Supporting Information

Reactivity of a Zinc Hexazene Complex.

*S. Gondzik, C. Wölper, R. Haack, G. Jansen, and S. Schulz**

Content

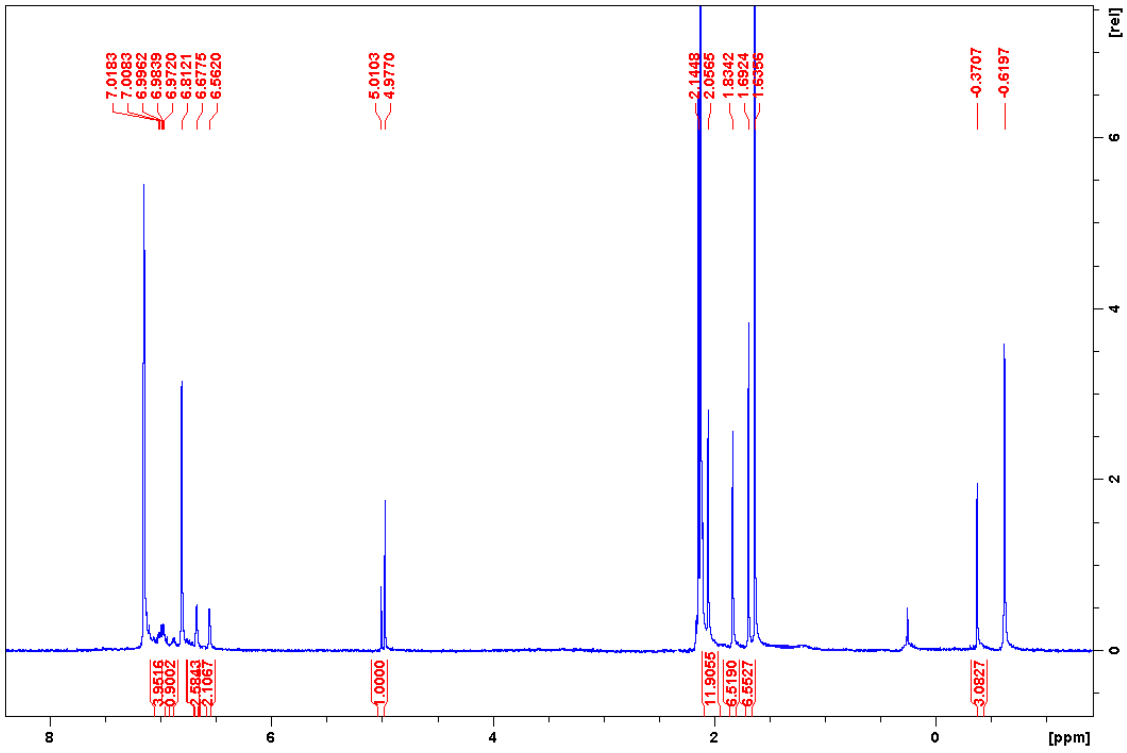

Figure S1. ^{1}H-NMR spectrum of [(^{Me}LZn)(μ-η^2:η^2-N_6Ph_2)(ZnMe)] (**2**) in C_6D_6.

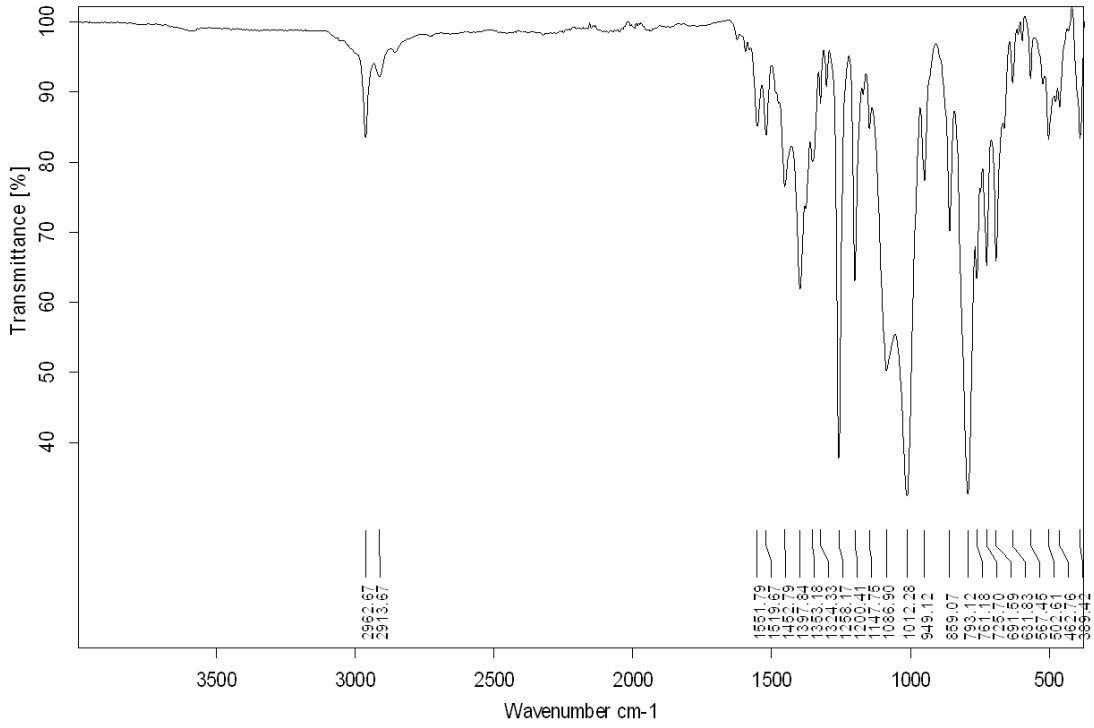

Figure S2. IR spectrum [(^{Me}LZn)(μ-η^2:η^2-N_6Ph_2)(ZnMe)] (**2**).

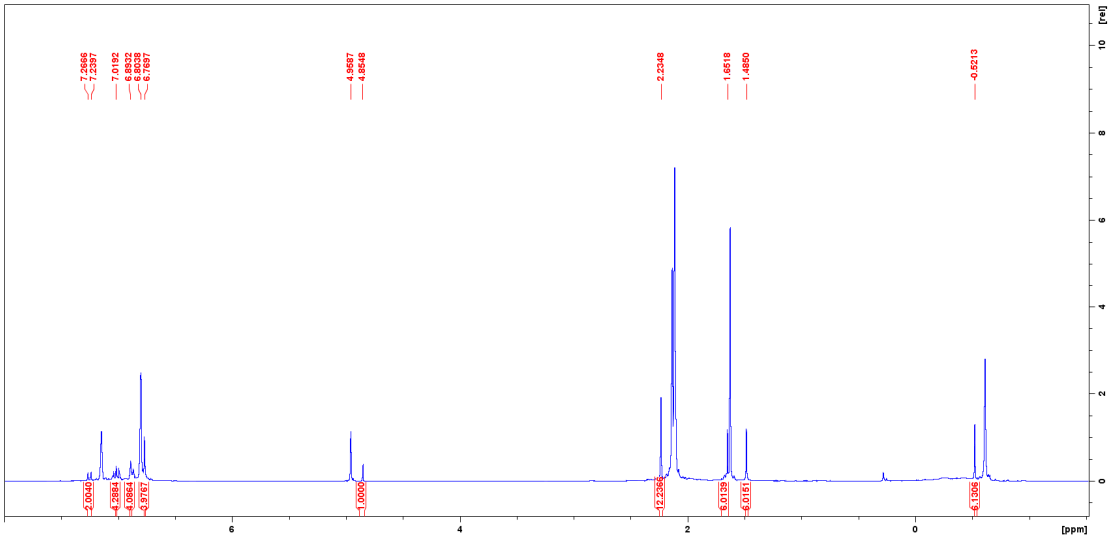

Figure S3. ^{1}H-NMR spectrum of [(^{Me}LZn)(μ-η^2:η^2-N_6Ph_2)($AlMe_2$)] (**3**) in C_6D_6.

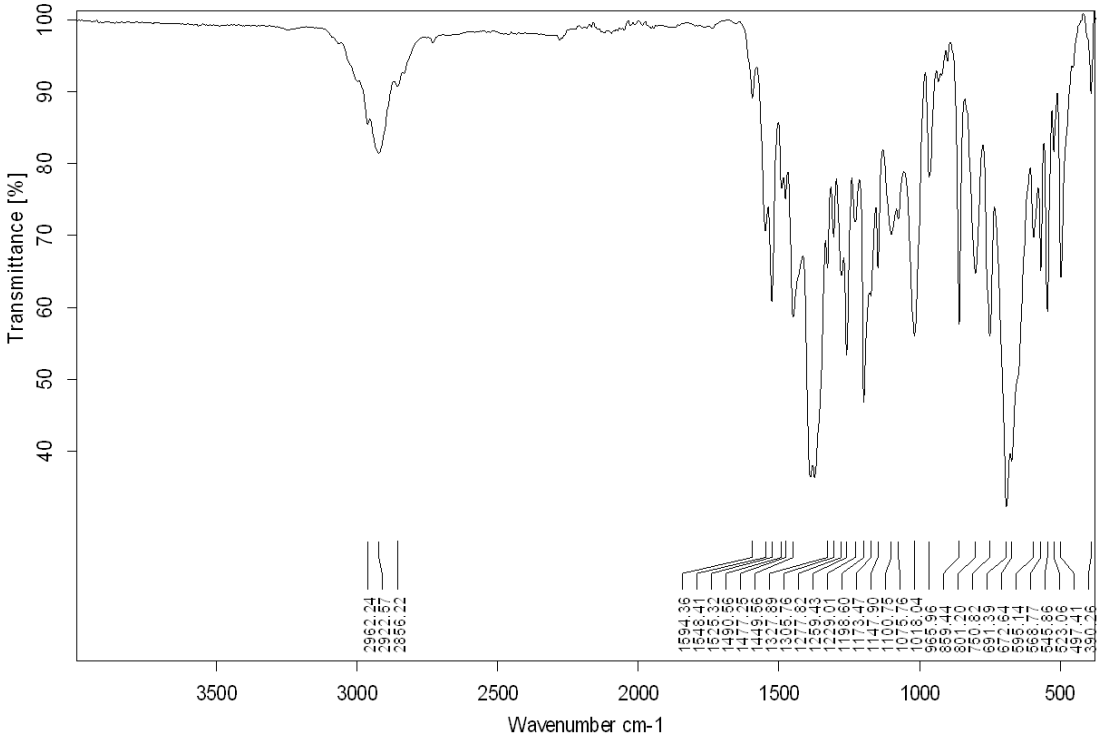

Figure S4. IR spectrum of [(^{Me}LZn)(μ-η^2:η^2-N_6Ph_2)($AlMe_2$)] (**3**).

