Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Exploring the reactivity of homoleptic organozinc compounds towards SO_2

Adam Tulewicz,* [a] Vadim Szejko,[b] Iwona Justyniak,[a] Małgorzata Wolska-Pietkiewicz [b] and Janusz Lewiński *[a,b]

[a] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

[b] Department of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

* E-mail: atulewicz@ichf.edu.pl; lewin@ch.pw.edu.pl

Table of Contents

I. NMR & IR spectra

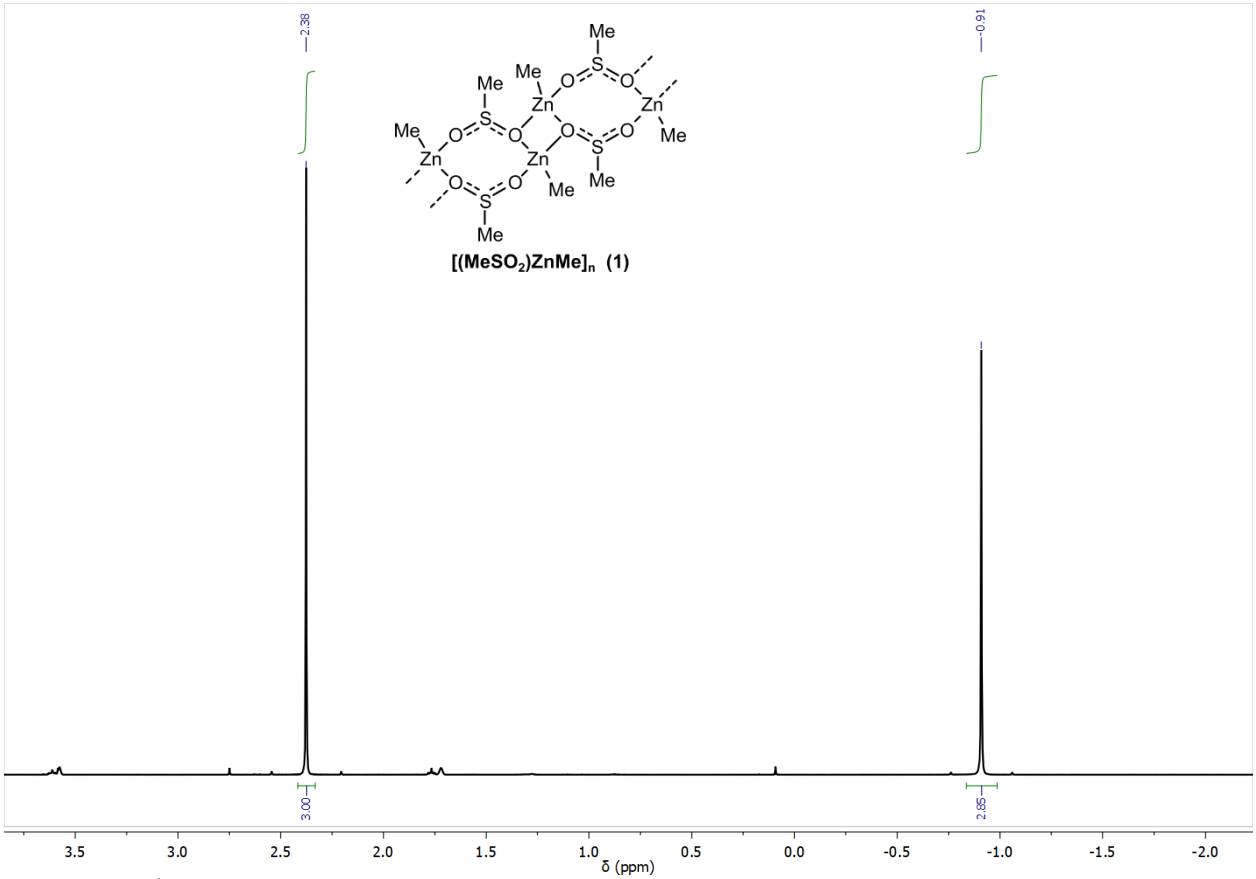

Figure S1. ^{1}H NMR (400 MHz, THF-d_8) spectrum of **[(MeSO$_2$ZnMe)$_2$]$_n$ (1)**.

