Supporting Information

for

Synthesis, Characterisation and Reactivity of a Zinc Triazenide for Potential Use in Vapor Deposition

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NMR Spectra

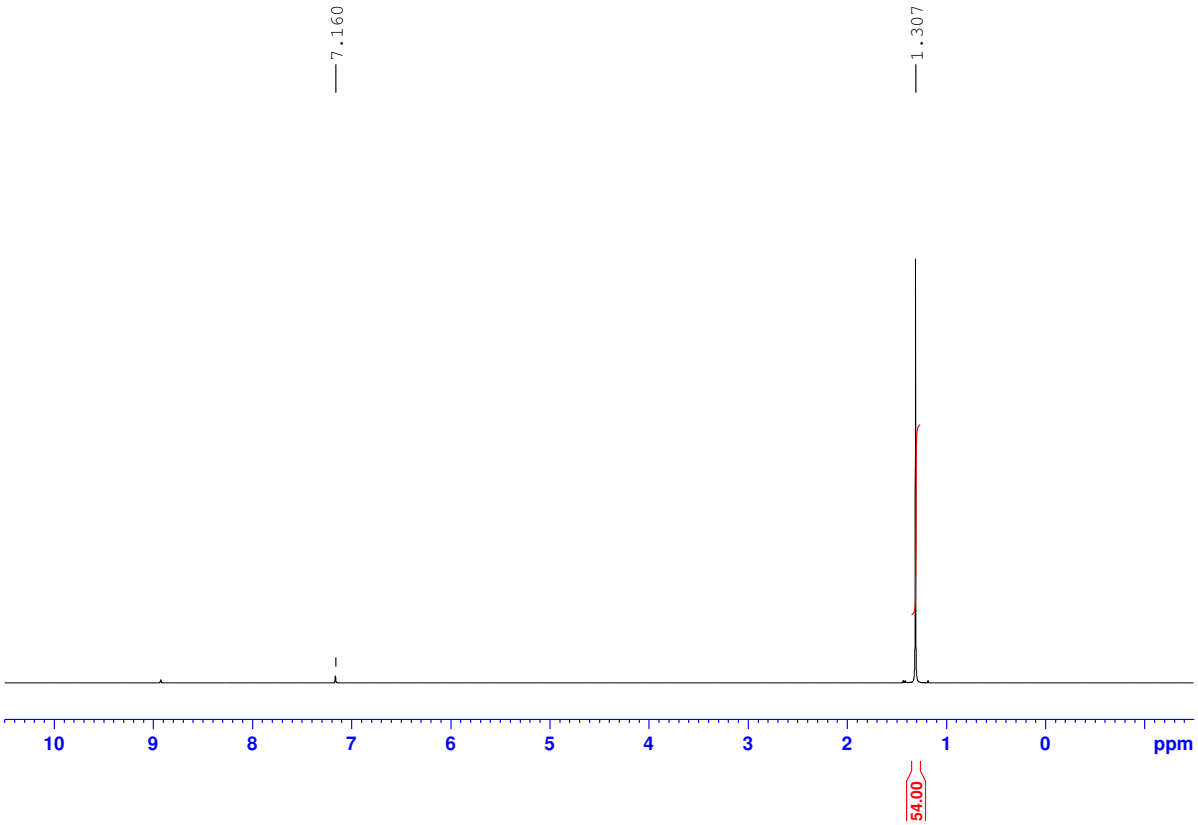

Figure S1: The ^{1}H NMR spectrum of **1** in C_6D_6 at 25 °C.

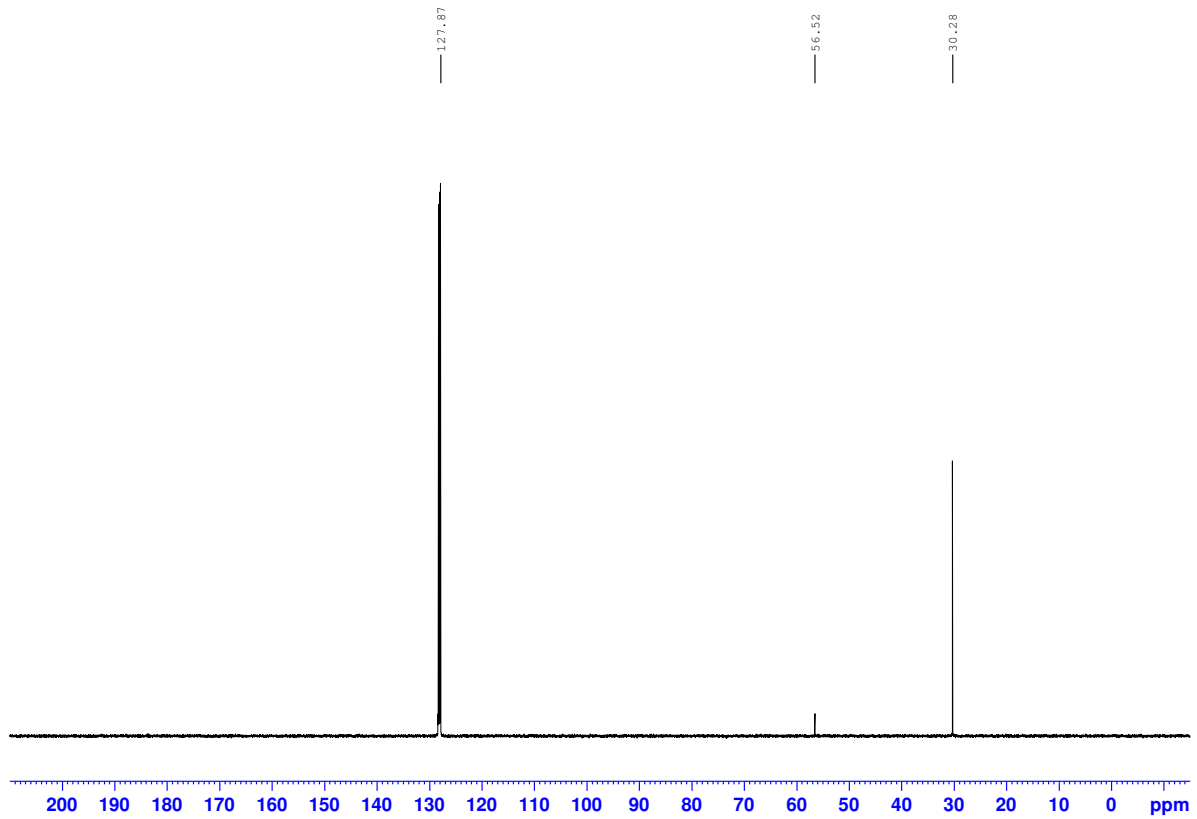

Figure S2: The ^{13}C NMR spectrum of **1** in C_6D_6 at 25 °C.