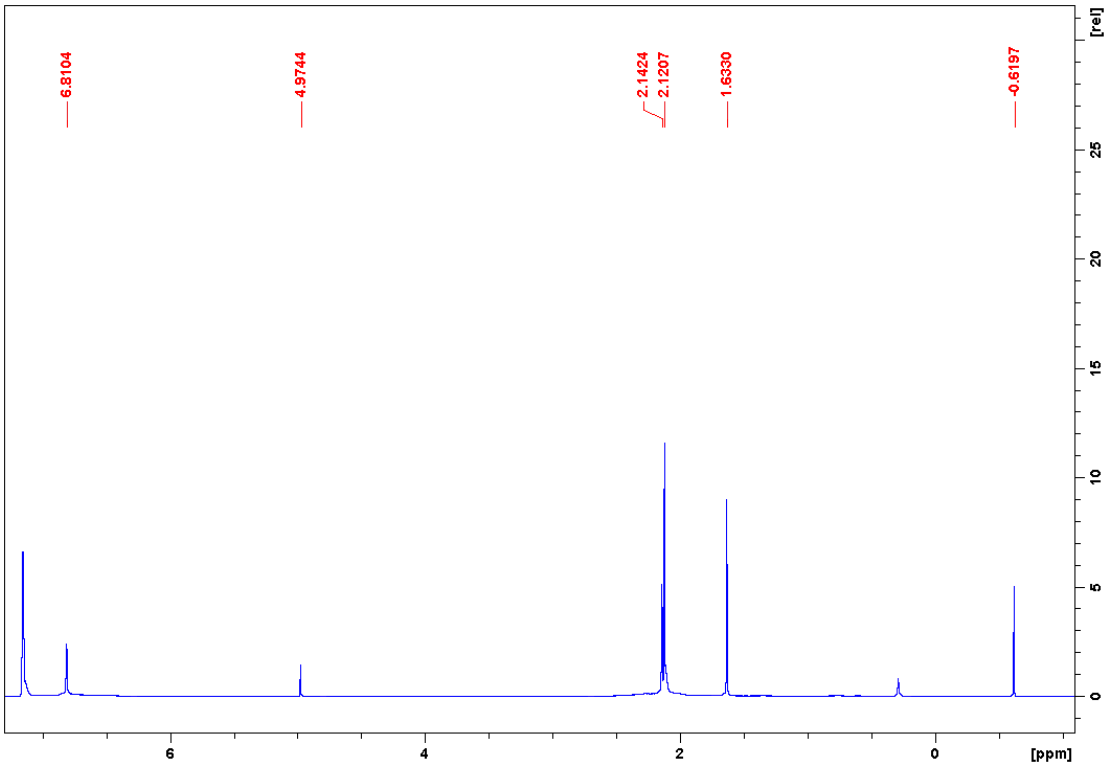

Figure S5. ^{1}H-NMR spectrum of [(^{Me}LZn)(μ-η^{2}:η^{2}-N_6Ph_2)(Li)] (**4**) in C_6D_6.

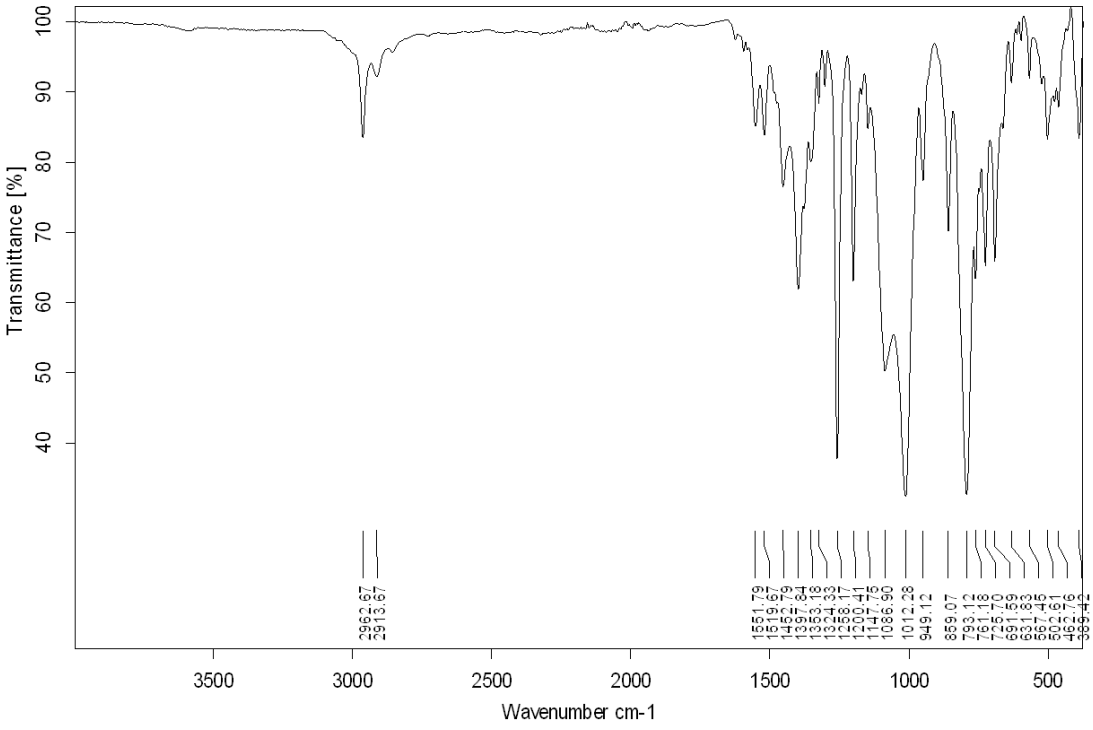

Figure S6. IR spectrum of [(^{Me}LZn)(μ-η^{2}:η^{2}-N_6Ph_2)(Li)] (**4**).

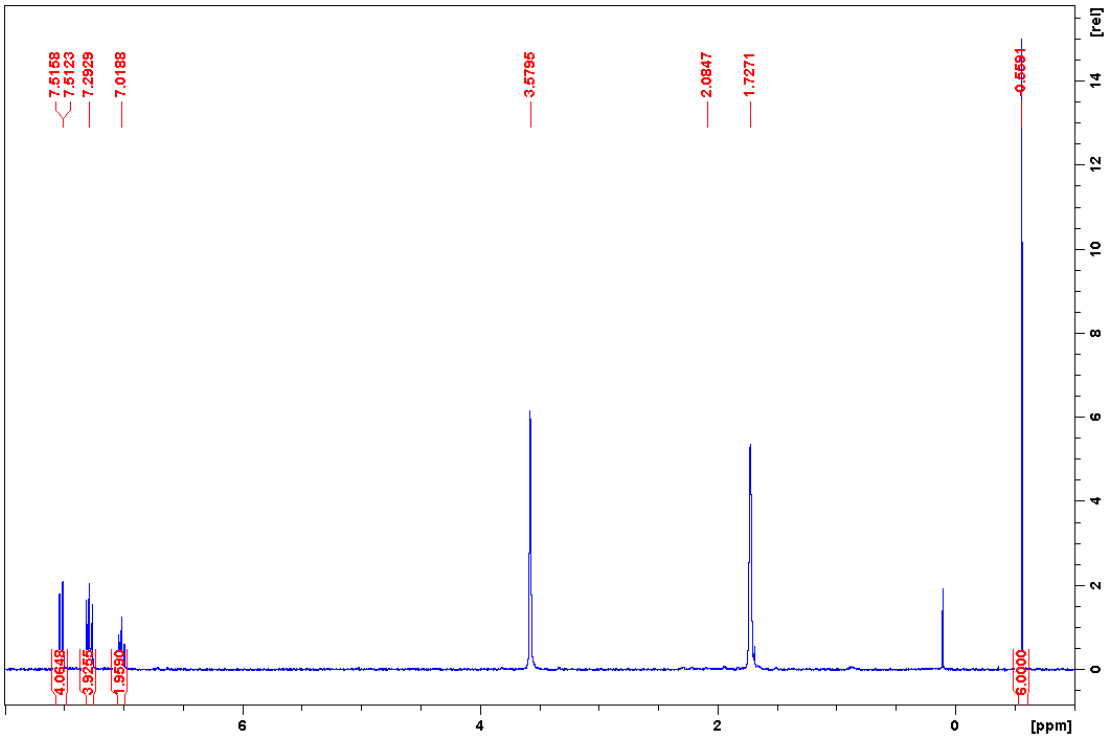

Figure S7. ^{1}H-NMR spectrum of [(ZnMe)$_2$(μ-η^2:η^2-N$_6$Ph$_2$)] (**5**) in THF-d$_8$.

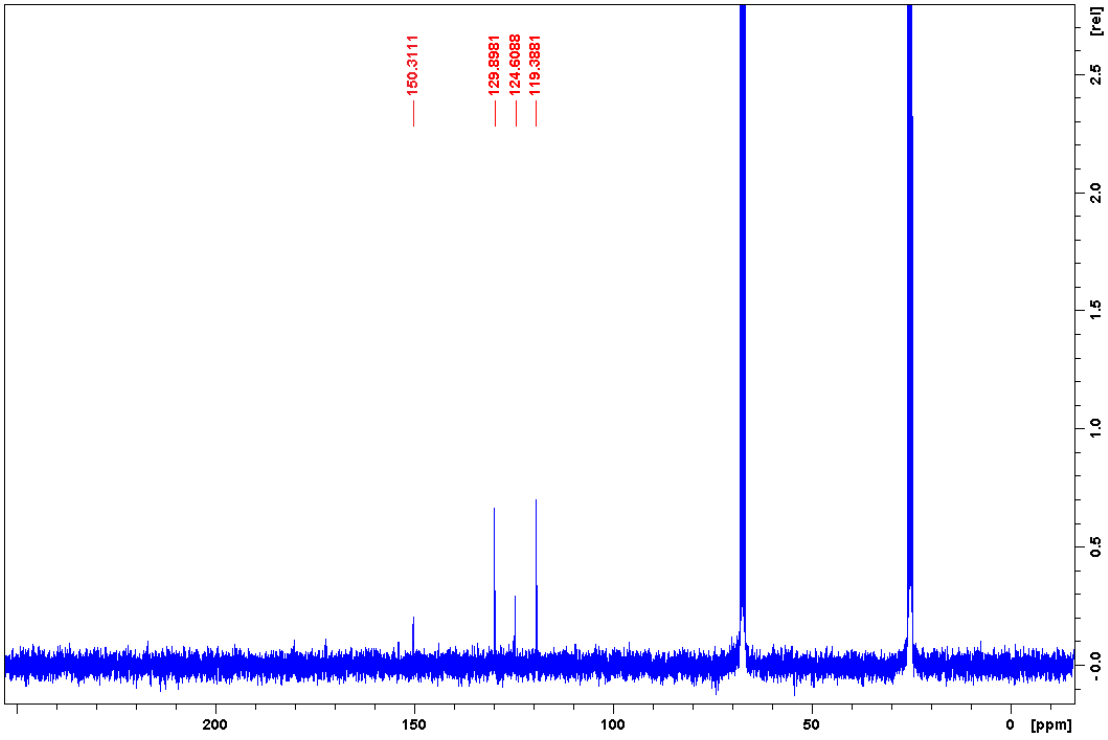

Figure S8. ^{13}C-NMR spectrum of [(ZnMe)$_2$(μ-η^2:η^2-N$_6$Ph$_2$)] (**5**) in THF-d$_8$.