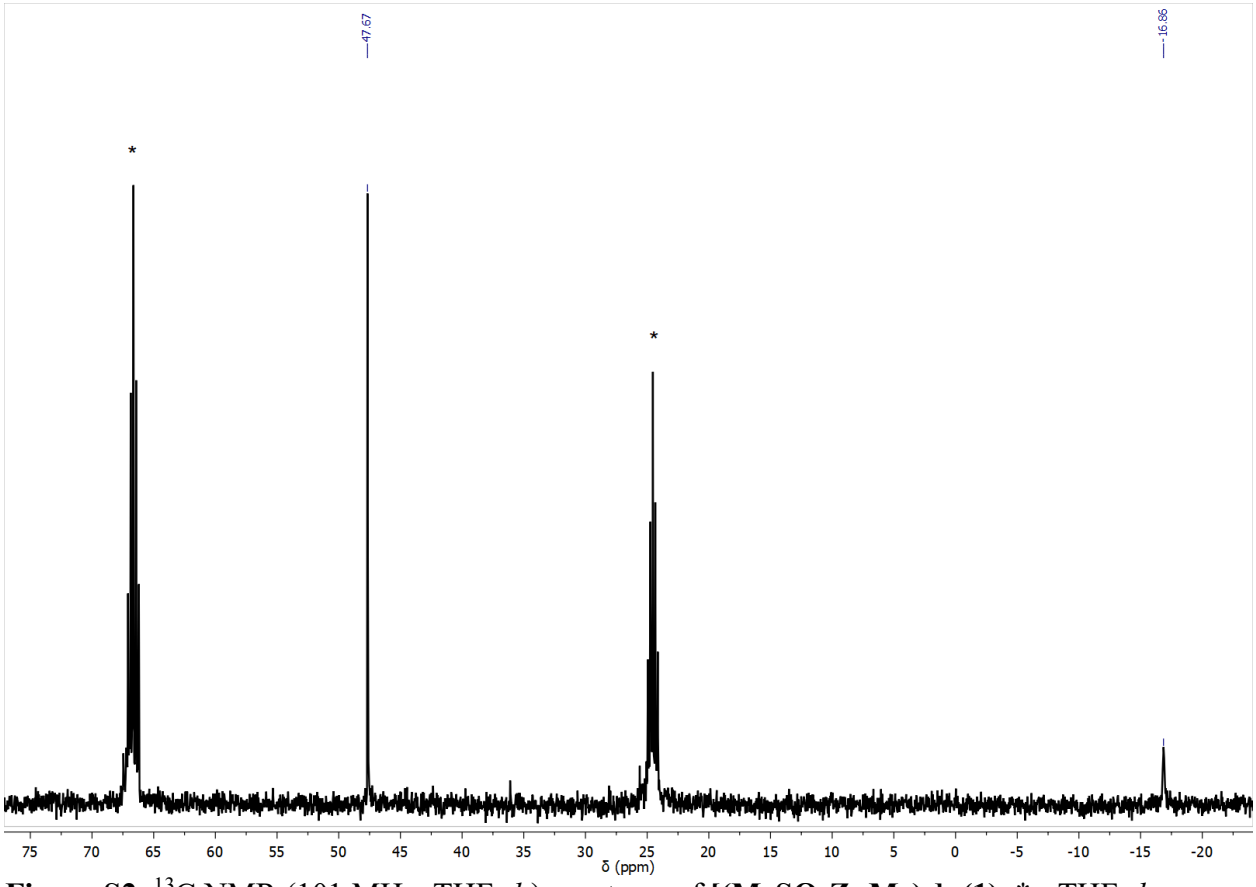

Figure S2. ^{13}C NMR (101 MHz, THF-d_8) spectrum of **[(MeSO$_2$ZnMe)$_2$]$_n$ (1)**. * - THF-d_8.