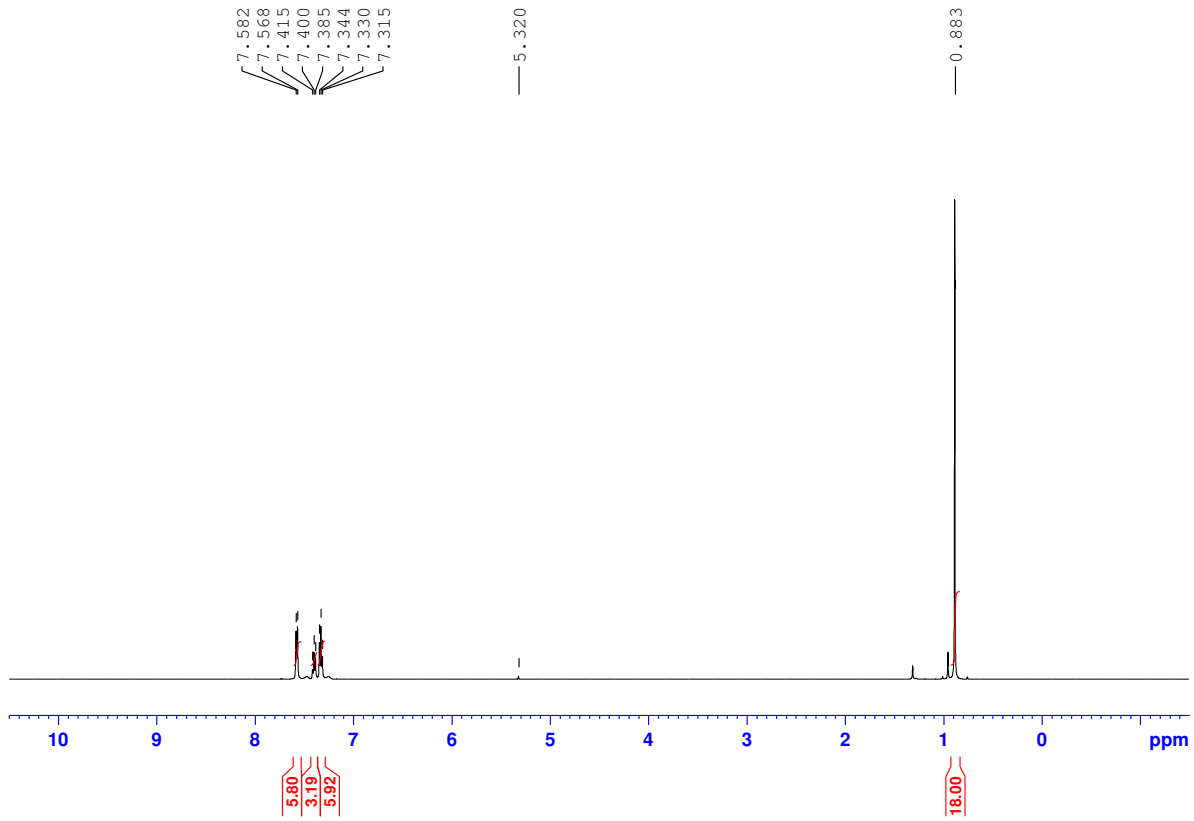

Figure S3: The ^{1}H NMR spectrum of **2** in CD_2Cl_2 at 25 °C.

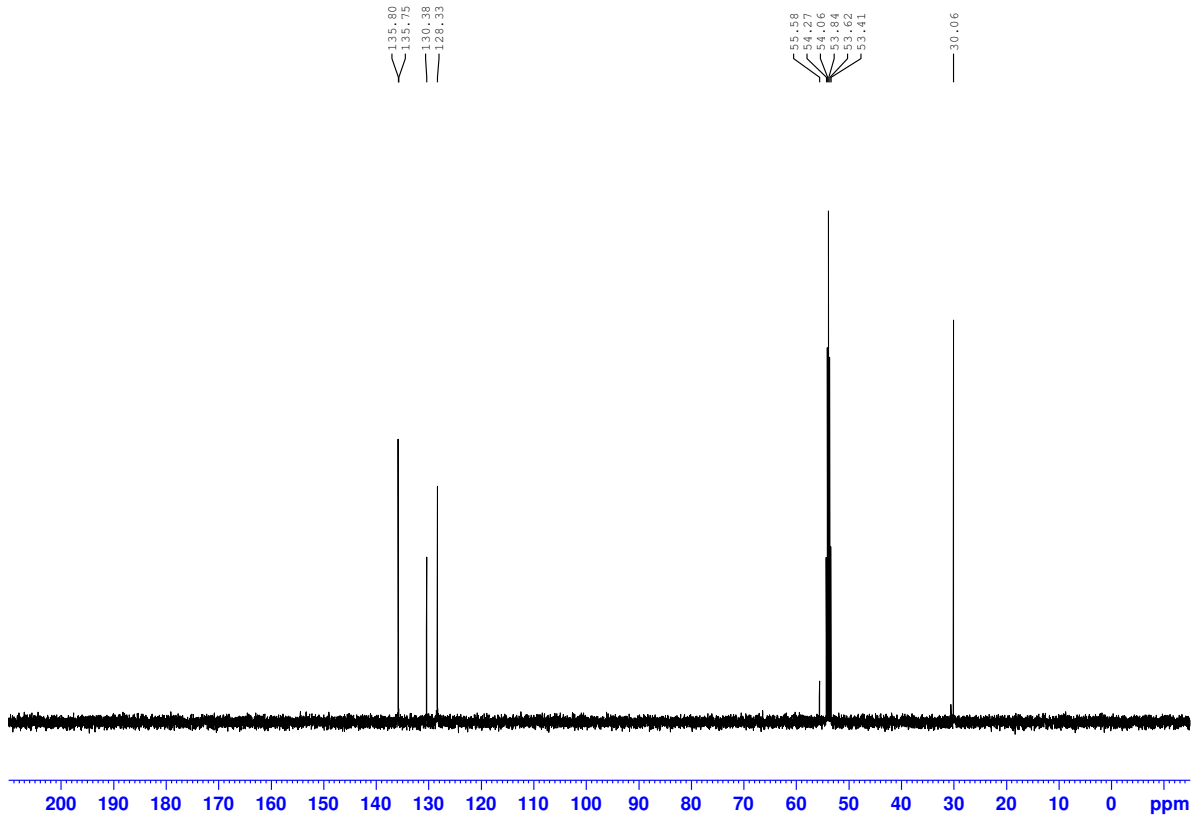

Figure S4: The ^{13}C NMR spectrum of **2** in CD_2Cl_2 at 25 °C.

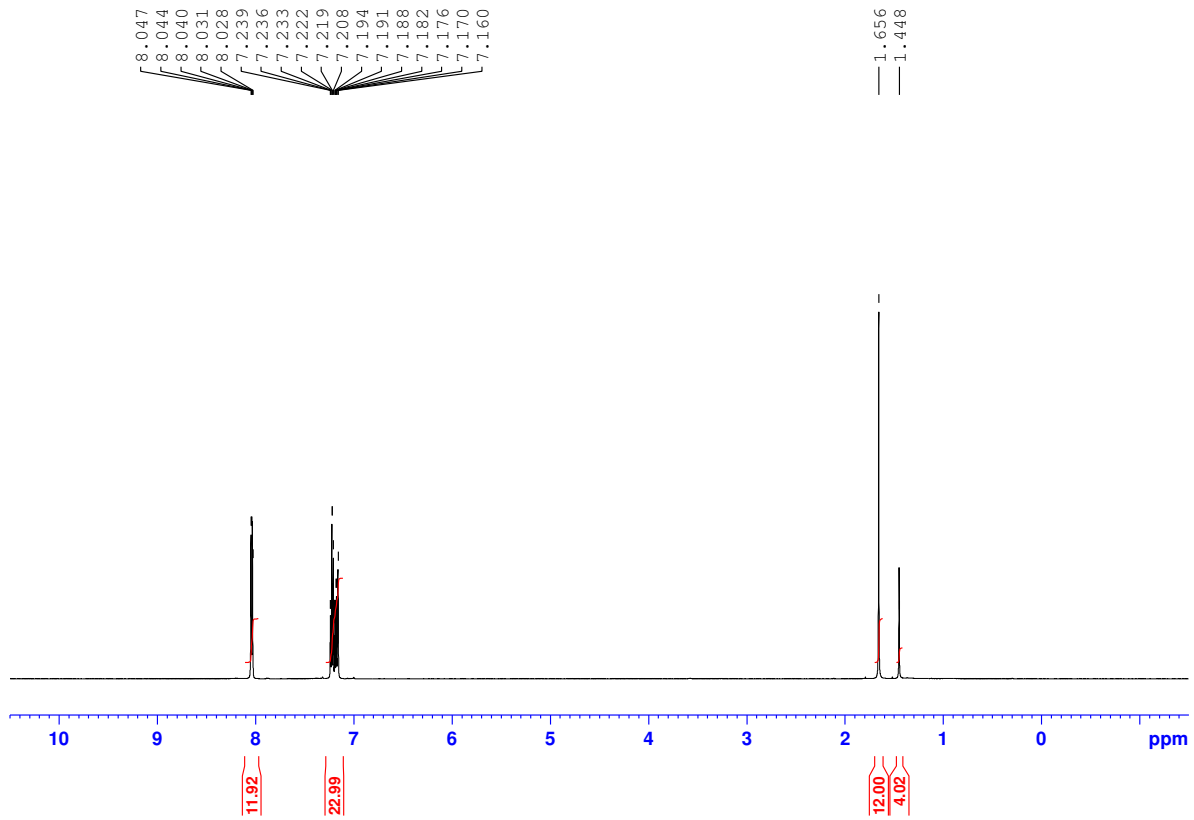

Figure S5: The ^{1}H NMR spectrum of **3** in C_6D_6 at 25 °C.

