203810	-4.15202914213406	-5.63148669499346	c
-1.37860401622163	-8.50128166908555	-2.50052430133330	c
0.62816712035134	-6.37343622398757	-5.27327418770053	h
-3.20926757626030	-5.11209487923373	-5.30680867080803	c
5.60410579047827	0.74935189745367	2.95828085691153	c
4.50810985956595	2.78918092152145	-0.30442332497566	h
7.68993736357948	0.55557073727143	-1.43829704973855	c
3.26481195055823	8.73902115402356	-0.62976684753140	c
0.02129065092189	10.68948873844395	-3.19399406941706	c
4.84510651874403	4.77662004669126	-4.02438752582256	h
3.77459126844625	6.59233767633540	-6.68431249438421	h
2.80580801712190	3.33346680987585	-6.34212421937324	h
-3.49808108685901	-1.11468868978652	4.55257540153558	c

-7.99509065264063	-0.44914024301600	4.10040208615106	c
-8.58782447030868	1.31830917530357	-1.15391581510774	h
-9.07940544563228	-2.03988031144963	-0.92061224264565	h
-7.27821466388863	-0.74896883512487	-3.49183551457085	h
-8.19865414785710	7.08789161629258	6.20630275326711	h
-4.17302089735869	7.70672817037583	6.82168983272233	c
-0.07086527324691	8.06455145254815	6.90740759260518	h
-8.83244943692187	10.61178220159715	-4.36243390192365	h
-8.22395214786647	7.55070974478210	-7.04644238251016	c
-7.22082006154449	4.27355282204829	-9.33390360090809	h
7.61292795606058	-5.12355415396532	1.96819995961854	h
6.28371209974671	-6.88601853119294	5.41915663502052	c
-0.51950999555352	-6.06280173413648	2.65262828579811	h
1.73407507574100	-7.41148641567573	5.82471533341974	c
6.06499438363500	-8.72522656417337	-1.05386588133059	h
7.88632408285232	-8.79008782283969	-4.73183833002391	c
4.47702307808465	-2.35213959687504	-6.00039241928502	h
6.99364956494891	-5.23571091814559	-7.50680263149707	c
-3.26541321873531	-8.73334234241727	-0.62678104163763	c
-0.02414769921681	-10.69032961969588	-3.18876219999129	c
-4.84077215572084	-4.77251124078129	-4.02971945076472	h
-3.77094749238414	-6.59479794376481	-6.68540984162390	h
-2.79828274328424	-3.33642193784740	-6.34883246847595	h
3.49326771284243	1.11991943558487	4.54909491975411	c
7.98952216715053	0.44308710610877	4.10635046167371	c
8.59079132729346	-1.32275835753827	-1.14782268717715	h
9.08639056513176	2.03455562962855	-0.91101431647431	h
7.28909294723596	0.74791353077403	-3.48716609557548	h
4.36263102369095	7.06096352204831	-0.06010641791644	h

3.77137338795294	11.07678971012541	0.51712792234412	c
-1.45306743810229	10.54625786639750	-4.66243656407004	h
0.51508034763716	13.03766772075323	-2.04903029149620	c
-1.62035392081876	-1.37015511251790	3.69063335896985	h
-3.75932434663012	-1.17487582214315	7.18923937771290	c
-9.69251264855031	-0.17432590224512	2.92858317671462	h
-8.26765204440601	-0.49705982879810	6.74604356259525	c
-4.44266639096115	8.58479454635758	8.69240290313153	h
-9.43491424275733	8.39619919828262	-8.51666005735121	h
8.20512005567922	-7.10392101864298	6.19407508113493	h
4.17876481434706	-7.71252029333785	6.81477209891792	c
0.07579710364173	-8.05932341836234	6.90631599116322	h
8.82364090264402	-10.61717720652863	-4.37612797771224	h
8.22228253311382	-7.55009819833161	-7.05486813584778	c
7.22673157039867	-4.26672423671045	-9.33672586992434	h
-4.36131220745914	-7.05346726284319	-0.05883039598360	h
-3.77457934022899	-11.06923492688373	0.52277629633880	c
1.45020877609252	-10.55050134667016	-4.65756337214998	h
-0.52063375254925	-13.03669761324371	-2.04125534104235	c
1.61791548875543	1.37932443618936	3.68313727004073	h
3.74942861252819	1.18175146138644	7.18621681809729	c
9.68856545139138	0.16309647809045	2.93807412957459	h
8.25695586059444	0.49245183786776	6.75249902178906	c
2.39342659525887	13.23953994236072	-0.18611440341079	c
5.25854436030304	11.21570478766997	1.97162473229055	h
-0.57697610898312	14.71885094620887	-2.62101316793127	h
-6.15281477784161	-0.85969441216168	8.30359730098470	c
-2.07834260245663	-1.48329349709670	8.38196475624768	h
-10.15832869284834	-0.25170960361590	7.59017577517612	h