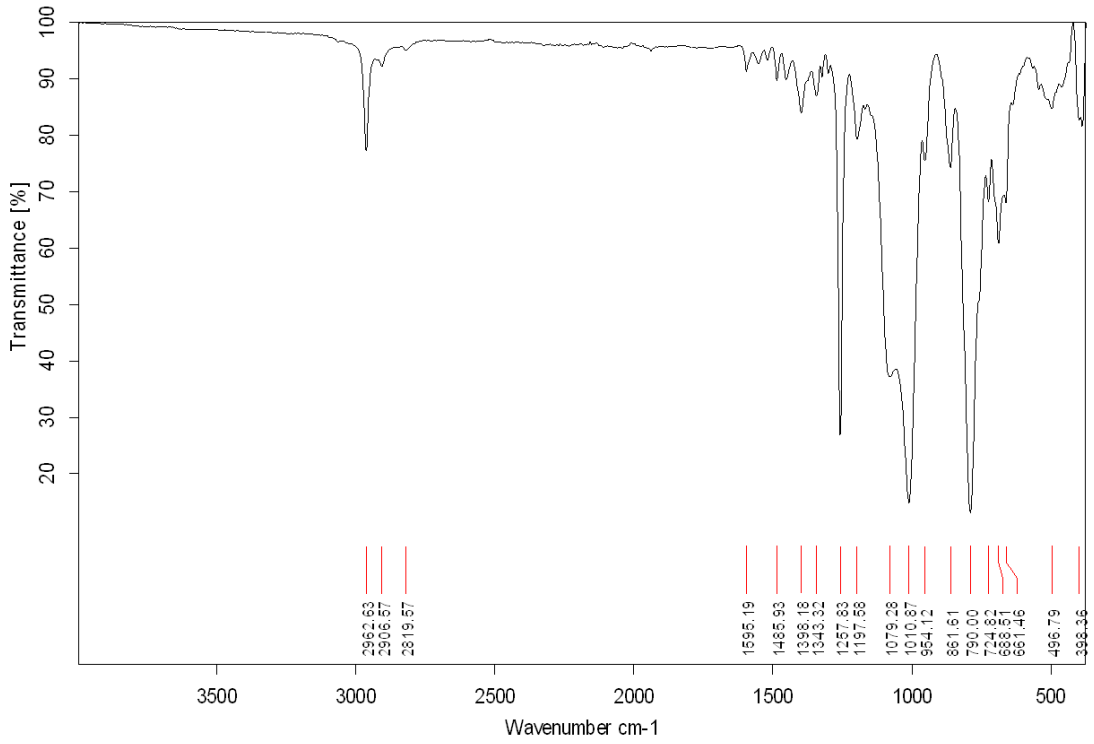

Figure S9. IR spectrum of $[(ZnMe)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)]$ (**5**).

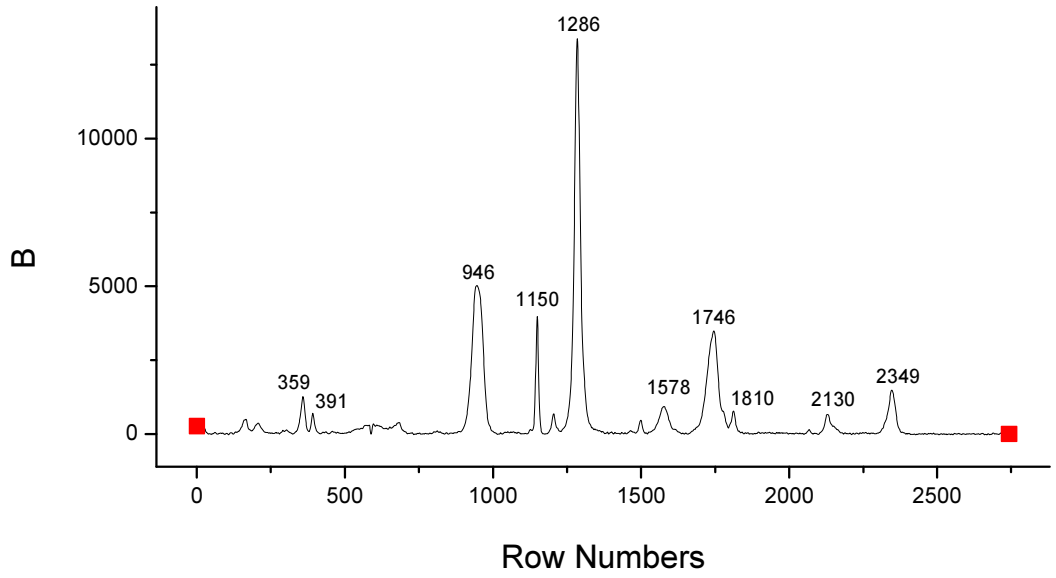

Figure S10. Raman spectrum of $[(ZnMe)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)]$ (**5**).

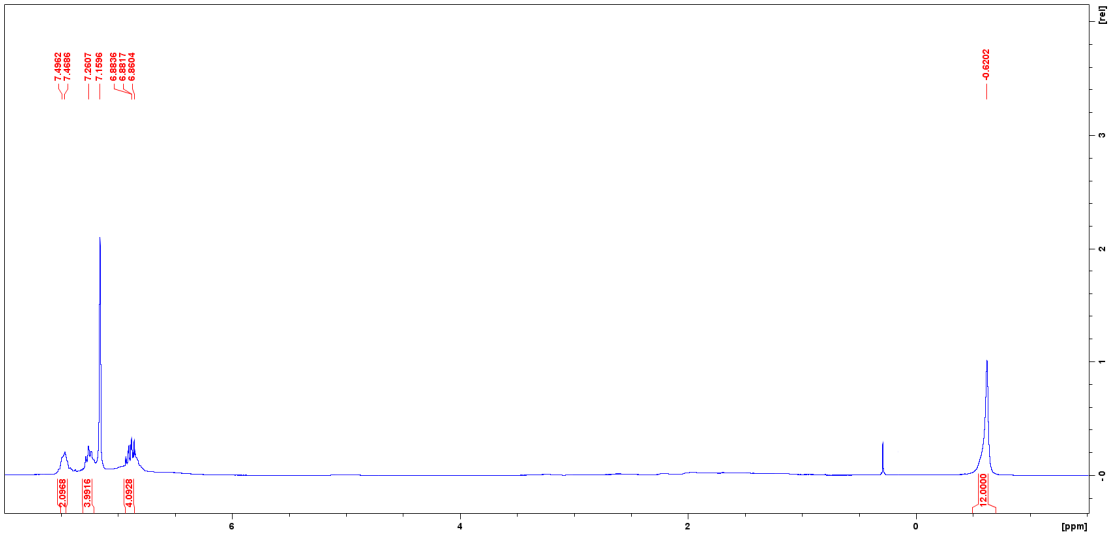

Figure S11. ^{1}H-NMR spectrum of $[(AlMe_2)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)]$ (**6**) in C_6D_6.

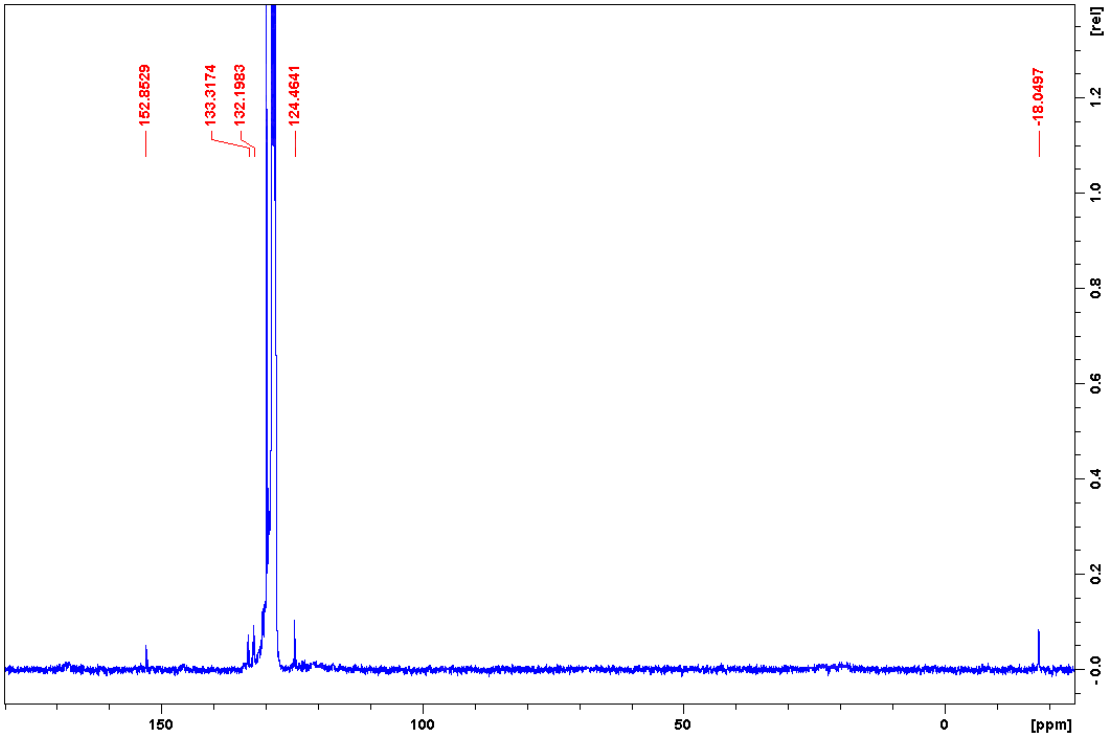

Figure S12. ^{13}C-NMR spectrum of $[(AlMe_2)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)]$ (**6**) in C_6D_6.