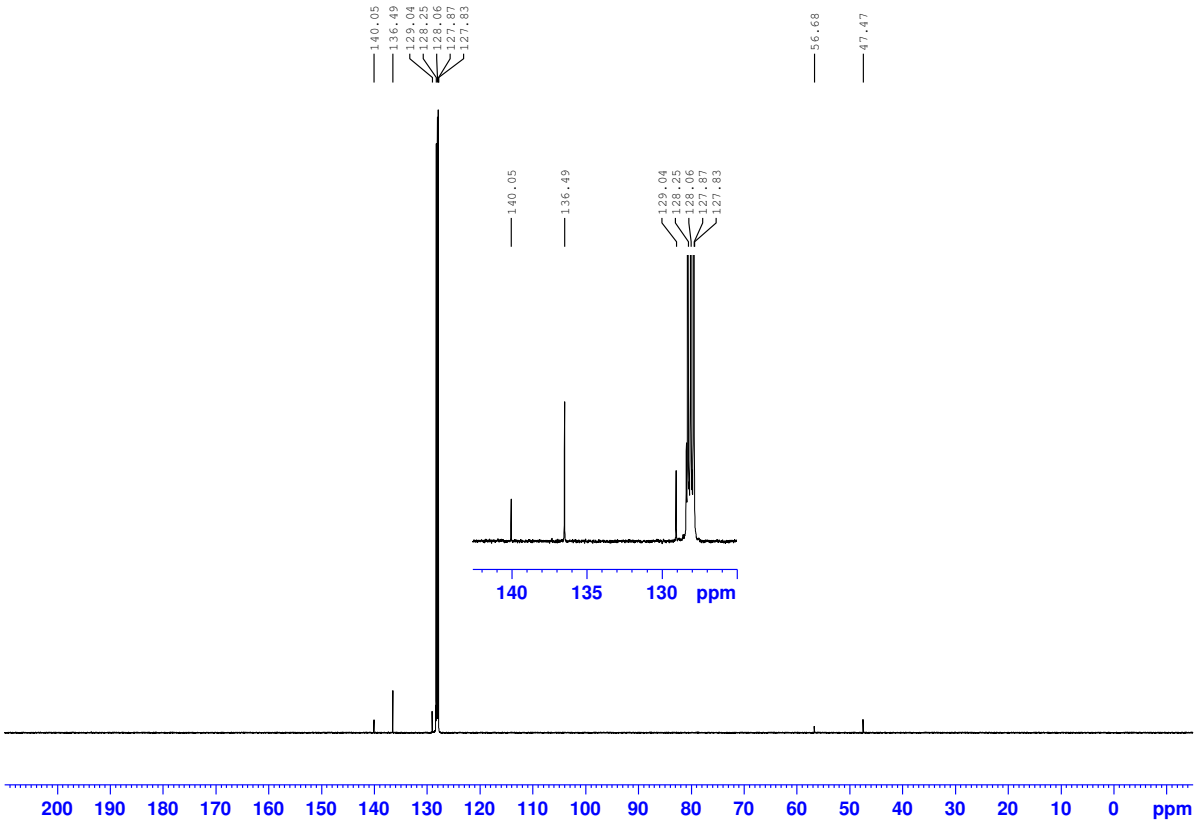

Figure S6: The ^{13}C NMR spectrum of **3** in C_6D_6 at 25 °C.

Solution State Thermolysis in Toluene-d_8

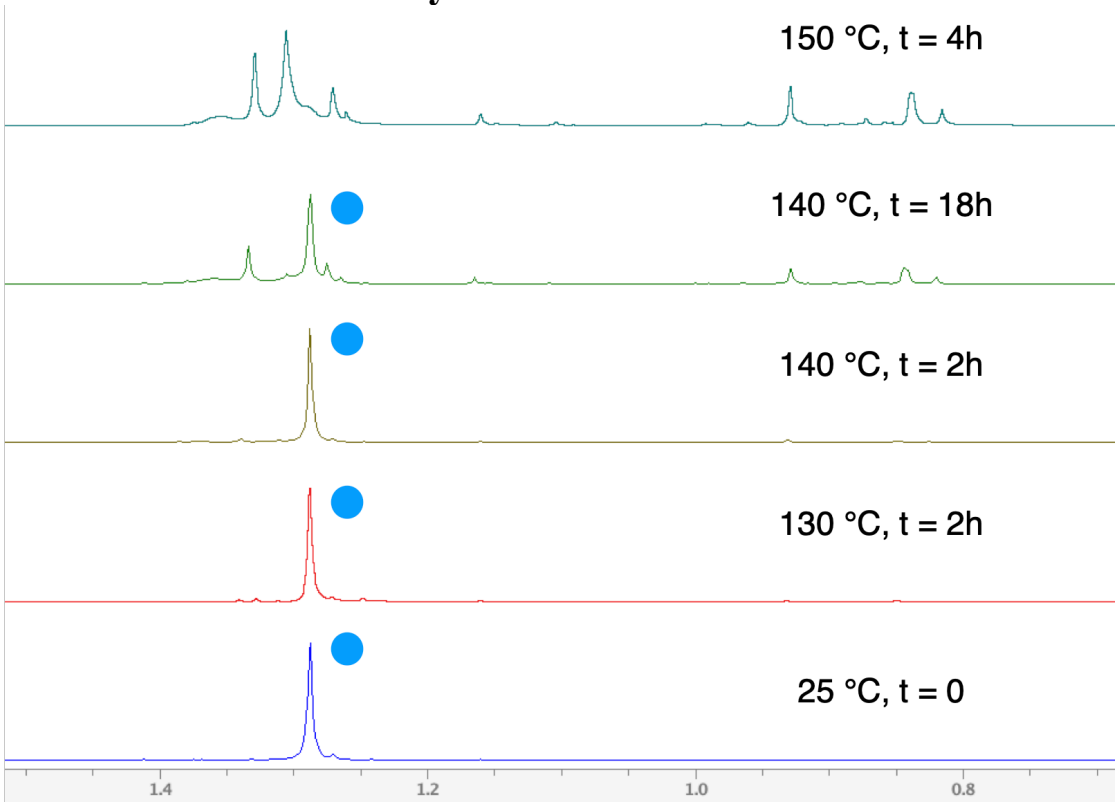

Figure S7: The ^{1}H NMR spectra of **1**, recorded during the decomposition study performed between 130 and 150 °C at various times. The light blue dots show the methyl peak of **1**. Compound **1** decomposed slowly at ~140 °C and rapidly at 150 °C.