4.44878514658365	-8.59270874016506	8.68443246556354	h
9.43160420499990	-8.39568546649441	-8.52637684134368	h
-2.39903178240298	-13.23432624320940	-0.17794551874856	c
-5.26166847522988	-11.20470243814798	1.97768213975005	h
0.56966137212087	-14.71970981361363	-2.61122481173252	h
6.13999301464412	0.86195148931995	8.30553750122211	c
2.06680971289258	1.49520453673031	8.37532270582335	h
10.14530525798848	0.24294980233036	7.60061049450778	h
2.78923599882276	15.07633033573133	0.71562490333674	h
-6.36584883535495	-0.90489605541812	10.37640743380364	h
-2.79700821408971	-15.06967257849809	0.72577670630641	h
6.34912279540513	0.90891697048774	10.37870325186430	h

Theoretical IR spectrum of 1_H

wave number (cm^{-1})	IR int. (km/mol)
8.47	0.00112
8.62	0.00682
12.49	0.13381
13.11	0.00895
22.46	0.16699
24.13	0.00276
25.28	0.02698
29.55	0.03179
32.16	0.00799
33.03	0.30472
41.73	0.11379
41.95	0.25027
46.26	0.26409
48.54	0.00190
53.11	0.72856
55.65	0.00634
57.33	0.00973
61.43	0.03148
67.52	0.14535
69.32	0.00054
77.16	0.08406
77.39	0.00717
80.05	0.04514
80.58	0.04988
86.23	0.02321
94.88	0.02647
98.66	0.00398
101.75	0.10425
103.23	0.28878
105.46	0.30369
119.13	0.23619
144.47	0.02150
173.71	0.48371
176.02	0.73306
182.73	2.26568
183.59	0.41385
186.17	0.15400
189.71	0.01125
195.73	2.31797
206.75	0.70589
207.90	1.12914
211.91	0.07384
218.41	0.04925
219.67	5.01821
242.08	1.33086
243.87	2.22404
246.90	0.09510
247.56	0.57665
257.94	0.05402
258.76	0.70583
262.66	21.93167
266.21	0.72913
275.36	27.73266
284.22	1.21984
302.45	27.61008
305.97	4.13212
312.79	0.82304
323.26	1.47097
326.99	0.28299
331.14	30.35168
342.94	0.53804
362.13	1.86308
371.72	1.34796
392.35	0.40433
395.99	0.07043
396.91	0.02636
403.12	0.60644
405.49	0.00308
405.80	2.86660
407.10	11.00621
409.58	0.00655
411.40	0.28975
412.30	0.05739
447.00	0.13824
447.29	35.01403
453.77	0.35733
457.03	18.30274
462.06	0.67250
463.64	11.28445
468.81	5.33922
470.76	9.81347
499.96	8.28502
504.41	76.87795

509.65	0.77599	703.93	34.34298	898.37	1.98713
511.99	42.71393	704.97	32.53578	898.46	1.68880
524.79	13.72717	706.30	0.61729	899.82	7.54442
528.74	183.97424	706.47	19.78119	907.69	0.35699
561.68	9.28138	715.41	162.10527	914.63	0.78851
561.86	1.12699	721.61	36.33105	914.78	0.77827
568.80	1.31565	727.32	133.81494	920.33	0.87700
571.33	27.67612	740.40	59.90144	920.49	2.21549
600.48	202.20750	740.77	0.57954	951.42	0.61882
606.20	62.45783	742.87	0.10724	951.58	0.05104
607.31	3.83805	743.79	50.87260	952.70	0.97310
609.19	2.78539	749.31	3.78570	960.09	1.66298
609.77	5.79994	750.89	8.98374	962.61	12.28293
610.08	0.36150	768.47	109.46966	962.79	1.76631
612.20	2.76132	769.15	3.12719	962.85	2.62361
613.17	77.75116	770.71	8.57181	963.12	1.56393
614.33	0.01624	770.75	15.99144	964.77	0.01669
615.91	3.40081	796.34	0.17488	967.02	1.82842
616.52	114.25030	809.80	319.66299	967.09	0.01799
653.13	10.10250	827.78	92.21023	968.94	70.39498
654.43	6.34543	829.40	1.49299	975.81	9.17554
672.10	4.19970	831.19	1.08033	976.68	0.32549
678.56	72.72431	832.49	1.02941	976.83	6.09008
695.38	114.99460	833.98	5.88195	982.00	0.49956
697.75	50.39826	840.90	0.07848	982.55	0.28200
698.82	45.77460	842.45	0.00404	982.64	1.37421
700.31	6.51985	842.74	1.83874	984.40	0.21915
700.45	13.37485	845.52	0.24404	984.50	0.58081
703.80	13.32086	846.52	0.54420	984.56	0.34765