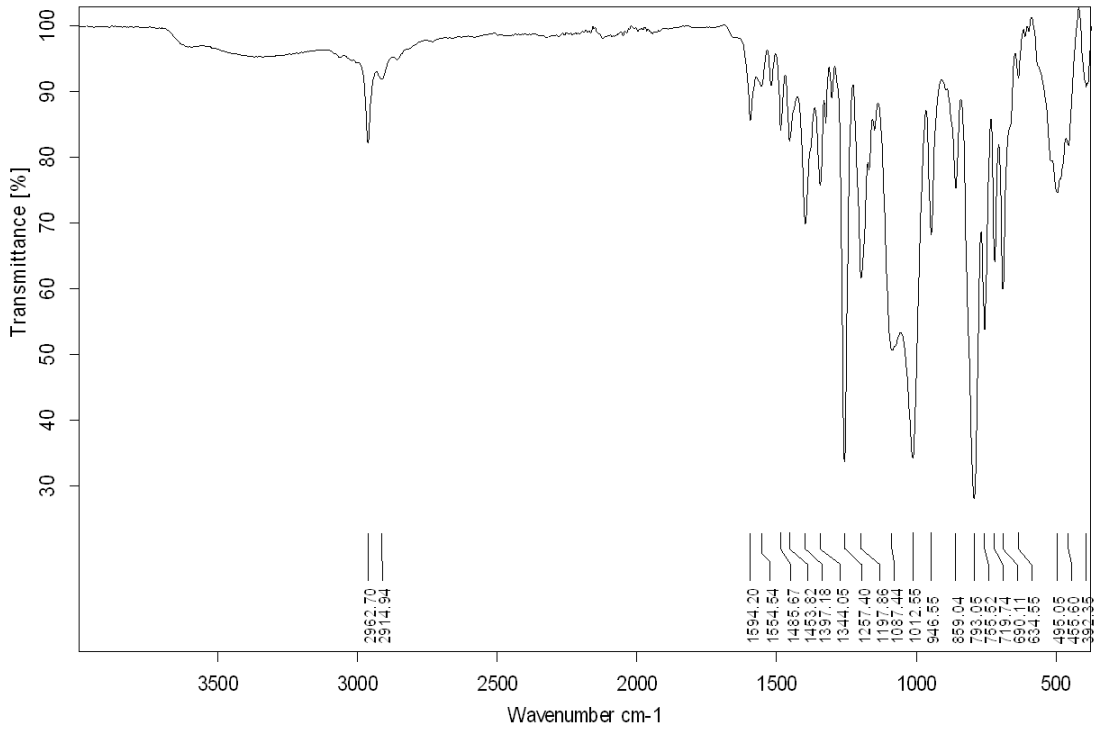

Figure S13. IR spectrum of $[(AlMe_2)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)]$ (**6**).

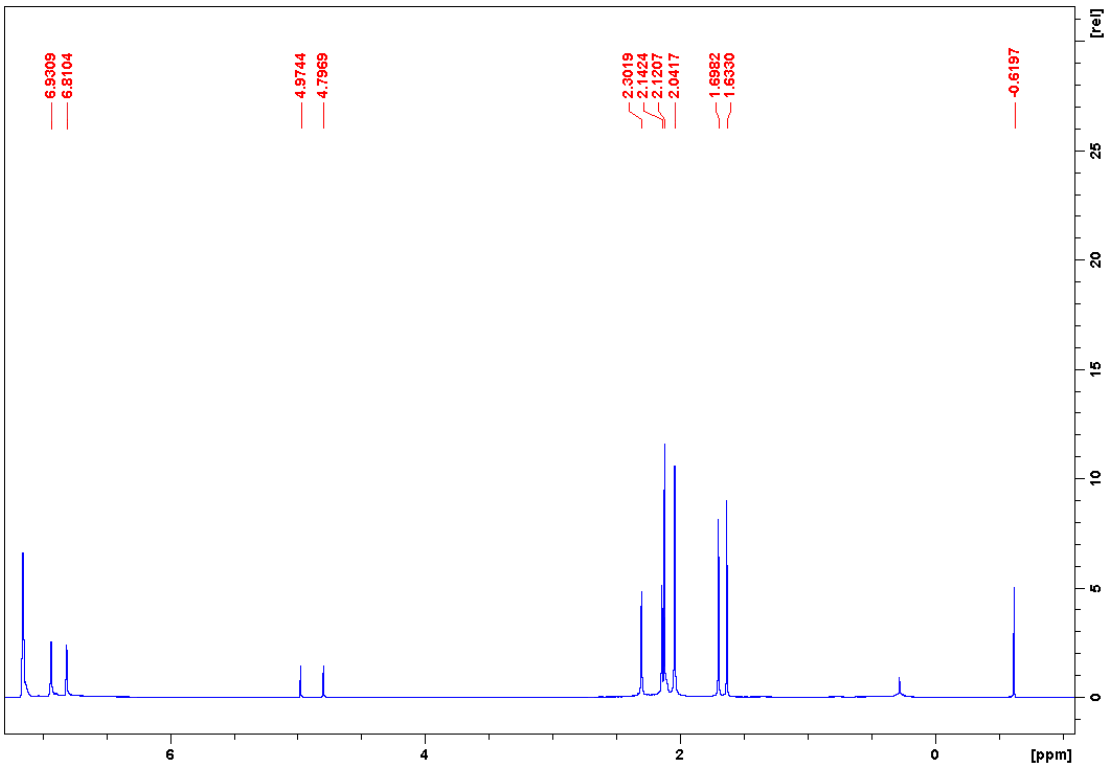

Figure S14. ^{1}H-NMR spectrum of $[(ZnMe)(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)(Li)]$ (**7**) in C_6D_6.

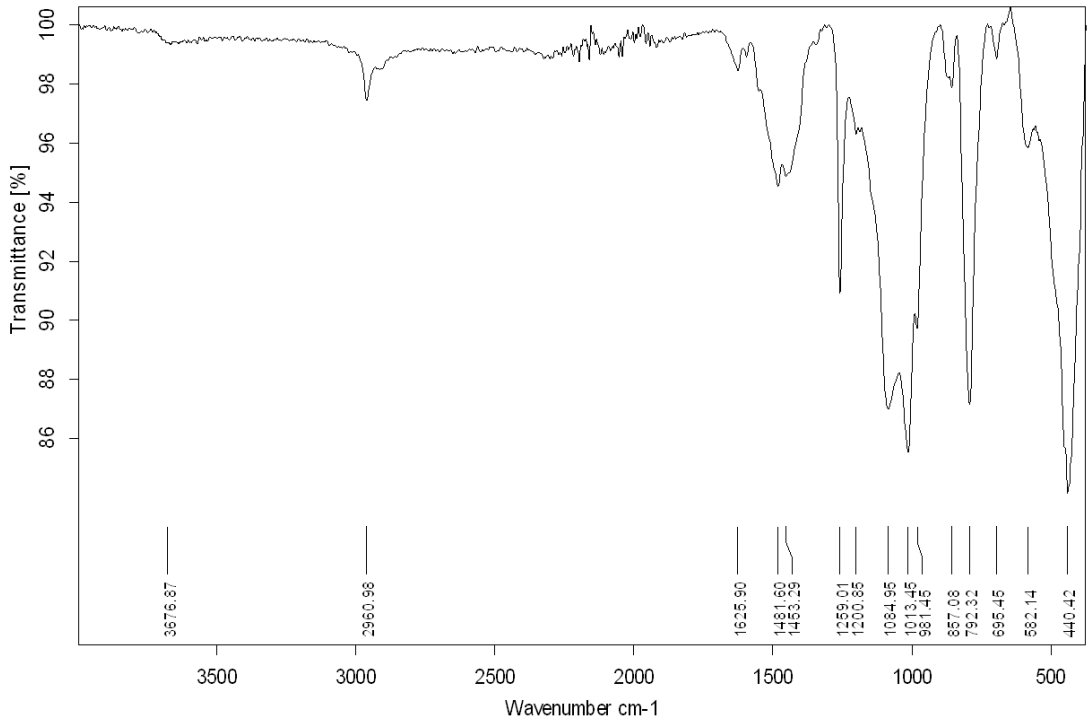

Figure S15. IR spectrum of [(ZnMe)(μ-η^2:η^2-N_6Ph_2)(Li)] (**7**).

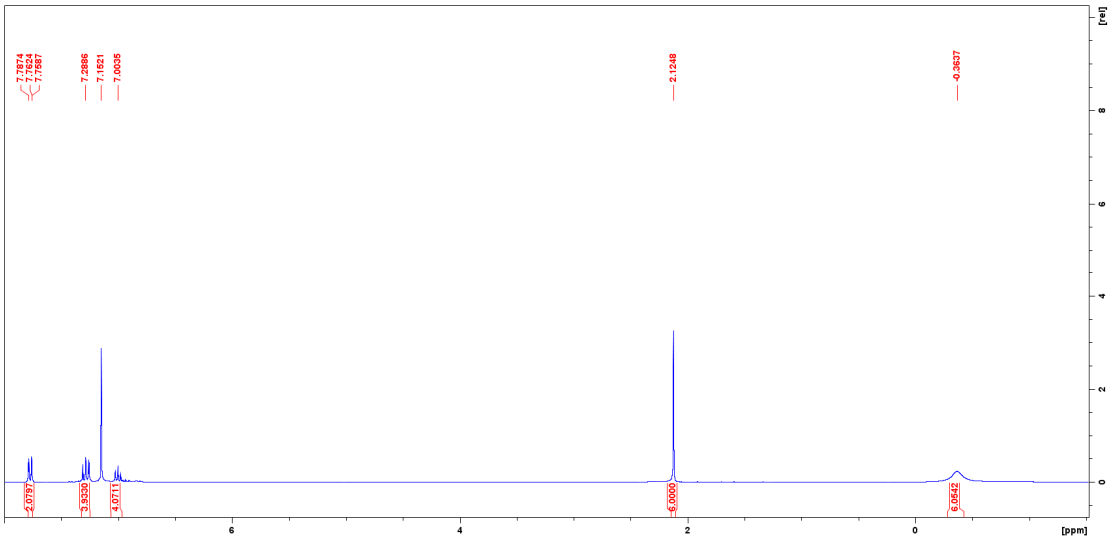

Figure S16. ^{1}H-NMR spectrum of [$(ZnMe)_2$(μ-η^2:η^2-N_6Ph_2)$(CH_3CN)_2$] (**8**) in C_6D_6.