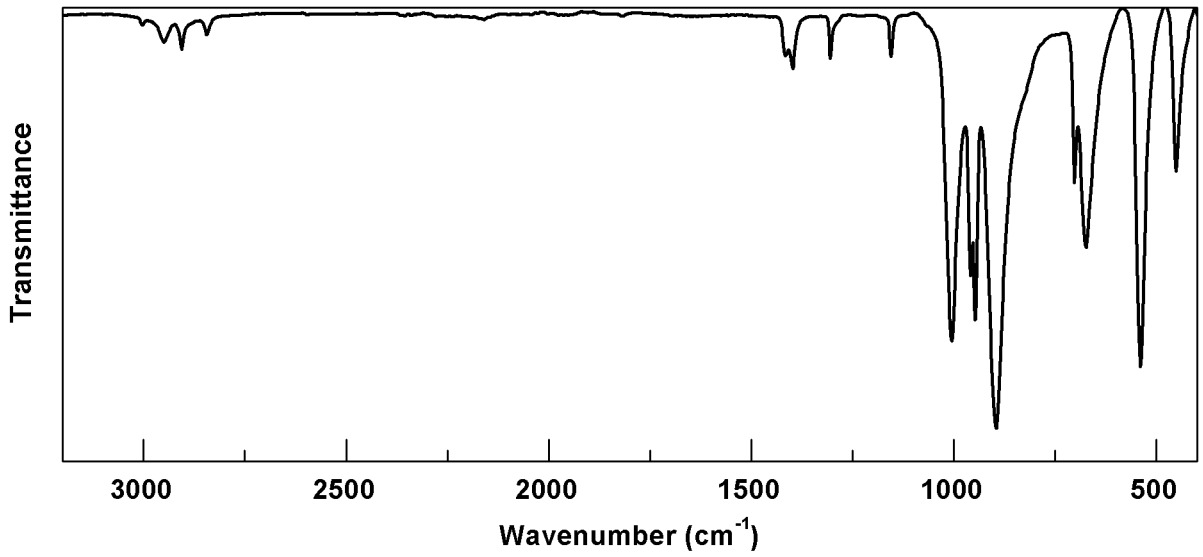

Figure S3. IR (ATR) spectrum of **[(MeSO$_2$ZnMe)$_2$]$_n$ (1)**.