Thermogravimetric Analysis

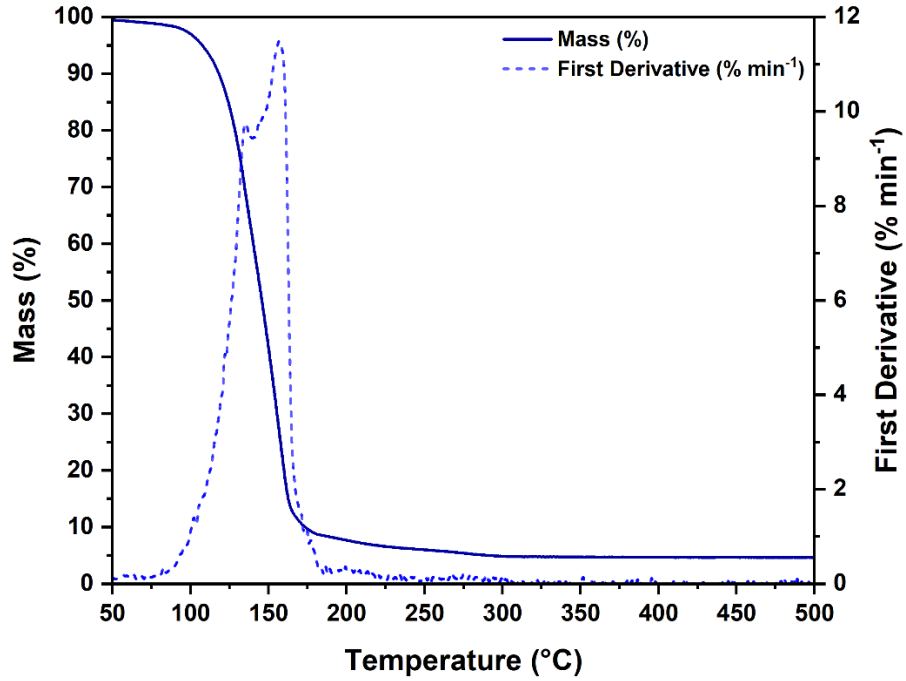

Figure S8: TGA ramp experiment of **1** showing its first derivative.

X-ray Crystallography

Table S1: Crystallographic data and structure refinement parameters for **1**, **2** and **3**.

	Compound 1	**Compound 2**	**Compound 3**
Empirical formula	$C_{32}H_{72}N_{12}Zn_2$	$C_{52}H_{66}N_6S_2Si_2Zn_2$	$C_{42}H_{46}N_2S_2Si_2Zn$
Formula weight/g mol^{-1}	755.75	1026.14	764.48
Temperature/K	120.15	120.01(10)	296
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_12_12_1$
***a*/Å**	10.46540(10)	17.7677(2)	10.986(5)
***b*/Å**	11.07540(10)	19.2736(2)	11.629(6)
***c*/Å**	18.2679(2)	16.2547(2)	31.308(15)
***α*/°**	90	90	90
***β*/°**	101.5640(10)	106.7230(10)	90
***γ*/°**	90	90	90
Volume/Å^3	2074.42(4)	5331.08(11)	4000(3)
Z	2	4	4
ρ_{calc}g/cm^3	1.210	1.279	1.27
μ/mm^{-1}	1.695	2.567	0.81
F(000)	816.0	2160.0	1608
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	Mo-Kα (λ = 0.71073 Å)
2Θrange for data collection/°	8.624 to 153.214	5.194 to 153.58	2.26 to 26.32
Reflections collected	24531	23238	7024
Independent reflections	4318 [R_{int} = 0.0345, R_{sigma} = 0.0205]	10967 [R_{int} = 0.0302, R_{sigma} = 0.0384]	6704 [R_{int} = 0.0335, R_{sigma} = 0.0313]
Data/restraints/parameters	4318/0/220	10967/12/613	6024/433/462
Goodness-of-fit on F^2	1.051	1.030	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0281, wR_2 = 0.0704	R_1 = 0.0308, wR_2 = 0.0760	R_1 = 0.0260, wR_2 = 0.0622
Final R indexes [all data]	R_1 = 0.0326, wR_2 = 0.0737	R_1 = 0.0385, wR_2 = 0.0803	R_1 = 0.0280, wR_2 = 0.0629
Largest diff. peak/hole/e Å^{-3}	0.47/-0.37	0.43/-0.50	0.27/-0.19

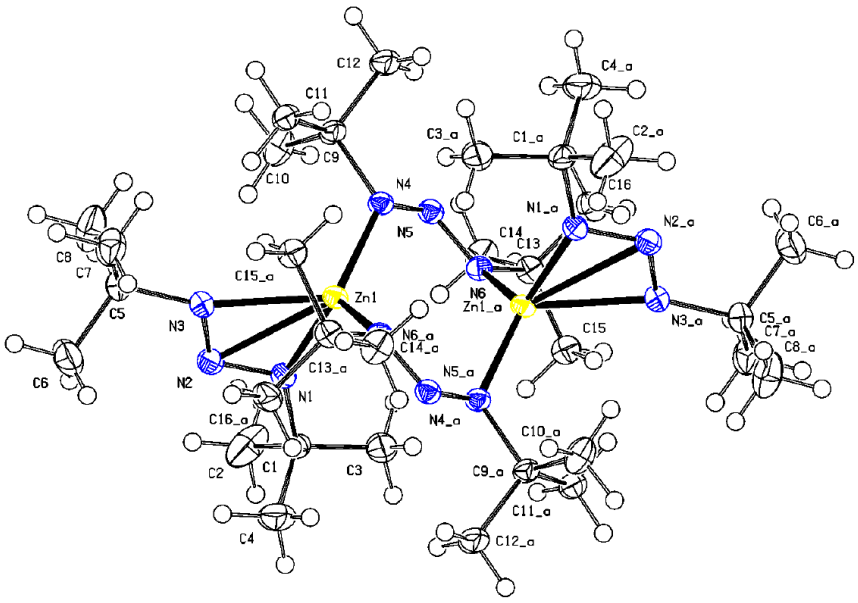

Figure S9: ORTEP drawing of **1** showing the naming scheme for the atomic centres.

Table S2: Selected bond parameters for **1** from crystal structure determination. The naming of the atomic centres are displayed in Figure S9.

Bond Lengths (Å)		Angles (°)		Dihedral Angles (°)	
Zn1--N1	2.0000(12)	N1--Zn1--N6	117.38(5)	Zn1--N1--N2--N3	1.47(13)
Zn1--N6	2.0298(12)	N1--Zn1--N4	116.53(5)	Zn1--N1--C1--C3	-22.8(2)
Zn1--N4	2.0241(12)	N1--Zn1--N3	59.15(5)	Zn1--N1--C1--C4	95.5(2)
Zn1--N3	2.3116(12)	N6--Zn1--N3	113.47(5)	Zn1--N1--C1--C2	-143.52(18)
N5--N6	1.2932(18)	N4--Zn1--N6	120.65(5)	Zn1--N6--C13--C15	48.87(14)
N5--N4	1.2955(18)	N4--Zn1--N3	114.10(5)	Zn1--N6--C13--C14	167.67(10)
N1--N2	1.3041(18)	N6--N5--N4	118.52(12)	Zn1--N6--C13--C16	-71.04(14)
N1--C1	1.4780(19)	N2--N1--Zn1	101.67(9)	Zn1--N4--C9--C11	42.83(15)
N6--C13	1.5037(18)	N2--N1--C1	113.62(12)	Zn1--N4--C9--C12	161.37(11)
N4--C9	1.5050(18)	C1--N1--Zn1	143.72(10)	Zn1--N4--C9--C10	-76.98(14)
N2--N3	1.2898(18)	N5--N6--Zn1	121.89(10)	Zn1--N3--C5--C8	89.2(3)
N3--C5	1.4964(19)	N5--N6--C13	110.20(11)	Zn1--N3--C5--C7	-29.2(4)
C13--C15	1.524(2)	C13--N6--Zn1	119.26(9)	Zn1--N3--C5--C6	-149.4(3)
C13--C14	1.529(2)	N5--N4--Zn1	120.73(9)	N5--N6--C13--C15	-162.77(12)
C13--C16	1.531(2)	N5--N4--C9	109.61(11)	N5--N6--C13--C14	-43.96(17)
C1--C3	1.510(2)	C9--N4--Zn1	120.85(9)	N5--N6--C13--C16	77.32(15)
C1--C4	1.537(2)	N3--N2--N1	111.58(12)	N5--N4--C9--C11	-169.53(12)
C1--C2	1.517(2)	N2--N3--Zn1	87.58(8)	N5--N4--C9--C12	-50.99(17)
C9--C11	1.523(2)	N2--N3--C5	112.06(12)	N5--N4--C9--C10	70.66(15)
C9--C12	1.532(2)	C5--N3--Zn1	160.32(10)	N1--N2--N3--Zn1	-1.24(11)
C9--C10	1.525(2)	N6--C13--C15	106.52(11)	N1--N2--N3--C5	177.53(12)
C5--C8	1.531(2)	N6--C13--C14	111.03(12)	N6--N5--N4--Zn1	-34.50(17)
C5--C7	1.523(2)	N6--C13--C16	108.70(12)	N6--N5--N4--C9	177.81(12)
C5--C6	1.520(2)	N1--C1--C3	106.97(12)	N4--N5--N6--Zn1	-35.04(17)
		N1--C1--C4	108.31(14)	N4--N5--N6--C13	177.58(12)
		N1--C1--C2	111.02(13)	N2--N1--C1--C3	171.57(13)
		N4--C9--C11	107.10(12)	N2--N1--C1--C4	-70.16(17)
		N4--C9--C12	110.02(12)	N2--N1--C1--C2	50.9(2)
		N4--C9--C10	108.91(13)	N2--N3--C5--C8	-87.17(17)
		N3--C5--C8	109.30(13)	N2--N3--C5--C7	154.46(14)
		N3--C5--C7	108.42(13)	N2--N3--C5--C6	34.24(19)
		N3--C5--C6	111.82(14)	C1--N1--N2--N3	172.83(12)

Table S3: Selected bond parameters for **2** from crystal structure determination.