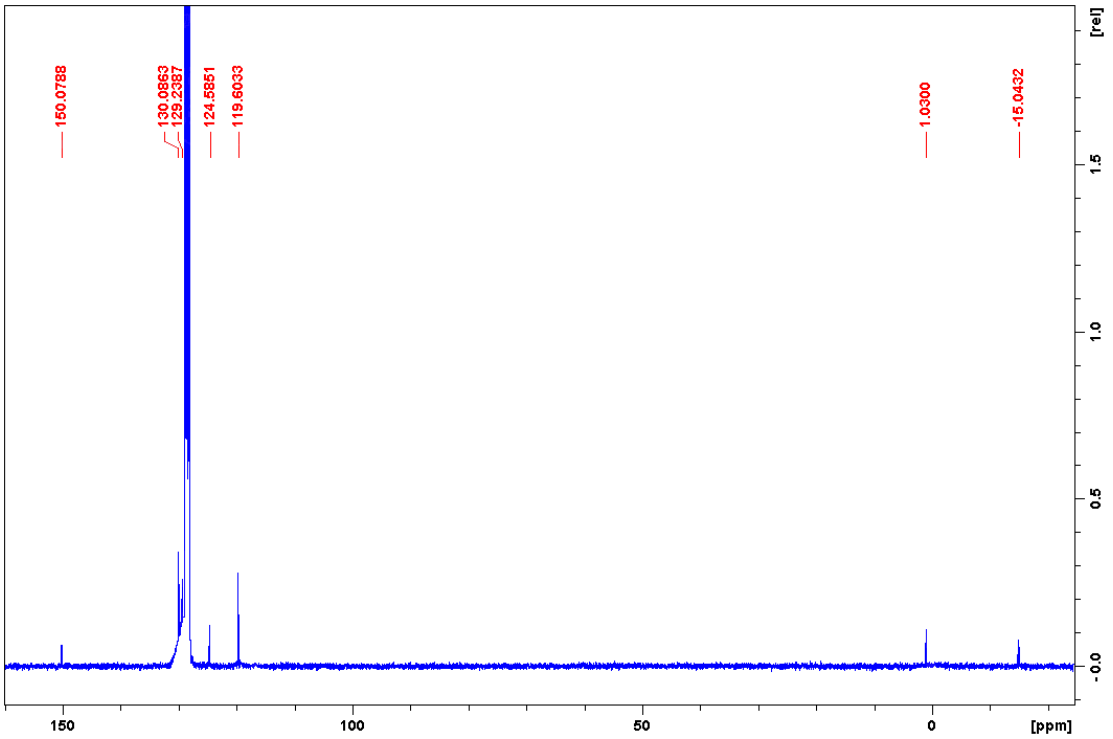

Figure S17. ^{13}C-NMR spectrum of $[(ZnMe)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)(CH_3CN)_2]$ (**8**) in C_6D_6.

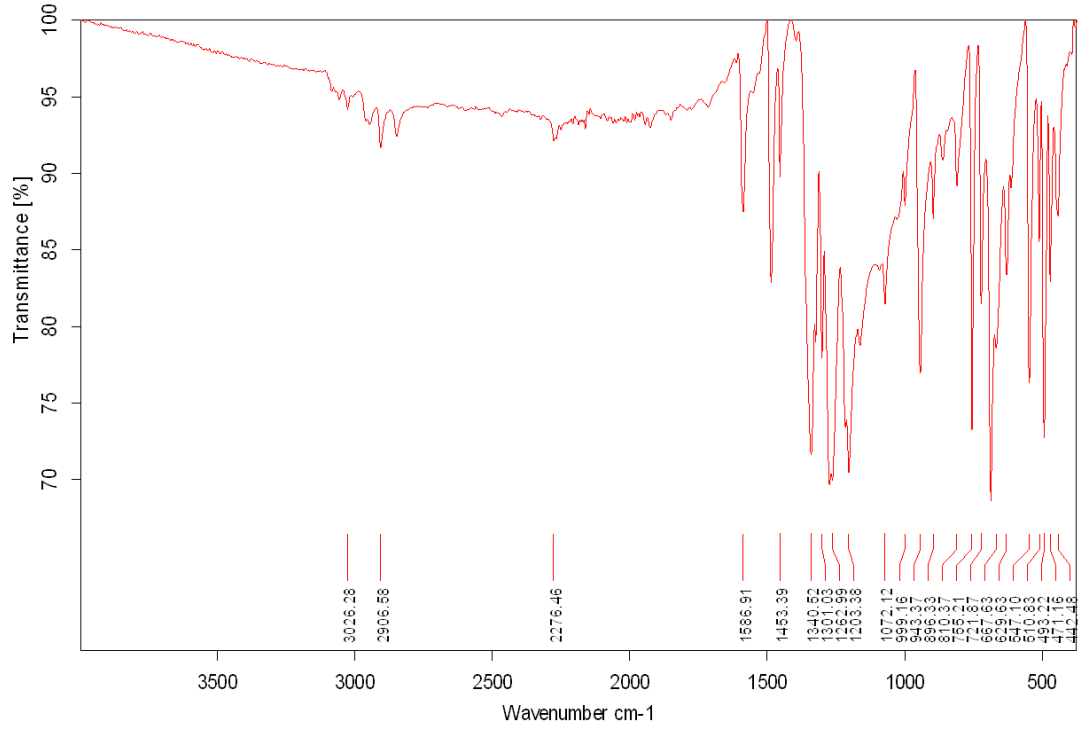

Figure S18. IR spectrum of $[(ZnMe)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)\ (CH_3CN)_2]$ (**8**).

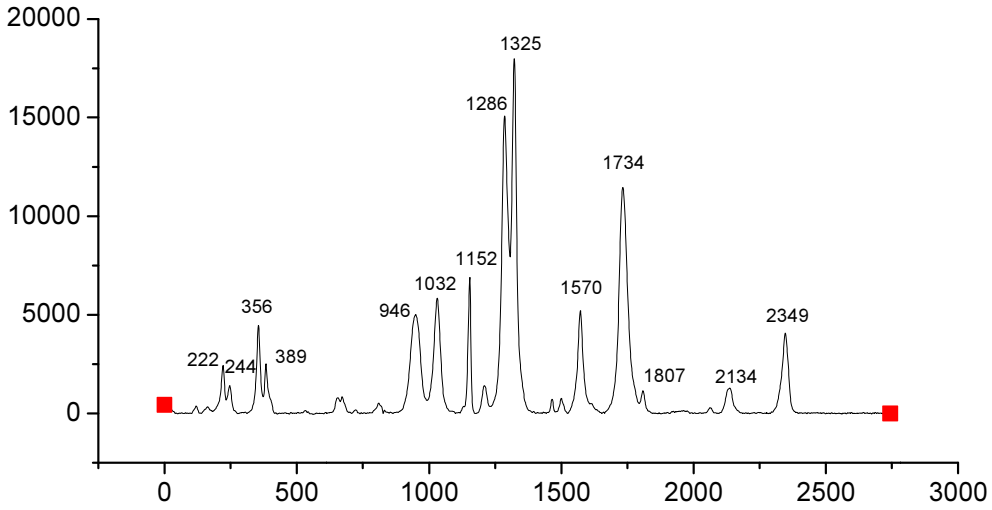

Figure S19. Raman spectrum of $[(ZnMe)_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_6Ph_2)\ (CH_3CN)_2]$ (**8**).

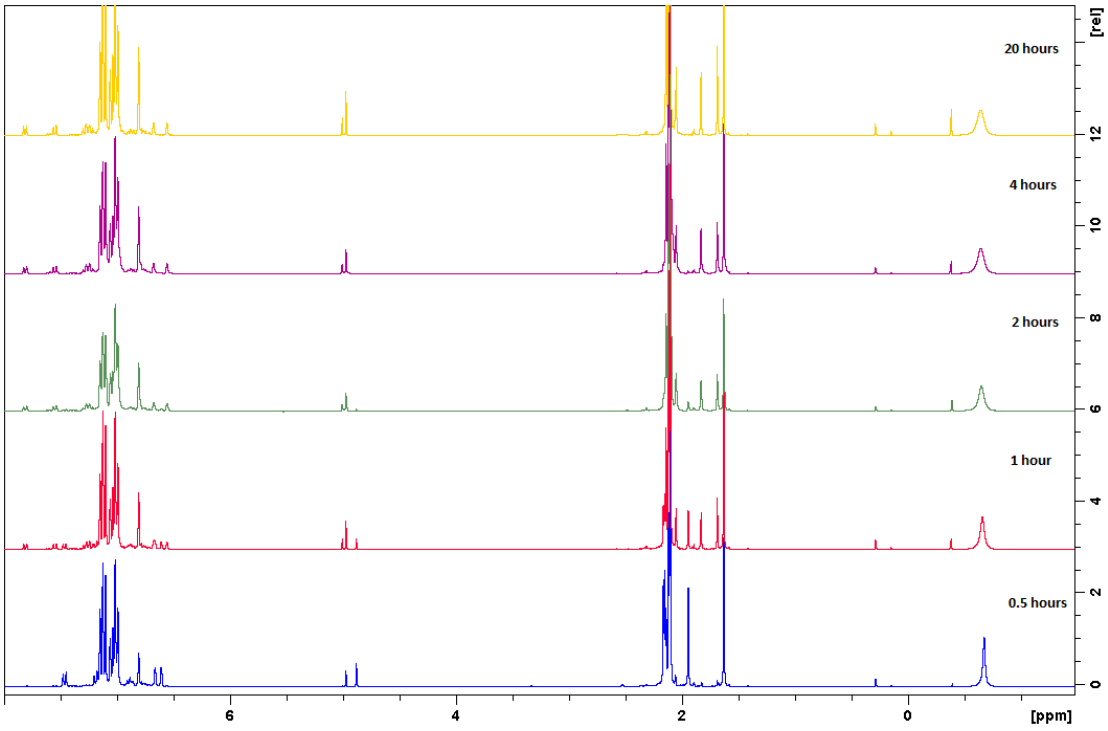

Figure S20. Time dependant ^{1}H NMR spectra of the reaction of **1** with one equivalent $ZnMe_2$.