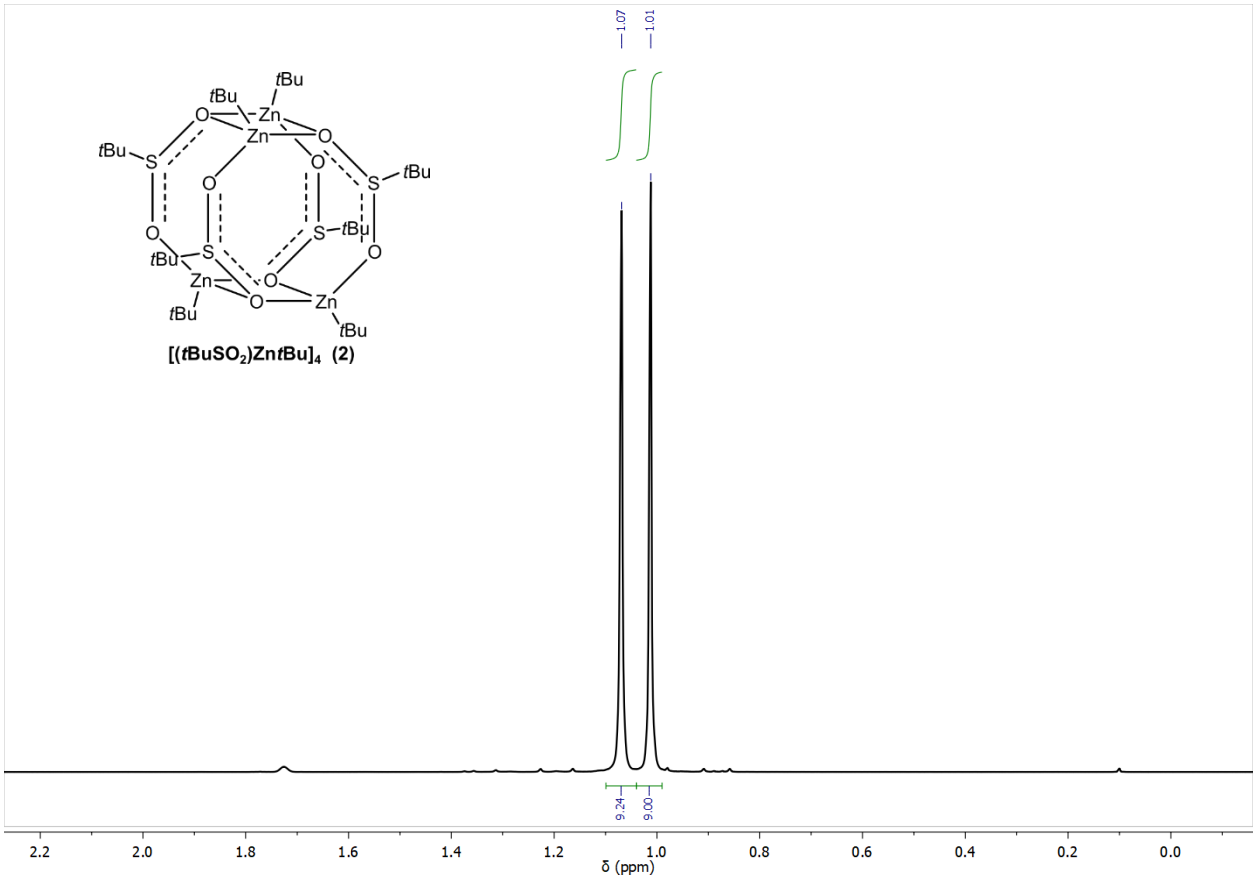

Figure S4. ^{1}H NMR (400 MHz, THF-d_8) spectrum of **[*t*BuSO$_2$Zn*t*Bu]$_4$ (2)**.