Bond Lengths (Å)		Angles (°)	
Zn2--S2	2.3583(4)	S2--Zn2--S2	117.38(5)
Zn2--S2	2.3529(4)	S2--Zn2--N5	116.53(5)
Zn2--N6	2.0387(13)	S2--Zn2--N5	59.15(5)
Zn2--N4	2.0573(14)	N6--Zn2--S2	113.47(5)
Zn2--N5	2.4979(14)	N6--Zn2--S2	120.65(5)
Zn1--S1	2.3645(4)	N6--Zn2--N4	114.10(5)
Zn1--S1	2.3348(4)	N6--Zn2--N5	118.52(12)

Zn1--N3	2.0579(15)	N4--Zn2--S2	101.67(9)
Zn1--N2	2.4938(15)	N4--Zn2--S2	113.62(12)
Zn1--N1	2.0392(14)	N4--Zn2--N5	143.72(10)
S1--Zn1	2.3645(4)	S1--Zn1--S1	121.89(10)
S1--Si1	2.1355(6)	S1--Zn1--N2	110.20(11)
S2--Zn2	2.3584(4)	S1--Zn1--N2	119.26(9)
S2--Si2	2.1372(6)	N3--Zn1--S1	120.73(9)
Si1--C15	1.8702(17)	N3--Zn1--S1	109.61(11)
Si1--C9	1.8731(16)	N3--Zn1--N2	120.85(9)
Si1--C21	1.8731(16)	N1--Zn1--S1	111.58(12)
Si2--C47	1.8806(17)	N1--Zn1--S1	87.58(8)
Si2--C41	1.8715(17)	N1--Zn1--N3	112.06(12)
Si2--C35	1.8672(18)	N1--Zn1--N2	160.32(10)
N6--N5	1.300(2)	Zn1--S1--Zn1	106.52(11)
N6--C31	1.480(2)	Si1--S1--Zn1	111.03(12)
N4--N5	1.298(2)	Si1--S1--Zn1	108.70(12)
N4--C27	1.479(2)	Zn2--S2--Zn2	109.22(13)
N3--N2	1.295(2)	Si2--S2--Zn2	111.21(13)
N3--C5	1.474(2)	Si2--S2--Zn2	110.12(13)
N2--N1	1.301(2)	C15--Si1--S1	106.97(12)
N1--C1	1.479(2)	C15--Si1--C9	108.31(14)
C15--C20	1.406(2)	C15--Si1--C21	111.02(13)
C15--C16	1.393(2)	C9--Si1--S1	109.78(14)
C9--C10	1.399(2)	C9--Si1--C21	110.56(16)
C9--C14	1.400(2)	C21--Si1--S1	110.13(18)
C21--C22	1.400(2)	C47--Si2--S2	107.10(12)
C21--C26	1.393(2)	C41--Si2--S2	110.02(12)
C47--C48	1.401(2)	C41--Si2--C47	108.91(13)
C47--C52	1.388(3)	C35--Si2--S2	109.17(14)
C41--C46	1.393(2)	C35--Si2--C47	110.75(13)
C41--C42	1.395(2)	C35--Si2--C41	110.82(14)
C10--C11	1.388(2)	N5--N6--Zn2	109.30(13)
C11--C12	1.389(3)	N5--N6--C31	108.42(13)
C22--C23	1.391(3)	C31--N6--Zn2	111.82(14)
C35--C40	1.390(2)	N5--N4--Zn2	108.74(16)
C35--C36	1.398(3)	N5--N4--C27	109.50(17)
C20--C19	1.387(3)	C27--N4--Zn2	109.02(15)

Table S4: Selected bond parameters for **3** from crystal structure determination.

Bond Lengths (Å)		Angles (°)	
Zn1--N2	2.155(2)	N2--Zn1--N1	83.99(9)
Zn1--N1	2.177(2)	N2--Zn1--S1	106.31(7)
Zn1--S1	2.2538(11)	N1--Zn1--S1	101.94(6)
Zn1--S2	2.2651(9)	N2--Zn1--S2	102.36(7)
Si1--C2	1.866(2)	N1--Zn1--S2	110.83(7)
Si1--C11	1.872(3)	S1--Zn1--S2	138.19(3)

Si1--C9	1.879(2)	C2--Si1--C11	108.52(10)
Si1--S2	2.0941(11)	C2--Si1--C9	110.60(10)
S1--Si2	2.0949(12)	C11--Si1--C9	104.78(10)
Si2--C8	1.871(2)	C2--Si1--S2	112.88(7)
Si2--C3	1.874(2)	C11--Si1--S2	113.69(8)
Si2--C5	1.878(2)	C9--Si1--S2	106.04(8)
N1--C30	1.441(4)	Si2--S1--Zn1	112.36(3)
N1--C37	1.456(4)	Si1--S2--Zn1	112.80(4)
N1--C21	1.465(4)	C8--Si2--C3	108.28(10)
C2--C12	1.383(3)	C8--Si2--C5	109.41(11)
C2--C10	1.384(3)	C3--Si2--C5	105.41(11)
C3--C6	1.388(3)	C8--Si2--S1	110.18(8)
C3--C13	1.391(3)	C3--Si2--S1	107.68(7)
N2--C44B	1.378(13)	C5--Si2--S1	115.55(8)
N2--C43	1.452(4)	C30--N1--C37	110.4(3)
N2--C41B	1.463(8)	C30--N1--C21	109.3(3)
N2--C44A	1.588(15)	C37--N1--C21	107.5(3)
N2--C41A	1.600(10)	C30--N1--Zn1	112.74(19)
C5--C32	1.369(4)	C37--N1--Zn1	105.8(2)
C5--C16	1.372(4)	C21--N1--Zn1	110.99(16)
C6--C17	1.372(3)	C12--C2--Si1	123.10(17)
C7--C8	1.381(3)	C10--C2--Si1	120.03(17)
C7--C14	1.379(4)	C6--C3--Si2	120.19(17)
C8--C28	1.390(3)	C13--C3--Si2	122.95(17)
C9--C31	1.371(3)	C44B--N2--C43	112.9(9)
C9--C23	1.375(3)	C44B--N2--C41B	82.9(16)
C10--C19	1.376(3)	C43--N2--C41B	123.1(6)
C11--C33	1.374(4)	C44B--N2--C44A	28.4(8)
C11--C24	1.380(4)	C43--N2--C44A	99.7(7)
C12--C20	1.385(4)	C41B--N2--C44A	110.9(11)
C13--C15	1.372(4)	C44B--N2--C41A	113.8(16)
C14--C18	1.363(4)	C43--N2--C41A	94.0(6)
C15--C27	1.372(4)	C41B--N2--C41A	35.3(3)
C16--C39	1.384(4)	C44A--N2--C41A	141.8(11)
C17--C27	1.369(4)	C44B--N2--Zn1	118.4(7)
C18--C35	1.359(5)	C43--N2--Zn1	113.47(17)
C19--C25	1.366(4)	C41B--N2--Zn1	103.0(3)
C20--C25	1.364(4)	C44A--N2--Zn1	105.7(7)
C22--C36	1.341(4)	C41A--N2--Zn1	101.0(3)
C22--C38	1.342(4)	C32--C5--Si2	121.5(2)
C23--C36	1.378(4)	C16--C5--Si2	120.5(2)
C24--C29	1.377(4)	C7--C8--Si2	120.67(18)
C26--C29	1.348(5)	C28--C8--Si2	123.00(19)
C26--C34	1.366(5)	C31--C9--Si1	122.51(18)
C28--C35	1.373(4)	C23--C9--Si1	122.22(18)
C31--C38	1.370(4)	C33--C11--Si1	122.4(2)