985.98	1.49425	1088.51	24.72386	1203.58	75.74904
986.06	2.85741	1088.68	42.66545	1268.33	28.98215
986.79	0.49741	1091.70	10.68383	1268.49	7.12139
986.80	0.03404	1092.10	73.79793	1282.21	7.43636
987.92	0.15952	1096.23	15.85815	1282.34	15.14751
987.97	0.33932	1097.07	1.93394	1292.44	2.59058
990.96	0.00080	1119.12	117.36256	1292.45	3.41221
1012.32	0.37092	1121.57	524.45534	1300.84	4.00518
1013.83	22.86776	1136.90	3.19036	1300.90	1.53242
1023.14	8.91148	1138.41	0.05068	1312.02	2.44823
1023.43	3.24329	1138.42	1.20441	1312.25	3.34743
1024.43	0.01500	1139.22	0.01020	1314.16	2.49255
1024.45	1.01211	1142.40	0.27793	1314.41	0.27437
1025.05	3.78664	1142.42	0.26953	1316.86	1.28298
1025.26	5.96253	1143.25	0.32656	1317.42	14.44466
1030.50	20.39036	1143.26	0.55818	1344.46	0.83954
1031.34	20.93737	1156.73	0.25949	1344.62	10.02457
1032.15	21.27919	1156.78	0.63328	1350.06	27.98037
1033.73	0.09513	1162.65	4.70697	1350.97	13.26602
1059.58	15.63848	1164.62	0.09201	1354.21	9.90344
1059.83	0.36761	1165.97	1.77087	1354.37	7.85152
1067.13	37.92187	1167.75	2.18838	1363.41	0.05784
1068.01	1.19127	1170.91	6.19782	1363.43	0.46093
1072.35	7.33921	1170.93	6.12002	1365.91	0.77425
1073.04	0.64697	1179.11	0.15895	1365.95	0.40324
1076.83	0.30369	1179.50	57.69385	1373.02	1.91955
1077.13	2.84299	1192.30	61.02729	1373.25	1.17536
1082.24	56.89523	1192.42	8.21670	1378.56	14.07930
1082.65	13.08614	1203.21	15.14272	1378.61	2.84997

1424.01	0.59445	1596.91	1.28194	3077.79	4.70264
1424.81	2.53335	1597.84	0.06745	3082.04	1.39031
1427.37	4.87300	1597.84	0.56787	3082.28	0.27169
1427.41	9.07980	1601.95	0.27889	3083.00	0.58484
1430.85	1.23502	1601.98	0.06526	3083.01	0.57956
1430.91	21.00648	1604.26	0.50215	3085.51	0.84245
1432.81	26.69182	1604.28	2.43716	3085.65	0.72105
1432.95	5.42921	1614.92	4.86282	3090.02	0.47377
1436.21	5.82034	1614.94	0.00812	3090.06	0.32980
1436.31	11.84286	1616.55	0.46873	3091.85	11.68978
1441.50	20.73502	1617.28	5.07230	3091.85	4.07347
1441.60	6.05886	1740.62	230.45828	3092.30	2.00639
1442.91	7.93725	2889.98	14.61033	3092.37	1.85797
1442.93	12.14021	2890.09	38.26532	3092.79	24.45941
1446.01	1.00348	2936.89	13.27158	3093.79	2.53409
1446.09	6.39799	2936.94	4.51093	3098.42	6.35994
1473.21	0.39478	2947.07	19.00699	3098.48	13.34474
1473.23	2.83250	2947.16	13.08718	3098.64	36.86553
1475.01	2.85483	2951.73	12.25115	3098.66	9.17064
1475.10	7.58802	2951.82	22.62769	3102.19	10.60067
1484.15	13.42954	3025.72	10.10414	3102.21	6.02447
1484.18	3.49151	3025.85	54.49554	3104.66	0.71792
1487.16	1.45751	3037.34	22.83999	3105.25	38.24634
1488.07	21.19555	3037.40	22.00007	3107.71	14.37876
1587.71	0.70235	3047.84	16.83367	3107.75	15.28481
1587.73	0.06721	3047.96	14.31753	3109.95	45.82131
1590.72	0.82494	3050.23	7.75806	3109.98	2.61430
1590.74	0.18554	3050.37	8.84434	3112.51	14.81150
1596.52	0.46025	3077.76	6.12773	3112.54	25.67417