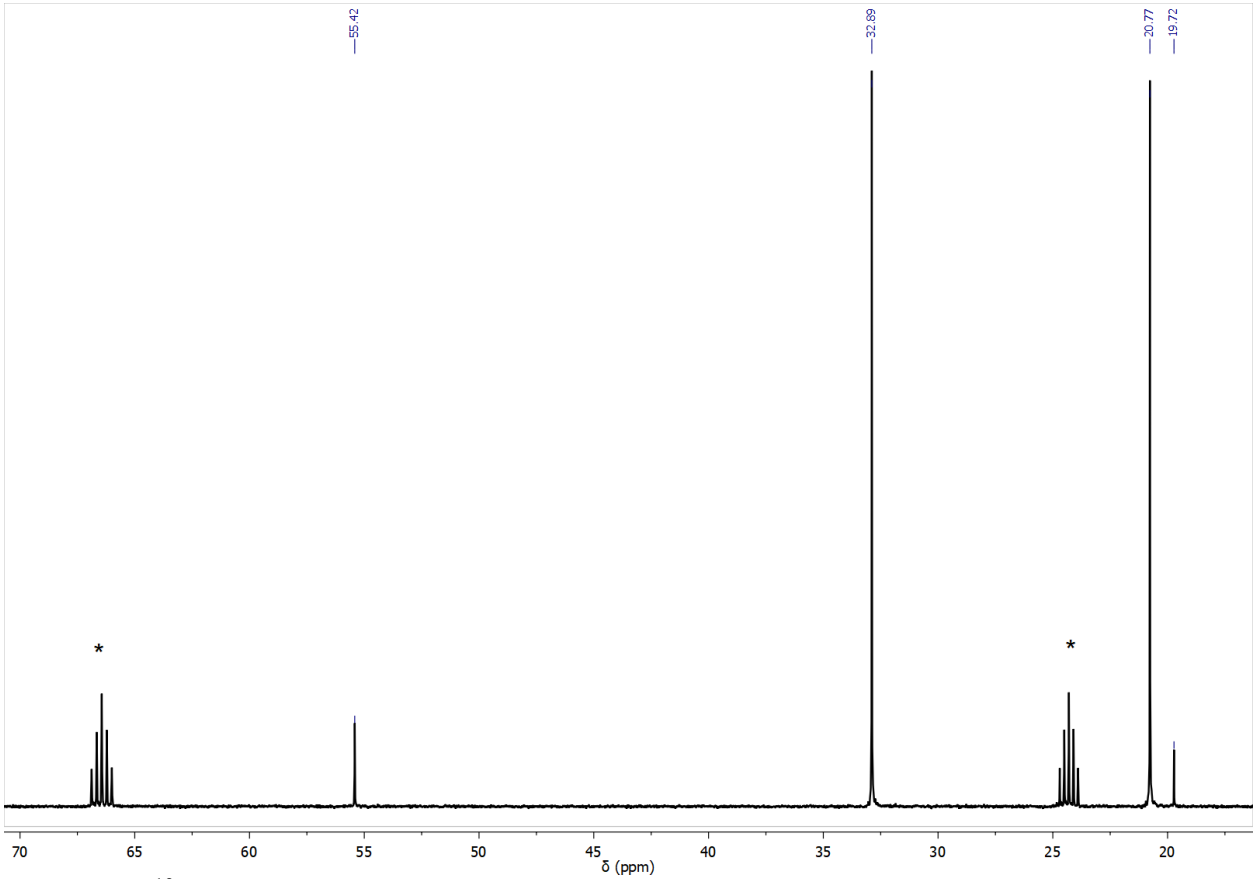

Figure S5. ^{13}C NMR (101 MHz, THF-d_8) spectrum of **[*t*BuSO$_2$Zn*t*Bu]$_4$ (2)**. * - THF-d_8.

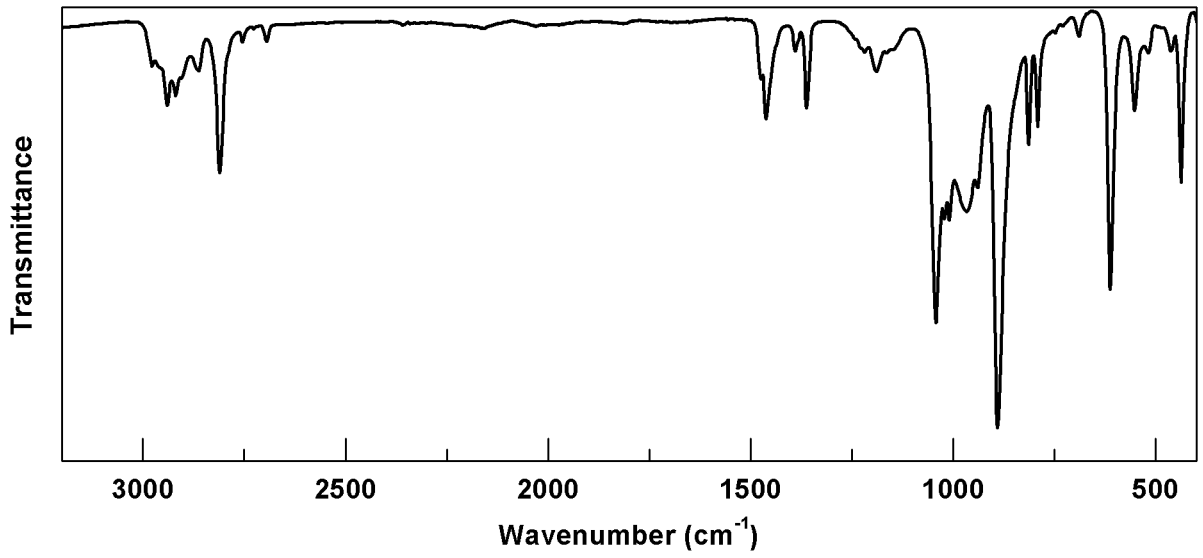

Figure S6. IR (ATR) spectrum of **[*t*BuSO$_2$Zn*t*Bu]$_4$ (2)** .