C32--C42	1.388(4)	C24--C11--Si1	120.5(2)
C33--C34	1.368(4)	C41A--C37--N1	120.0(5)
C37--C41A	1.261(9)	N1--C37--C41B	115.7(4)
C37--C41B	1.457(10)	C37--C41A--N2	118.3(7)
C39--C40	1.357(5)	C37--C41B--N2	114.9(6)
C40--C42	1.369(5)		

Computational Details

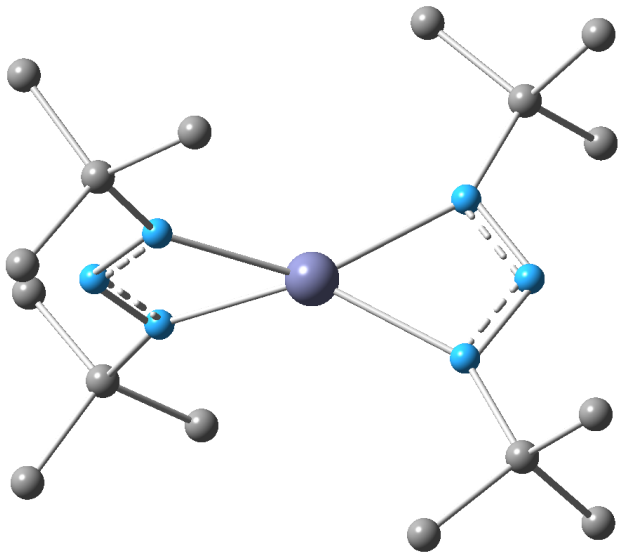

Figure S10: DFT optimized geometry of monomeric **1**.

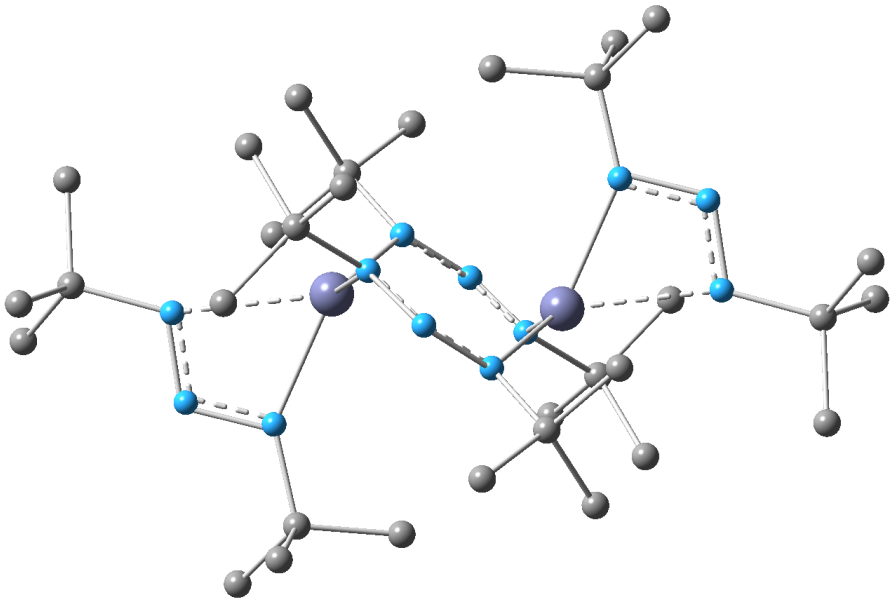

Figure S11: DFT optimized geometry of dimeric **1**.

Table S5: Average bond lengths (Å) and angles (°) from DFT optimized geometries of monomeric and dimeric **1**, as well as dimeric **1** from X-ray crystallography.

	Monomer	Dimer (DFT)	Dimer (X-ray)
Zn–Zn	N/A	3.289	
Zn–N (chel)	2.063	2.031, 2.294	2.0000(12), 2.3116(12)

Zn–N (bridge)	N/A	2.059	2.0269(12)
N–N (chel)	1.288	1.285	1.3041(18), 1.2898(18)
N–N (bridge)	N/A	1.280	1.2932(18), 1.2955(18)
N–C (chel)	1.470	1.480	1.4780(19), 1.4964(19)
N–C (bridge)	N/A	1.503	1.5037(18), 1.5050(18)
N–Zn–N (chel-bite)	61.5	58.8	59.15(5)
N–N–N (chel)	110.0	112.4	111.58(12)
N–N–N (bridge)	N/A	120.6	118.52(12)

Table S6: Total energies and thermochemical corrections (in Hartrees) from gas phase energy calculations and vibrational analysis at 298.15 K for monomeric and dimeric **1**.

	Monomer	Dimer
E(B3LYP)	-2739.7554	-5479.5636
ZPE	0.517499	1.042615
H	0.549254	1.104031
G	0.451969	0.951915

Natural Bond Orbital Analysis

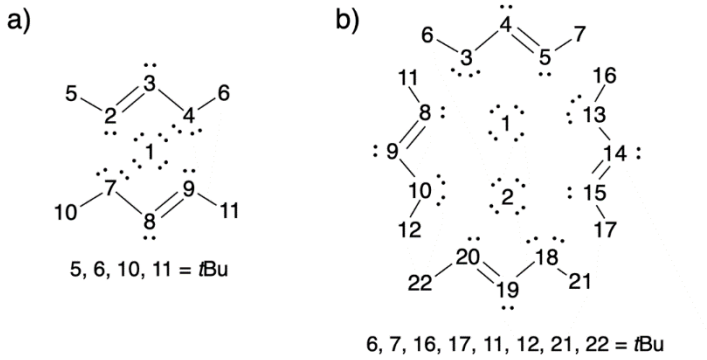

Figure S12: Natural Lewis structures for monomeric **1** (a) and dimeric **1** (b).

Table S7: Average NBO charges (from Natural Population Analysis) for monomeric and dimeric **1**

	Monomeric **1**	Dimeric **1**	
Zn	1.432	1.473	
	N/A	**Bridging L**	**Chelating L**
N_term	-0.521	-0.520	-0.539
N_cent	0.014	-0.003	0.000
C_tert	0.097	0.104	0.116
C_prim	-0.601	-0.604	-0.613
H	0.207	0.207	0.211

Table S8: Natural electron configurations of atoms in monomeric **1**

Zn 1	[core]4s(0.56)3d(9.97)5p(0.03)
N 2	[core]2s(1.40)2p(4.07)3s(0.01)3p(0.03)3d(0.01)
N 3	[core]2s(1.38)2p(3.57)3s(0.01)3p(0.01)3d(0.01)
N 4	[core]2s(1.40)2p(4.07)3s(0.01)3p(0.03)3d(0.01)
C 5	[core]2s(0.94)2p(2.94)3p(0.01)
C 6	[core]2s(0.94)2p(2.94)3p(0.01)
N 7	[core]2s(1.40)2p(4.07)3s(0.01)3p(0.03)3d(0.01)
N 8	[core]2s(1.38)2p(3.57)3s(0.01)3p(0.01)3d(0.01)
N 9	[core]2s(1.40)2p(4.07)3s(0.01)3p(0.03)3d(0.01)
C 10	[core]2s(0.94)2p(2.94)3p(0.01)
C 11	[core]2s(0.94)2p(2.94)3p(0.01)
C 12	[core]2s(1.11)2p(3.48)3d(0.01)
H 13	1s(0.78)
H 14	1s(0.80)
H 15	1s(0.79)
C 16	[core]2s(1.11)2p(3.47)3d(0.01)
H 17	1s(0.79)
H 18	1s(0.79)
H 19	1s(0.79)
C 20	[core]2s(1.11)2p(3.48)3d(0.01)
H 21	1s(0.80)
H 22	1s(0.78)
H 23	1s(0.79)
C 24	[core]2s(1.11)2p(3.48)3d(0.01)
H 25	1s(0.80)
H 26	1s(0.78)
H 27	1s(0.79)
C 28	[core]2s(1.11)2p(3.47)3d(0.01)
H 29	1s(0.79)
H 30	1s(0.79)
H 31	1s(0.79)
C 32	[core]2s(1.11)2p(3.48)3d(0.01)
H 33	1s(0.78)
H 34	1s(0.80)
H 35	1s(0.79)
C 36	[core]2s(1.11)2p(3.48)3d(0.01)
H 37	1s(0.78)