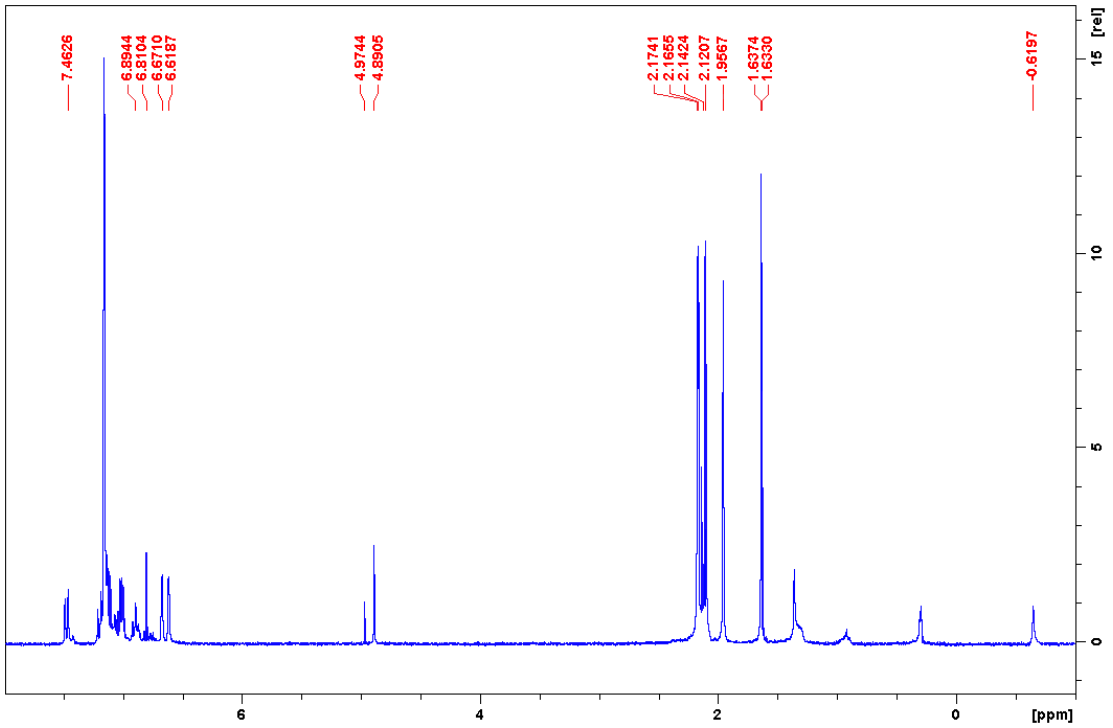

Figure S21. ^{1}H NMR spectrum of the reaction of **1** with one equivalent $ZnMe_2$ after five days.

Single-crystal X-ray analyses

The crystals were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 100 K. The structures were solved by Direct Methods (SHELXS-97)[1] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-97)[2]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2) except for **1** where the corrections was done numerically by face-indexing. Hydrogen atoms were refined using a riding model or rigid methyl groups. CCDC 1011108 (**1**),CCDC 1011107 (**2**), CCDC 1011105 (**3**), and CCDC 1011106 (**5**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic details of **5** and **8**

	6	**10**
Empirical formula	C_{35} H_{56} Al Bi N_2	C_{35} H_{56} Bi Ga N_2
M	740.77	783.51
Crystal size [mm]	0.28 × 0.24 × 0.21	0.480 × 0.413 × 0.254
T [K]	100(1)	100(1)
Crystal system	triclinic	triclinic
Space group	P -1	P -1
a [Å]	11.5940(15)	9.0994(6)
b [Å]	12.2244(16)	12.0444(9)
c [Å]	12.6546(16)	16.5176(12)
α [°]	72.804(6)	74.379(2)
β [°]	88.915(6)	79.774(2)
γ [°]	89.682(6)	85.921(2)
V [Å^3]	1713.1(4)	1715.2(2)
Z	2	2
D_{calc} [g · cm^{-1}]	1.436	1.517
μ(MoK_α [mm^{-1}])	5.196	5.932
Transmissions	0.54/0.38	0.44/0.12
F(000)	752	788
Index ranges	$-16 \le h \le 16$	$-13 \le h \le 13$
	$-16 \le k \le 17$	$-17 \le k \le 17$
	$-17 \le l \le 17$	$-23 \le l \le 23$
θ_{max} [°]	30.086	30.978
Reflections collected	48941	55296
Independent reflections	9813	10747
R_{int}	0.0251	0.0508
Refined parameters	365	365
R_1 [$I > 2\sigma(I)$][a]	0.0175	0.0278
wR_2 [all data][a]	0.0437	0.0693
GooF[b]	1.042	1.046
$\Delta\rho_{final}$ (max/min) [e · Å^{-3}]	1.407/-0.592	2.736/-2.248

[a] $R(F) = \Sigma\, ||F_o| - |F_c||/\Sigma|F_o|$; $wR(F^2) = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\, \Sigma\{w(F_o^2)^2\}]^{0,5}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$ mit $P = [F_o^2 + 2F_c^2]/3$, a and b are constants chosen by the programme; [b] GoF = $[\Sigma\{w(F_o^2 - F_c^2)^2\}/(n-p)]^{0,5}$ with n data and p parameters.

Computational Studies

All geometries were fully optimized using tightened convergence criteria and improved integration grids at the density functional theory level, employing the BP86 exchange-correlation functional [3] including a third-generation dispersion correction [4] as implemented in the Turbomole V6.3 quantum chemistry program package [5]. A quadruple-zeta valence quality Gaussian type function basis set termed def2-QZVP [6] has been used throughout. Atom coordinates, energies, atomic partial charges (NPA[7]) and frequencies of the optimized geometry are given below.

Calculated Structures and Frequencies

$(MeZn)_2N_6Ph_2$ 5'

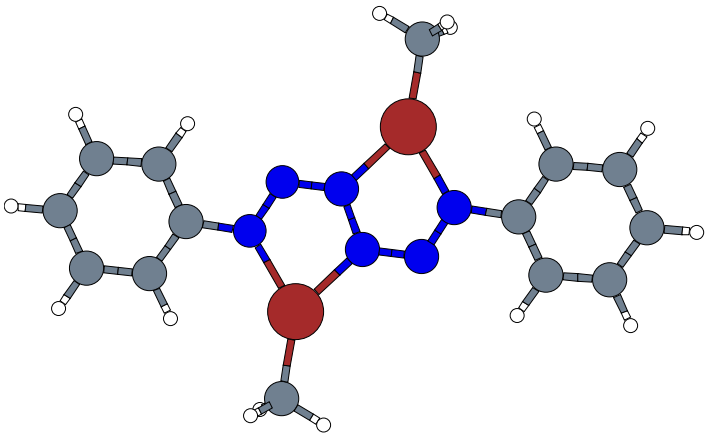

Table S2. Energy (in Hartree) and atomic coordinates (in Å):

Energy = -4431.534602474

Zn	-1.4632389	-1.8652546	0.0000000
N	-2.2684863	0.0035715	0.0000000
N	-1.4188166	0.9959064	0.0000000
N	-0.1498589	0.6807072	0.0000000
C	-3.6349251	0.3716939	0.0000000
C	-4.5772988	-0.6693790	0.0000000
H	-4.2291036	-1.7032547	0.0000000
C	-5.9419066	-0.3859529	0.0000000
H	-6.6600169	-1.2051756	0.0000000
C	-6.3851513	0.9383935	0.0000000
H	-7.4510882	1.1616770	0.0000000
C	-5.4465408	1.9764828	0.0000000
H	-5.7837111	3.0128606	0.0000000
C	-4.0808434	1.7057441	0.0000000

H	-3.3530019	2.5131391	0.0000000
C	-2.0024576	-3.7408876	0.0000000
H	-2.6106709	-3.9720493	0.8862172
H	-1.1349959	-4.4139142	0.0000000
H	-2.6106709	-3.9720493	-0.8862172
N	2.2684863	-0.0035715	0.0000000
N	1.4188166	-0.9959064	0.0000000
N	0.1498589	-0.6807072	0.0000000
C	3.6349251	-0.3716939	0.0000000
C	4.5772988	0.6693790	0.0000000
H	4.2291036	1.7032547	0.0000000
C	5.9419066	0.3859529	0.0000000
H	6.6600169	1.2051756	0.0000000
C	6.3851513	-0.9383935	0.0000000
H	7.4510882	-1.1616770	0.0000000
C	5.4465408	-1.9764828	0.0000000
H	5.7837111	-3.0128606	0.0000000
C	4.0808434	-1.7057441	0.0000000
H	3.3530019	-2.5131391	0.0000000
Zn	1.4632389	1.8652546	0.0000000
C	2.0024576	3.7408876	0.0000000
H	2.6106709	3.9720493	-0.8862172
H	1.1349959	4.4139142	0.0000000
H	2.6106709	3.9720493	0.8862172

Table S3. **Atomic populations according to NPA:**

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 Zn	1.36711	6.64749	12.03317	9.95206	0.00016	0.00000
2 N	-0.49968	3.39473	4.09563	0.00628	0.00289	0.00014
3 N	-0.02242	3.39604	3.60937	0.01469	0.00211	0.00022
4 N	-0.37705	3.41064	3.95647	0.00705	0.00276	0.00014
5 C	0.09765	2.88263	3.00954	0.00494	0.00454	0.00070
6 C	-0.22723	2.96866	3.25103	0.00351	0.00336	0.00067
7 H	0.22692	0.77168	0.00104	0.00028	0.00008	0.00000
8 C	-0.21302	2.97153	3.23441	0.00330	0.00307	0.00070
9 H	0.22534	0.77329	0.00099	0.00029	0.00008	0.00000
10 C	-0.22712	2.97416	3.24592	0.00327	0.00306	0.00071
11 H	0.22409	0.77446	0.00104	0.00032	0.00009	0.00000
12 C	-0.20643	2.97308	3.22636	0.00321	0.00308	0.00070
13 H	0.22422	0.77438	0.00103	0.00029	0.00009	0.00000
14 C	-0.23341	2.97120	3.25471	0.00354	0.00328	0.00069
15 H	0.24225	0.75631	0.00105	0.00031	0.00009	0.00000
16 C	-1.27167	3.27531	3.98637	0.00780	0.00134	0.00085
17 H	0.22334	0.77399	0.00224	0.00035	0.00009	0.00000
18 H	0.22377	0.77331	0.00250	0.00033	0.00009	0.00000
19 H	0.22334	0.77399	0.00224	0.00035	0.00009	0.00000
20 N	-0.49968	3.39473	4.09563	0.00628	0.00289	0.00014
21 N	-0.02242	3.39604	3.60937	0.01469	0.00211	0.00022

22 N	-0.37705	3.41064	3.95647	0.00705	0.00276	0.00014
23 C	0.09765	2.88263	3.00954	0.00494	0.00454	0.00070
24 C	-0.22723	2.96866	3.25103	0.00351	0.00336	0.00067
25 H	0.22692	0.77168	0.00104	0.00028	0.00008	0.00000
26 C	-0.21302	2.97153	3.23441	0.00330	0.00307	0.00070
27 H	0.22534	0.77329	0.00099	0.00029	0.00008	0.00000
28 C	-0.22712	2.97416	3.24592	0.00327	0.00306	0.00071
29 H	0.22409	0.77446	0.00104	0.00032	0.00009	0.00000
30 C	-0.20643	2.97308	3.22636	0.00321	0.00308	0.00070
31 H	0.22422	0.77438	0.00103	0.00029	0.00009	0.00000
32 C	-0.23341	2.97120	3.25471	0.00354	0.00328	0.00069
33 H	0.24225	0.75631	0.00105	0.00031	0.00009	0.00000
34 Zn	1.36711	6.64749	12.03317	9.95206	0.00016	0.00000
35 C	-1.27167	3.27531	3.98637	0.00780	0.00134	0.00085
36 H	0.22334	0.77399	0.00224	0.00035	0.00009	0.00000
37 H	0.22377	0.77331	0.00250	0.00033	0.00009	0.00000
38 H	0.22334	0.77399	0.00224	0.00035	0.00009	0.00000