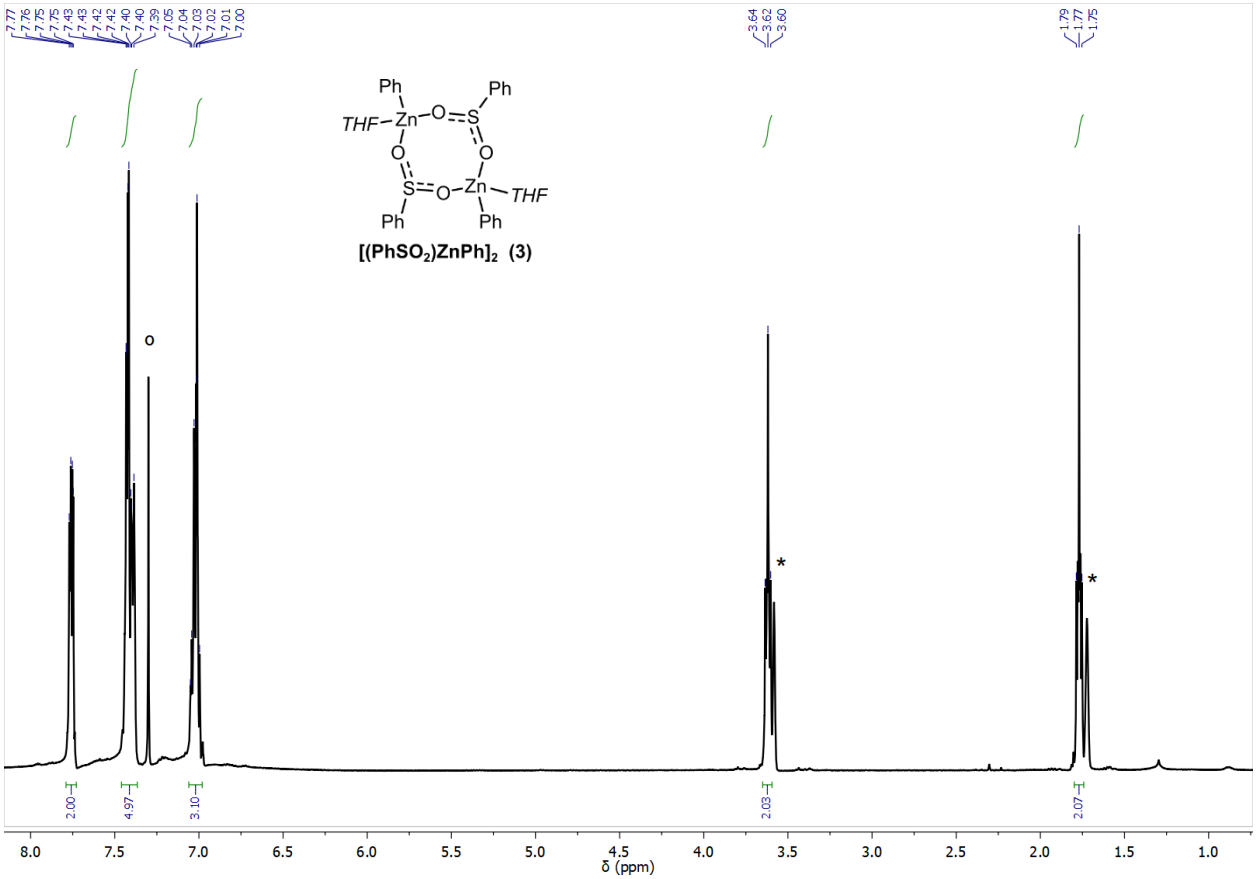

Figure S7. ^{1}H NMR (400 MHz, THF-d_8) spectrum of **[(PhSO₂)ZnPh]₂·2THF (3)**. * - THF-d_8, º - benzene.