H 38	1s(0.79)
H 39	1s(0.80)
C 40	[core]2s(1.11)2p(3.48)3d(0.01)
H 41	1s(0.78)
H 42	1s(0.80)
H 43	1s(0.79)
C 44	[core]2s(1.11)2p(3.47)3d(0.01)
H 45	1s(0.79)
H 46	1s(0.79)
H 47	1s(0.79)
C 48	[core]2s(1.11)2p(3.48)3d(0.01)
H 49	1s(0.78)
H 50	1s(0.80)
H 51	1s(0.79)
C 52	[core]2s(1.11)2p(3.47)3d(0.01)
H 53	1s(0.79)
H 54	1s(0.79)
H 55	1s(0.79)
C 56	[core]2s(1.11)2p(3.48)3d(0.01)
H 57	1s(0.80)
H 58	1s(0.78)
H 59	1s(0.79)

Table S9: Natural electron configurations of atoms in dimeric **1**

Zn 1	[core]4s(0.50)3d(9.97)4p(0.01)4d(0.01)5p(0.03)
Zn 2	[core]4s(0.50)3d(9.97)4p(0.01)4d(0.01)5p(0.03)
N 3	[core]2s(1.42)2p(4.03)3s(0.01)3p(0.02)3d(0.01)
N 4	[core]2s(1.37)2p(3.59)3s(0.01)3p(0.01)3d(0.01)
N 5	[core]2s(1.40)2p(4.11)3s(0.01)3p(0.03)3d(0.01)
C 6	[core]2s(0.94)2p(2.93)3p(0.01)
C 7	[core]2s(0.94)2p(2.94)3p(0.01)
N 8	[core]2s(1.41)2p(4.08)3s(0.01)3p(0.02)3d(0.01)
N 9	[core]2s(1.35)2p(3.61)3s(0.02)3p(0.01)3d(0.01)
N 10	[core]2s(1.41)2p(4.09)3s(0.01)3p(0.02)3d(0.01)
C 11	[core]2s(0.95)2p(2.91)3p(0.01)
C 12	[core]2s(0.95)2p(2.91)3p(0.01)
N 13	[core]2s(1.41)2p(4.09)3s(0.01)3p(0.02)3d(0.01)
N 14	[core]2s(1.35)2p(3.61)3s(0.02)3p(0.01)3d(0.01)
N 15	[core]2s(1.41)2p(4.08)3s(0.01)3p(0.02)3d(0.01)
C 16	[core]2s(0.95)2p(2.91)3p(0.01)
C 17	[core]2s(0.95)2p(2.91)3p(0.01)
N 18	[core]2s(1.42)2p(4.03)3s(0.01)3p(0.02)3d(0.01)
N 19	[core]2s(1.37)2p(3.59)3s(0.01)3p(0.01)3d(0.01)
N 20	[core]2s(1.40)2p(4.11)3s(0.01)3p(0.03)3d(0.01)
C 21	[core]2s(0.94)2p(2.93)3p(0.01)
C 22	[core]2s(0.94)2p(2.94)3p(0.01)
C 23	[core]2s(1.11)2p(3.49)3d(0.01)
H 24	1s(0.78)
H 25	1s(0.80)
H 26	1s(0.79)
C 27	[core]2s(1.10)2p(3.48)3d(0.01)
H 28	1s(0.80)
H 29	1s(0.79)
H 30	1s(0.79)
C 31	[core]2s(1.11)2p(3.48)3d(0.01)

H 32 1s(0.80)
H 33 1s(0.79)
H 34 1s(0.79)
C 35 [core]2s(1.11)2p(3.48)3d(0.01)
H 36 1s(0.80)
H 37 1s(0.78)
H 38 1s(0.79)
C 39 [core]2s(1.10)2p(3.49)3d(0.01)
H 40 1s(0.79)
H 41 1s(0.78)
H 42 1s(0.80)
C 43 [core]2s(1.11)2p(3.48)3d(0.01)
H 44 1s(0.79)
H 45 1s(0.80)
H 46 1s(0.79)
C 47 [core]2s(1.10)2p(3.49)3d(0.01)
H 48 1s(0.79)
H 49 1s(0.79)
H 50 1s(0.79)
C 51 [core]2s(1.11)2p(3.50)3d(0.01)
H 52 1s(0.77)
H 53 1s(0.80)
H 54 1s(0.79)
C 55 [core]2s(1.11)2p(3.49)3d(0.01)
H 56 1s(0.79)
H 57 1s(0.79)
H 58 1s(0.78)
C 59 [core]2s(1.11)2p(3.49)3d(0.01)
H 60 1s(0.78)
H 61 1s(0.79)
H 62 1s(0.79)
C 63 [core]2s(1.11)2p(3.49)3d(0.01)
H 64 1s(0.80)
H 65 1s(0.79)
H 66 1s(0.78)
C 67 [core]2s(1.10)2p(3.51)3d(0.01)
H 68 1s(0.79)
H 69 1s(0.79)
H 70 1s(0.79)
C 71 [core]2s(1.10)2p(3.51)3d(0.01)
H 72 1s(0.79)
H 73 1s(0.79)
H 74 1s(0.79)
C 75 [core]2s(1.11)2p(3.49)3d(0.01)
H 76 1s(0.79)
H 77 1s(0.78)
H 78 1s(0.79)
C 79 [core]2s(1.11)2p(3.49)3d(0.01)
H 80 1s(0.80)
H 81 1s(0.78)
H 82 1s(0.79)
C 83 [core]2s(1.11)2p(3.50)3d(0.01)
H 84 1s(0.80)
H 85 1s(0.77)
H 86 1s(0.79)

C 87	[core]2s(1.10)2p(3.49)3d(0.01)
H 88	1s(0.79)
H 89	1s(0.79)
H 90	1s(0.79)
C 91	[core]2s(1.11)2p(3.49)3d(0.01)
H 92	1s(0.78)
H 93	1s(0.79)
H 94	1s(0.79)
C 95	[core]2s(1.11)2p(3.48)3d(0.01)
H 96	1s(0.79)
H 97	1s(0.79)
H 98	1s(0.80)
C 99	[core]2s(1.11)2p(3.48)3d(0.01)
H100	1s(0.78)
H101	1s(0.80)
H102	1s(0.79)
C103	[core]2s(1.10)2p(3.49)3d(0.01)
H104	1s(0.78)
H105	1s(0.79)
H106	1s(0.80)
C107	[core]2s(1.11)2p(3.48)3d(0.01)
H108	1s(0.79)
H109	1s(0.80)
H110	1s(0.79)
C111	[core]2s(1.10)2p(3.48)3d(0.01)
H112	1s(0.79)
H113	1s(0.80)
H114	1s(0.79)
C115	[core]2s(1.11)2p(3.49)3d(0.01)
H116	1s(0.80)
H117	1s(0.78)
H118	1s(0.79)