3113.02	24.07135	3116.11	16.40553	3134.09	2.67639
3114.45	1.18489	3116.88	3.78440	3134.30	4.20814
3115.84	3.39893	3118.74	27.02632		
3115.99	24.93623	3118.79	3.50106		

Theoretical IR spectrum of 1_D

wave number (cm^{-1})	IR int. (km/mol)
8.47	0.00114
8.63	0.00685
12.49	0.13393
13.11	0.00900
22.47	0.16753
24.14	0.00276
25.29	0.02702
29.57	0.03190
32.17	0.00807
33.04	0.30721
41.75	0.11431
41.96	0.25084
46.22	0.26899
48.56	0.00189
53.12	0.73296
55.69	0.00636
57.37	0.00969
61.47	0.03107
67.56	0.14582
69.37	0.00053
77.18	0.08220
77.42	0.00731
80.04	0.04851
80.62	0.05032
86.29	0.02329
94.93	0.02627
98.74	0.00403
101.82	0.10749
103.28	0.28662
105.52	0.30577
119.09	0.22845
144.42	0.02305
173.80	0.39666
176.03	0.74124
182.54	2.48280
183.72	0.41272
186.29	0.15794
189.64	0.00411
195.67	2.50766
206.83	0.71389
207.66	1.20450
212.01	0.07048
218.45	0.05940
219.41	5.88171
241.88	1.30719
243.72	2.98153
246.52	0.01958
247.68	0.62124
258.55	0.08069
258.93	0.50503
261.52	24.85637
266.43	0.73803
273.98	19.68844
283.63	1.16383
297.07	7.24592
301.92	30.26957
313.43	0.85473
323.11	3.22530
327.58	0.24027
329.80	29.59228
342.35	0.61386
361.07	4.61264
371.75	1.35166
392.24	0.39277
395.95	1.38646
397.33	0.02003

398.69	5.38511	609.41	2.78878	750.55	30.87338
403.61	0.22010	610.18	1.02003	769.11	110.70007
405.95	0.00319	610.29	0.41535	770.33	2.97278
406.47	0.07820	610.99	2.27610	771.65	21.41787
410.04	0.00605	612.43	0.07700	771.74	1.88622
411.77	0.01997	614.53	0.01488	797.12	0.15997
412.75	0.05867	616.17	3.44683	808.35	228.51526
438.99	22.78478	620.96	15.85939	820.98	223.11608
446.12	123.55530	653.69	9.42049	831.94	2.87297
447.26	0.15551	654.47	1.84893	833.30	3.87758
453.64	0.37235	672.37	4.07311	835.03	1.01220
457.05	25.85726	678.23	52.17140	835.07	2.73766
462.36	0.71372	697.69	173.22366	843.55	0.05594
464.68	30.85889	699.20	50.98950	845.08	0.00375
469.08	5.45994	700.92	14.60030	845.20	0.83486
470.96	17.42182	701.92	8.04523	848.18	0.25618
500.08	7.94206	702.04	11.50036	849.12	0.57772
505.91	152.45950	704.30	23.85608	900.74	2.37250
509.99	0.82163	704.80	27.60807	900.84	1.54592
514.15	0.36661	706.27	19.50608	902.32	7.32202
522.93	60.65475	707.94	5.09529	910.27	0.35451
528.64	183.06021	707.98	10.04170	917.27	0.70846
542.44	58.55147	722.14	35.96603	917.37	0.64521
562.37	0.76479	725.20	68.50482	923.03	0.96537
566.42	60.33851	741.83	79.06136	923.19	2.51924
569.13	1.43564	742.28	0.33643	954.09	0.60607
578.26	85.09336	744.35	0.25624	954.26	0.07998
607.57	3.55861	744.84	35.65709	955.40	0.93394
608.47	1.53021	750.19	4.24689	962.68	4.51999