Table S4. **Vibrational frequencies:**

mode	symmetry	wave number [cm^{-1}]	IR intensity km/mol	selection rules	
				IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	9.68	0.06914	YES	NO
8	bg	13.92	0.00000	NO	YES
9	au	19.75	0.12144	YES	NO
10	au	42.30	0.00130	YES	NO
11	bu	50.19	1.43433	YES	NO
12	bg	58.74	0.00000	NO	YES
13	au	59.86	0.03096	YES	NO
14	ag	72.34	0.00000	NO	YES
15	bu	75.87	2.23792	YES	NO
16	bg	80.70	0.00000	NO	YES
17	bg	96.00	0.00000	NO	YES
18	ag	113.17	0.00000	NO	YES
19	au	127.50	0.63412	YES	NO
20	au	131.98	6.51509	YES	NO
21	bu	165.28	7.89533	YES	NO
22	ag	170.37	0.00000	NO	YES
23	bg	193.88	0.00000	NO	YES
24	ag	195.30	0.00000	NO	YES
25	ag	232.59	0.00000	NO	YES
26	bu	250.78	35.51517	YES	NO

27	au	297.78	0.36690	YES	NO
28	bg	318.70	0.00000	NO	YES
29	bu	323.64	20.16063	YES	NO
30	bg	400.07	0.00000	NO	YES
31	au	400.16	0.06030	YES	NO
32	au	411.27	1.25457	YES	NO
33	bu	457.42	9.97904	YES	NO
34	ag	501.76	0.00000	NO	YES
35	bg	512.91	0.00000	NO	YES
36	au	514.99	16.67325	YES	NO
37	ag	552.96	0.00000	NO	YES
38	bu	557.74	53.81187	YES	NO
39	ag	600.07	0.00000	NO	YES
40	bu	606.84	4.85414	YES	NO
41	bg	612.62	0.00000	NO	YES
42	ag	612.72	0.00000	NO	YES
43	bu	627.44	32.34927	YES	NO
44	bg	681.39	0.00000	NO	YES
45	au	681.50	45.40479	YES	NO
46	au	702.24	60.91268	YES	NO
47	bg	702.29	0.00000	NO	YES
48	bu	709.12	158.03931	YES	NO
49	ag	714.73	0.00000	NO	YES
50	bu	728.61	27.46369	YES	NO
51	bg	750.50	0.00000	NO	YES
52	au	751.28	76.25223	YES	NO
53	ag	764.59	0.00000	NO	YES
54	au	814.69	0.03005	YES	NO
55	bg	815.17	0.00000	NO	YES
56	ag	882.46	0.00000	NO	YES
57	bg	892.00	0.00000	NO	YES
58	au	892.44	6.60435	YES	NO
59	bu	946.53	209.09462	YES	NO
60	bg	950.27	0.00000	NO	YES
61	au	950.39	0.10277	YES	NO
62	bg	965.42	0.00000	NO	YES
63	au	965.51	0.15227	YES	NO
64	ag	986.77	0.00000	NO	YES
65	bu	987.31	0.43385	YES	NO
66	ag	1021.66	0.00000	NO	YES
67	bu	1022.44	7.86486	YES	NO
68	ag	1031.16	0.00000	NO	YES
69	ag	1084.23	0.00000	NO	YES
70	bu	1085.31	9.36695	YES	NO
71	bu	1158.83	7.07026	YES	NO
72	ag	1158.92	0.00000	NO	YES
73	bu	1171.21	32.76174	YES	NO
74	ag	1172.61	0.00000	NO	YES
75	ag	1180.80	0.00000	NO	YES
76	bu	1181.36	18.76580	YES	NO

77	ag	1194.05	0.00000	NO	YES
78	bu	1203.71	297.42945	YES	NO
79	bu	1263.63	289.00549	YES	NO
80	ag	1278.69	0.00000	NO	YES
81	bu	1293.86	1587.04846	YES	NO
82	ag	1313.51	0.00000	NO	YES
83	bu	1324.41	184.33636	YES	NO
84	ag	1338.96	0.00000	NO	YES
85	bu	1347.44	223.04034	YES	NO
86	ag	1360.62	0.00000	NO	YES
87	bu	1414.03	0.68949	YES	NO
88	ag	1414.08	0.00000	NO	YES
89	au	1416.31	1.36165	YES	NO
90	bg	1416.42	0.00000	NO	YES
91	ag	1446.89	0.00000	NO	YES
92	bu	1447.08	8.57522	YES	NO
93	bu	1477.64	111.55055	YES	NO
94	ag	1478.59	0.00000	NO	YES
95	ag	1572.49	0.00000	NO	YES
96	bu	1572.82	9.83481	YES	NO
97	bu	1588.29	21.56286	YES	NO
98	ag	1588.56	0.00000	NO	YES
99	bu	2953.58	42.10137	YES	NO
100	ag	2953.66	0.00000	NO	YES
101	bg	3025.17	0.00000	NO	YES
102	au	3025.20	22.04068	YES	NO
103	ag	3038.07	0.00000	NO	YES
104	bu	3038.10	21.17421	YES	NO
105	ag	3085.12	0.00000	NO	YES
106	bu	3085.13	7.90309	YES	NO
107	bu	3094.52	2.94891	YES	NO
108	ag	3094.65	0.00000	NO	YES
109	bu	3104.65	28.91376	YES	NO
110	ag	3104.74	0.00000	NO	YES
111	bu	3118.82	49.46870	YES	NO
112	ag	3119.02	0.00000	NO	YES
113	ag	3136.06	0.00000	NO	YES
114	bu	3136.51	5.53874	YES	NO

$(MeZn)_2N_6Ph_2(CH_3CN)_2$ 8'

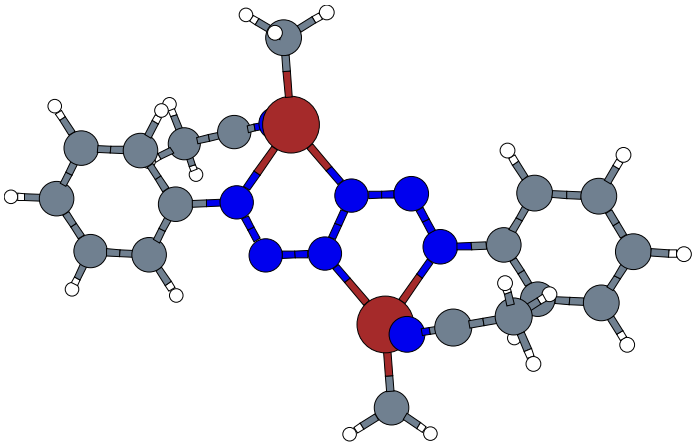

Table S5. Energy (in Hartree) and atomic coordinates (in Å):

Energy = -4697.212867496

Zn	0.8099729	1.2385025	-1.8964781
N	-1.0776776	1.6226900	-1.1617356
N	-1.4804858	0.8794138	-0.1600291
N	-0.6210870	0.0301877	0.3212106
N	-0.3427151	0.0937091	-3.5833725
C	-2.0766614	2.3825418	-1.7883976
C	-3.4569622	2.1686920	-1.6010759
H	-3.7835926	1.4115877	-0.8919006
C	-4.3809177	2.9106544	-2.3337976
H	-5.4460501	2.7337284	-2.1833310
C	-3.9589403	3.8659903	-3.2667080
H	-4.6889516	4.4353658	-3.8403362
C	-2.5888537	4.0826080	-3.4506868
H	-2.2440257	4.8258949	-4.1690876
C	-1.6557830	3.3498886	-2.7205275
H	-0.5859729	3.5032163	-2.8678851
C	2.2495415	2.2265570	-2.8010906
H	3.0976374	1.5671256	-3.0340815
H	2.6312557	3.0518576	-2.1830122
H	1.8965259	2.6564692	-3.7499778
C	-1.3105001	0.3103306	-4.1867108
C	-2.5324397	0.6112596	-4.9064186
H	-3.0184284	1.4820393	-4.4432720
H	-3.2158349	-0.2455204	-4.8635877
H	-2.3082801	0.8401320	-5.9553958
N	1.0776776	-1.6226900	1.1617356
N	1.4804858	-0.8794138	0.1600291
N	0.6210870	-0.0301877	-0.3212106
C	2.0766614	-2.3825418	1.7883976
C	3.4569622	-2.1686920	1.6010759
H	3.7835926	-1.4115877	0.8919006
C	4.3809177	-2.9106544	2.3337976

H	5.4460501	-2.7337284	2.1833310
C	3.9589403	-3.8659903	3.2667080
H	4.6889516	-4.4353658	3.8403362
C	2.5888537	-4.0826080	3.4506868
H	2.2440257	-4.8258949	4.1690876
C	1.6557830	-3.3498886	2.7205275
H	0.5859729	-3.5032163	2.8678851
Zn	-0.8099729	-1.2385025	1.8964781
N	0.3427151	-0.0937091	3.5833725
C	-2.2495415	-2.2265570	2.8010906
H	-3.0976374	-1.5671256	3.0340815
H	-2.6312557	-3.0518576	2.1830122
H	-1.8965259	-2.6564692	3.7499778
C	1.3105001	-0.3103306	4.1867108
C	2.5324397	-0.6112596	4.9064186
H	3.0184284	-1.4820393	4.4432720
H	3.2158349	0.2455204	4.8635877
H	2.3082801	-0.8401320	5.9553958