Atomic coordinates for optimized structures of **1**

Table S10: Cartesian coordinates for the optimized structure of monomeric **1**

Atom	X	Y	Z
30	0.000007	0.000017	0.000303
7	-1.772307	-0.743832	-0.748661
7	-2.510705	-0.000291	-0.00003
7	-1.772643	0.743358	0.748846
6	-2.440627	-1.666261	-1.677582
6	-2.44139	1.665755	1.677492
7	1.772661	-0.748686	0.743520
7	2.510719	0.00030	-0.000014
7	1.772311	0.749207	-0.743278
6	2.441401	-1.677683	1.665570
6	2.440611	1.678177	-1.665671
6	-3.302695	-2.671005	-0.900252
1	-4.090813	-2.152967	-0.353285
1	-3.765791	-3.388593	-1.580933

1	-2.69180	-3.22061	-0.181496
6	-1.312504	-2.394507	-2.410909
1	-0.682394	-1.683207	-2.948837
1	-0.682423	-2.9374	-1.703368
1	-1.718024	-3.108151	-3.129556
6	-3.302661	-0.881925	-2.676882
1	-3.765808	-1.557594	-3.399155
1	-4.090731	-0.338518	-2.155041
1	-2.691734	-0.159415	-3.221508
6	-3.303693	0.881364	2.676519
1	-3.767167	1.55701	3.398603
1	-4.09152	0.337856	2.154416
1	-2.692882	0.158938	3.221386
6	-1.313611	2.394161	2.411189
1	-0.683607	1.682956	2.949366
1	-0.683347	2.937104	1.70385
1	-1.719467	3.107783	3.129667
6	-3.303296	2.670378	0.899824
1	-4.091183	2.152241	0.352618
1	-3.766683	3.387954	1.580317
1	-2.692213	3.220006	0.181244
6	3.301955	0.90082	-2.671018
1	4.090073	0.353384	-2.153471
1	2.690551	0.18247	-3.220588
1	3.765022	1.581534	-3.388592
6	3.303367	2.676891	-0.881384
1	4.091467	2.15458	-0.338477
1	3.766502	3.399194	-1.557028
1	2.692958	3.221527	-0.158445
6	1.312474	2.412175	-2.393219
1	0.68188	1.70505	-2.936061
1	0.68288	2.950139	-1.681491
1	1.717981	3.130871	-3.10682
6	3.303756	-2.67639	0.880835
1	4.0916	-2.154078	0.337558
1	3.767207	-3.39872	1.556235
1	2.692985	-3.220997	0.158179
6	1.313614	-2.411687	2.393653
1	0.683296	-1.70457	2.936823
1	0.683665	-2.949628	1.682221
1	1.719462	-3.130407	3.107036
6	3.303251	-0.90036	2.670509
1	3.76667	-1.581097	3.387835
1	4.091115	-0.352918	2.152584

1	2.692126	-0.18202	3.220403

Table S11: Cartesian coordinates for the optimized structure of dimeric **1**

Atom	X	Y	Z
30	-1.635826	0.112492	0.12469
30	1.635824	-0.112497	-0.124656
7	-3.921474	0.0848	-0.065349
7	-3.783963	-0.566377	-1.160815
7	-2.548318	-0.72189	-1.486503
6	-5.342193	0.307703	0.31711
6	-2.276467	-1.552471	-2.671016
7	-0.886625	-1.305631	1.42037
7	-0.061654	-2.211233	1.050203
7	0.797275	-1.973088	0.13097
6	-1.768734	-1.808935	2.528151
6	1.64477	-3.179467	-0.161112
7	-0.797311	1.97307	-0.131148
7	0.061683	2.211203	-1.050319
7	0.886717	1.305621	-1.420398
6	-1.64488	3.179425	0.16083
6	1.768931	1.808953	-2.528083
7	3.921529	-0.084876	0.06551
7	3.783935	0.566326	1.160945
7	2.548264	0.721827	1.486565
6	5.34228	-0.307863	-0.316783
6	2.276303	1.552656	2.670877
6	-6.170932	0.770191	-0.891651
1	-6.209534	-0.000602	-1.659208
1	-7.191315	1.001819	-0.578697
1	-5.734734	1.668042	-1.333207
6	-5.379492	1.399199	1.38823
1	-4.794936	1.122695	2.265463
1	-4.993447	2.341543	1.001506
1	-6.408496	1.561987	1.713505
6	-5.932742	-0.992071	0.885431
1	-6.983716	-0.854386	1.150098
1	-5.864144	-1.791594	0.14651
1	-5.394047	-1.304827	1.780381
6	-3.25086	-1.239561	-3.812414
1	-2.98226	-1.817603	-4.699141
1	-4.274637	-1.48531	-3.534659
1	-3.212183	-0.17847	-4.065315
6	-0.849381	-1.218349	-3.097958
1	-0.781211	-0.177731	-3.413517

1	-0.163587	-1.356778	-2.26363
1	-0.531067	-1.857304	-3.923628
6	-2.379551	-3.030982	-2.267921
1	-3.398067	-3.264179	-1.953542
1	-2.112475	-3.687104	-3.099683
1	-1.711346	-3.236993	-1.431846
6	-2.187334	3.002752	1.578954
1	-2.703483	2.05231	1.69374
1	-1.379727	3.044862	2.309228
1	-2.903294	3.792255	1.810523
6	-2.780705	3.235403	-0.868882
1	-3.361621	2.314778	-0.851714
1	-3.448861	4.074272	-0.662308
1	-2.364851	3.361733	-1.869658
6	-0.829256	4.475692	0.102979
1	-1.46245	5.309077	0.413709
1	0.026465	4.429275	0.776694
1	-0.463862	4.676792	-0.901612
6	0.938624	2.495222	-3.61896
1	0.437753	3.381947	-3.235847
1	1.591497	2.794562	-4.441126
1	0.180825	1.816991	-4.013955
6	2.785081	2.790666	-1.932051
1	3.49491	3.124257	-2.691903
1	2.269248	3.663603	-1.530772
1	3.340834	2.318065	-1.123519
6	2.477648	0.596007	-3.126461
1	3.117127	0.905468	-3.954107
1	3.111936	0.115027	-2.385174
1	1.758255	-0.132785	-3.499865
6	-2.477478	-0.59599	3.126496
1	-3.111823	-0.115078	2.385216
1	-3.116899	-0.905435	3.954193
1	-1.758101	0.132856	3.499827
6	-0.938304	-2.495071	3.619019
1	-1.591094	-2.794384	4.441261
1	-0.437411	-3.381796	3.235935
1	-0.180513	-1.816763	4.013899
6	-2.784862	-2.790756	1.93226
1	-3.494639	-3.124311	2.692176
1	-3.340675	-2.318261	1.123708
1	-2.269003	-3.663706	1.531041
6	2.780563	-3.235629	0.868625
1	3.448673	-4.074517	0.661979

1	3.361532	-2.315033	0.851564
1	2.364678	-3.362037	1.869378
6	2.18729	-3.002695	-1.579198
1	2.903173	-3.792249	-1.810825
1	1.379709	-3.044642	-2.309509
1	2.703545	-2.052297	-1.693859
6	0.82903	-4.475667	-0.10342
1	0.463599	-4.676841	0.901143
1	-0.026675	-4.429085	-0.777145
1	1.462145	-5.30908	-0.414233
6	2.379023	3.031077	2.267362
1	3.397472	3.264428	1.95288
1	1.710742	3.236688	1.431252
1	2.11182	3.687373	3.098946
6	3.25084	1.240289	3.8123
1	4.274542	1.486202	3.534417
1	2.982153	1.818518	4.698878
1	3.212429	0.17926	4.065501
6	0.849319	1.218332	3.098005
1	0.163439	1.356391	2.263685
1	0.7814	0.177784	3.413852
1	0.530915	1.85744	3.923522
6	5.933052	0.991958	-0.884763
1	5.864455	1.79134	-0.14569
1	6.984043	0.854203	-1.149325
1	5.394504	1.304954	-1.779718
6	5.379611	-1.399149	-1.388114
1	4.993412	-2.341528	-1.00163
1	4.795203	-1.122407	-2.265372
1	6.408642	-1.561983	-1.713278
6	6.17078	-0.770681	0.892015
1	7.191198	-1.002329	0.579189
1	6.209312	-0.000053	1.659742
1	5.734431	-1.66859	1.333304