964.21	12.73031	1025.70	1.16191	1146.68	0.20425
964.80	1.25865	1026.63	4.69246	1146.70	0.17812
965.49	0.73322	1026.73	7.33163	1147.54	0.28614
965.53	0.86249	1032.49	20.29615	1147.55	0.60552
966.71	0.09409	1033.09	26.42526	1160.83	0.30269
969.52	0.14128	1033.98	13.26578	1160.87	0.30942
969.65	15.64889	1035.82	0.03622	1166.66	6.07865
969.95	55.51365	1061.73	16.76798	1168.64	0.04556
978.48	6.08755	1062.08	0.24327	1170.04	1.90400
979.57	0.25303	1069.31	38.71147	1171.81	2.33479
979.70	4.73290	1070.10	1.27007	1174.78	5.73300
983.03	0.24625	1074.94	8.35651	1174.88	9.43363
983.09	0.62666	1075.54	0.33304	1180.31	0.32738
983.73	1.25666	1079.35	1.34096	1180.57	55.18746
984.88	0.34970	1079.70	3.44978	1193.94	63.04421
984.92	0.52506	1083.61	58.78044	1194.06	7.89221
985.05	0.22774	1084.01	11.92100	1204.14	17.70160
986.53	1.73381	1090.70	26.67476	1204.42	69.05439
986.56	2.51879	1090.90	44.95617	1254.36	140.83769
989.38	0.47923	1092.89	10.18671	1271.37	31.08975
989.63	0.00099	1093.34	71.79770	1271.66	1.82165
990.49	0.18676	1098.09	17.05223	1285.57	7.62621
990.66	0.20666	1099.09	2.31755	1285.71	14.57539
993.23	0.11527	1119.75	109.60005	1296.09	4.23947
1014.18	0.50869	1121.90	501.34256	1296.10	1.99327
1015.62	21.02083	1141.16	2.39449	1304.54	3.99698
1024.44	7.26175	1142.68	0.05171	1304.61	1.21596
1024.60	3.37896	1142.69	1.10407	1315.94	2.47170
1025.69	0.05445	1143.51	0.00989	1316.26	5.88262

1318.26	2.45198	1444.59	0.12050	2900.60	14.75554
1318.56	0.37303	1447.06	10.76199	2900.70	38.25787
1320.99	0.82399	1447.25	21.08180	2947.75	12.81255
1321.63	10.82616	1448.95	1.91783	2947.79	4.89226
1348.47	10.13524	1449.10	1.54966	2958.36	19.46068
1349.07	5.74893	1475.68	0.51196	2958.45	13.05366
1354.00	26.05129	1475.70	2.94075	2963.12	12.89961
1355.18	7.19777	1477.53	3.16651	2963.21	22.31480
1358.35	10.26850	1477.63	7.78595	3036.63	10.15379
1358.54	6.59680	1486.34	14.12266	3036.75	54.95916
1363.86	0.05687	1486.37	2.99890	3048.28	24.00514
1363.87	0.36512	1489.40	1.46858	3048.34	21.37254
1366.22	0.71340	1490.32	21.02876	3058.81	16.30968
1366.30	0.24949	1588.35	0.67497	3058.92	15.14970
1373.38	2.03506	1588.39	0.12162	3061.24	7.82787
1373.62	1.37726	1591.33	0.80110	3061.38	9.00487
1379.89	16.61329	1591.35	0.11685	3089.06	6.18488
1380.09	5.08042	1597.09	0.48041	3089.09	4.76092
1429.23	3.45900	1597.49	1.48207	3093.36	1.42433
1429.72	7.15214	1598.43	0.60749	3093.60	0.27603
1429.90	10.16881	1598.43	0.02786	3094.29	0.59343
1430.34	0.31729	1602.59	0.27300	3094.30	0.58859
1434.32	20.35394	1602.63	0.00728	3096.81	0.84543
1434.38	1.56696	1604.87	0.49076	3096.95	0.73550
1436.72	24.06196	1604.89	2.49942	3101.36	0.48533
1436.81	3.65057	1615.47	4.91700	3101.40	0.33488
1441.53	5.26154	1615.49	0.01298	3103.13	11.71221
1441.62	13.72100	1617.11	0.47262	3103.13	4.10443
1444.45	19.61909	1617.85	4.76767	3103.62	1.98004

3103.69	1.83767	3115.96	0.72658	3125.80	1.26637
3104.10	24.73850	3116.55	38.64878	3127.13	3.56114
3105.10	2.57701	3119.02	14.37386	3127.28	25.00497
3109.74	9.37736	3119.06	15.44546	3127.42	16.62534
3109.79	16.71071	3121.20	46.27898	3128.19	3.73696
3109.91	33.63825	3121.23	2.65040	3130.06	26.91451
3109.94	6.44533	3123.81	14.99161	3130.11	3.49038
3113.49	10.74179	3123.85	25.99582	3145.50	2.66906
3113.52	6.10222	3124.35	24.05113	3145.71	4.20168

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