Table S6. **Atomic populations according to NPA:**

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 Zn	1.42046	6.59444	12.02439	9.96051	0.00020	0.00000
2 N	-0.49698	3.39168	4.09518	0.00726	0.00272	0.00014
3 N	-0.02448	3.39428	3.61357	0.01428	0.00212	0.00022
4 N	-0.34198	3.41242	3.91975	0.00710	0.00256	0.00014
5 N	-0.42562	3.56990	3.83781	0.01612	0.00150	0.00028
6 C	0.10359	2.88139	3.00469	0.00531	0.00432	0.00070
7 C	-0.24638	2.97341	3.26552	0.00359	0.00318	0.00068
8 H	0.24422	0.75435	0.00105	0.00030	0.00008	0.00000
9 C	-0.21922	2.97320	3.23906	0.00327	0.00300	0.00069
10 H	0.22424	0.77437	0.00102	0.00028	0.00008	0.00000
11 C	-0.25361	2.97410	3.27248	0.00334	0.00300	0.00070
12 H	0.22424	0.77430	0.00105	0.00031	0.00009	0.00000
13 C	-0.22544	2.97199	3.24643	0.00335	0.00298	0.00069
14 H	0.22547	0.77317	0.00099	0.00028	0.00008	0.00000
15 C	-0.24001	2.97148	3.26101	0.00366	0.00319	0.00066
16 H	0.23524	0.76343	0.00099	0.00026	0.00008	0.00000
17 C	-1.27829	3.27568	3.99313	0.00735	0.00131	0.00081
18 H	0.21873	0.77864	0.00222	0.00034	0.00008	0.00000
19 H	0.21448	0.78285	0.00224	0.00034	0.00008	0.00000
20 H	0.21041	0.78710	0.00206	0.00035	0.00009	0.00000
21 C	0.36179	2.88102	2.74915	0.00383	0.00402	0.00018
22 C	-0.75019	3.12663	3.61626	0.00475	0.00128	0.00126
23 H	0.28898	0.70925	0.00115	0.00044	0.00017	0.00000
24 H	0.26596	0.73277	0.00070	0.00040	0.00017	0.00000
25 H	0.26436	0.73438	0.00069	0.00040	0.00017	0.00000
26 N	-0.49698	3.39168	4.09518	0.00726	0.00272	0.00014
27 N	-0.02448	3.39428	3.61357	0.01428	0.00212	0.00022

28 N	-0.34198	3.41242	3.91975	0.00710	0.00256	0.00014
29 C	0.10359	2.88139	3.00469	0.00531	0.00432	0.00070
30 C	-0.24638	2.97341	3.26552	0.00359	0.00318	0.00068
31 H	0.24422	0.75435	0.00105	0.00030	0.00008	0.00000
32 C	-0.21922	2.97320	3.23906	0.00327	0.00300	0.00069
33 H	0.22424	0.77437	0.00102	0.00028	0.00008	0.00000
34 C	-0.25361	2.97410	3.27248	0.00334	0.00300	0.00070
35 H	0.22424	0.77430	0.00105	0.00031	0.00009	0.00000
36 C	-0.22544	2.97199	3.24643	0.00335	0.00298	0.00069
37 H	0.22547	0.77317	0.00099	0.00028	0.00008	0.00000
38 C	-0.24001	2.97148	3.26101	0.00366	0.00319	0.00066
39 H	0.23524	0.76343	0.00099	0.00026	0.00008	0.00000
40 Zn	1.42046	6.59444	12.02439	9.96051	0.00020	0.00000
41 N	-0.42562	3.56990	3.83781	0.01612	0.00150	0.00028
42 C	-1.27829	3.27568	3.99313	0.00735	0.00131	0.00081
43 H	0.21873	0.77864	0.00222	0.00034	0.00008	0.00000
44 H	0.21448	0.78285	0.00224	0.00034	0.00008	0.00000
45 H	0.21041	0.78710	0.00206	0.00035	0.00009	0.00000
46 C	0.36179	2.88102	2.74915	0.00383	0.00402	0.00018
47 C	-0.75019	3.12663	3.61626	0.00475	0.00128	0.00126
48 H	0.28898	0.70925	0.00115	0.00044	0.00017	0.00000
49 H	0.26596	0.73277	0.00070	0.00040	0.00017	0.00000
50 H	0.26436	0.73438	0.00069	0.00040	0.00017	0.00000

Table S7. **Vibrational frequencies:**

mode	symmetry	wave number [cm^{-1}]	IR intensity km/mol	selection rules	
				IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	10.97	4.49928	YES	NO
8	au	19.36	2.44170	YES	NO
9	ag	25.49	0.00000	NO	YES
10	au	29.38	0.71008	YES	NO
11	ag	39.23	0.00000	NO	YES
12	au	45.97	0.50992	YES	NO
13	ag	46.73	0.00000	NO	YES
14	au	48.66	2.80545	YES	NO
15	au	54.16	0.71274	YES	NO
16	ag	62.54	0.00000	NO	YES
17	au	68.78	1.83169	YES	NO
18	ag	72.54	0.00000	NO	YES
19	ag	76.10	0.00000	NO	YES

20	au	79.86	0.46595	YES	NO
21	ag	81.13	0.00000	NO	YES
22	au	85.48	4.69169	YES	NO
23	ag	90.96	0.00000	NO	YES
24	au	100.05	35.99800	YES	NO
25	ag	105.30	0.00000	NO	YES
26	ag	119.22	0.00000	NO	YES
27	au	119.94	4.48899	YES	NO
28	ag	126.38	0.00000	NO	YES
29	au	131.40	41.54998	YES	NO
30	au	143.46	4.87364	YES	NO
31	ag	149.35	0.00000	NO	YES
32	au	157.44	6.55565	YES	NO
33	ag	167.12	0.00000	NO	YES
34	au	172.94	13.68430	YES	NO
35	ag	194.47	0.00000	NO	YES
36	ag	200.73	0.00000	NO	YES
37	ag	231.67	0.00000	NO	YES
38	au	233.54	22.49792	YES	NO
39	au	298.36	16.79047	YES	NO
40	ag	329.57	0.00000	NO	YES
41	au	334.78	3.88169	YES	NO
42	ag	379.34	0.00000	NO	YES
43	au	379.38	1.74410	YES	NO
44	au	388.45	4.40457	YES	NO
45	ag	388.53	0.00000	NO	YES
46	au	405.92	0.06981	YES	NO
47	ag	406.03	0.00000	NO	YES
48	au	422.89	0.55483	YES	NO
49	au	451.13	10.87546	YES	NO
50	ag	494.93	0.00000	NO	YES
51	au	517.17	23.90951	YES	NO
52	ag	519.93	0.00000	NO	YES
53	ag	541.96	0.00000	NO	YES
54	au	544.27	57.67901	YES	NO
55	ag	592.69	0.00000	NO	YES
56	au	606.15	2.46663	YES	NO
57	ag	611.11	0.00000	NO	YES
58	au	623.08	9.19512	YES	NO
59	ag	624.42	0.00000	NO	YES
60	au	688.48	47.58569	YES	NO
61	ag	688.90	0.00000	NO	YES
62	au	693.26	55.27074	YES	NO
63	ag	693.84	0.00000	NO	YES
64	ag	700.43	0.00000	NO	YES
65	au	700.53	118.42751	YES	NO
66	au	720.30	64.48236	YES	NO
67	ag	753.74	0.00000	NO	YES
68	au	755.30	84.57570	YES	NO
69	ag	756.91	0.00000	NO	YES

70	ag	823.59	0.00000	NO	YES
71	au	823.60	0.32902	YES	NO
72	ag	859.96	0.00000	NO	YES
73	au	890.42	17.34133	YES	NO
74	ag	890.59	0.00000	NO	YES
75	au	921.93	1.61508	YES	NO
76	ag	922.02	0.00000	NO	YES
77	au	942.72	183.81694	YES	NO
78	au	955.07	0.04837	YES	NO
79	ag	955.09	0.00000	NO	YES
80	ag	967.02	0.00000	NO	YES
81	au	967.13	2.67875	YES	NO
82	ag	984.92	0.00000	NO	YES
83	au	985.90	4.54878	YES	NO
84	ag	1011.80	0.00000	NO	YES
85	au	1011.97	18.67161	YES	NO
86	ag	1018.06	0.00000	NO	YES
87	au	1020.04	1.44722	YES	NO
88	ag	1020.87	0.00000	NO	YES
89	au	1021.09	0.68108	YES	NO
90	ag	1028.16	0.00000	NO	YES
91	ag	1078.56	0.00000	NO	YES
92	au	1078.67	11.42694	YES	NO
93	au	1154.54	0.41154	YES	NO
94	ag	1154.70	0.00000	NO	YES
95	au	1166.71	84.67362	YES	NO
96	ag	1168.73	0.00000	NO	YES
97	au	1172.46	2.64922	YES	NO
98	ag	1172.51	0.00000	NO	YES
99	ag	1191.77	0.00000	NO	YES
100	au	1200.82	501.92037	YES	NO
101	au	1269.14	1405.83713	YES	NO
102	ag	1290.34	0.00000	NO	YES
103	au	1298.56	476.93345	YES	NO
104	ag	1309.31	0.00000	NO	YES
105	au	1330.15	223.47330	YES	NO
106	ag	1338.53	0.00000	NO	YES
107	au	1351.51	545.74967	YES	NO
108	ag	1355.23	0.00000	NO	YES
109	au	1355.31	45.77132	YES	NO
110	ag	1370.42	0.00000	NO	YES
111	au	1409.83	6.26600	YES	NO
112	ag	1409.95	0.00000	NO	YES
113	ag	1413.61	0.00000	NO	YES
114	au	1413.74	16.86302	YES	NO
115	au	1414.48	0.56685	YES	NO
116	ag	1414.58	0.00000	NO	YES
117	au	1417.90	1.31171	YES	NO
118	ag	1417.97	0.00000	NO	YES
119	ag	1443.86	0.00000	NO	YES

120	au	1444.79	6.51695	YES	NO
121	au	1474.87	137.05214	YES	NO
122	ag	1476.03	0.00000	NO	YES
123	ag	1563.74	0.00000	NO	YES
124	au	1564.06	16.63077	YES	NO
125	au	1586.42	128.25524	YES	NO
126	ag	1587.22	0.00000	NO	YES
127	au	2269.31	45.79132	YES	NO
128	ag	2269.31	0.00000	NO	YES
129	au	2946.72	72.55277	YES	NO
130	ag	2946.87	0.00000	NO	YES
131	ag	2965.27	0.00000	NO	YES
132	au	2965.27	26.55679	YES	NO
133	ag	3019.36	0.00000	NO	YES
134	au	3019.44	40.47378	YES	NO
135	ag	3024.50	0.00000	NO	YES
136	au	3024.52	35.13571	YES	NO
137	au	3038.10	14.22247	YES	NO
138	ag	3038.10	0.00000	NO	YES
139	au	3052.11	0.14846	YES	NO
140	ag	3052.12	0.00000	NO	YES
141	au	3084.63	11.52439	YES	NO
142	ag	3084.70	0.00000	NO	YES
143	au	3090.77	8.66078	YES	NO
144	ag	3090.87	0.00000	NO	YES
145	ag	3100.98	0.00000	NO	YES
146	au	3101.04	24.80297	YES	NO
147	au	3114.95	54.09021	YES	NO
148	ag	3115.06	0.00000	NO	YES
149	ag	3129.53	0.00000	NO	YES
150	au	3129.57	5.24807	YES	NO

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