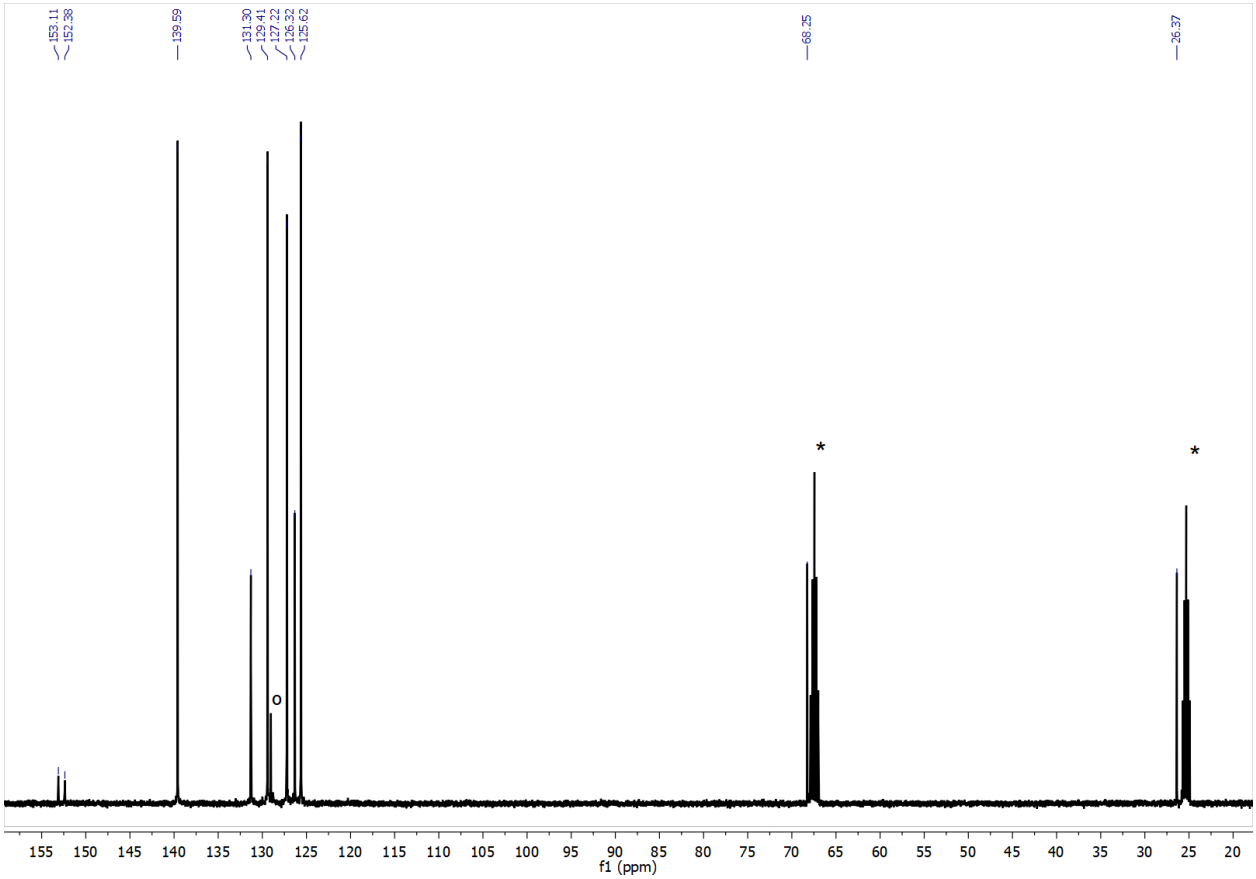

Figure S8. ^{13}C NMR (101 MHz, THF-d_8) spectrum of **[(PhSO₂)ZnPh]₂·2THF (3)**. * - THF-d_8, º - benzene.

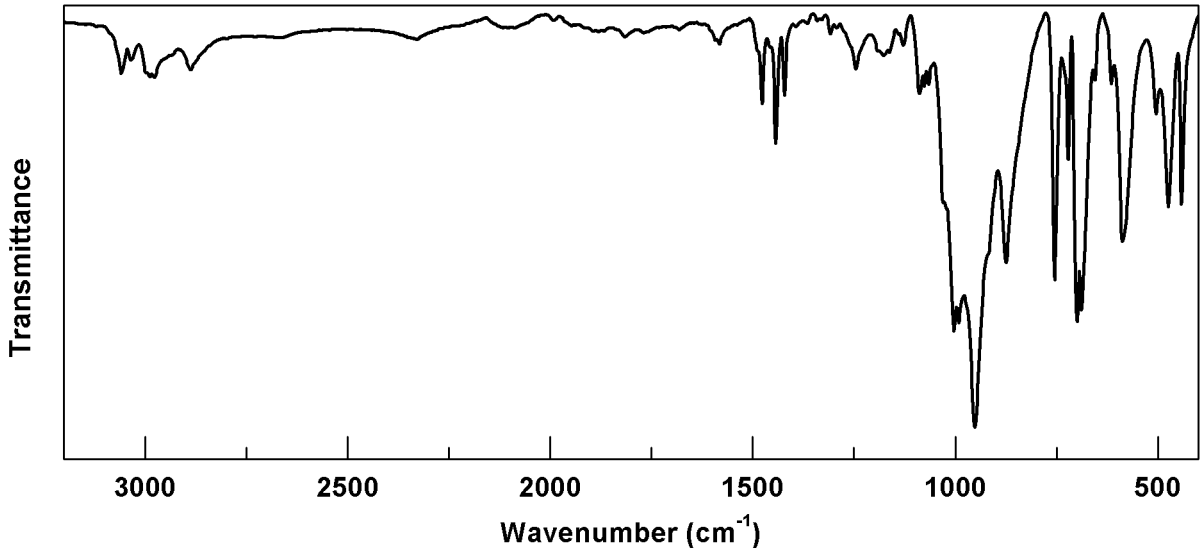

Figure S9. IR (ATR) spectrum of **[(PhSO$_2$)ZnPh]$_2$·2THF (3)**.

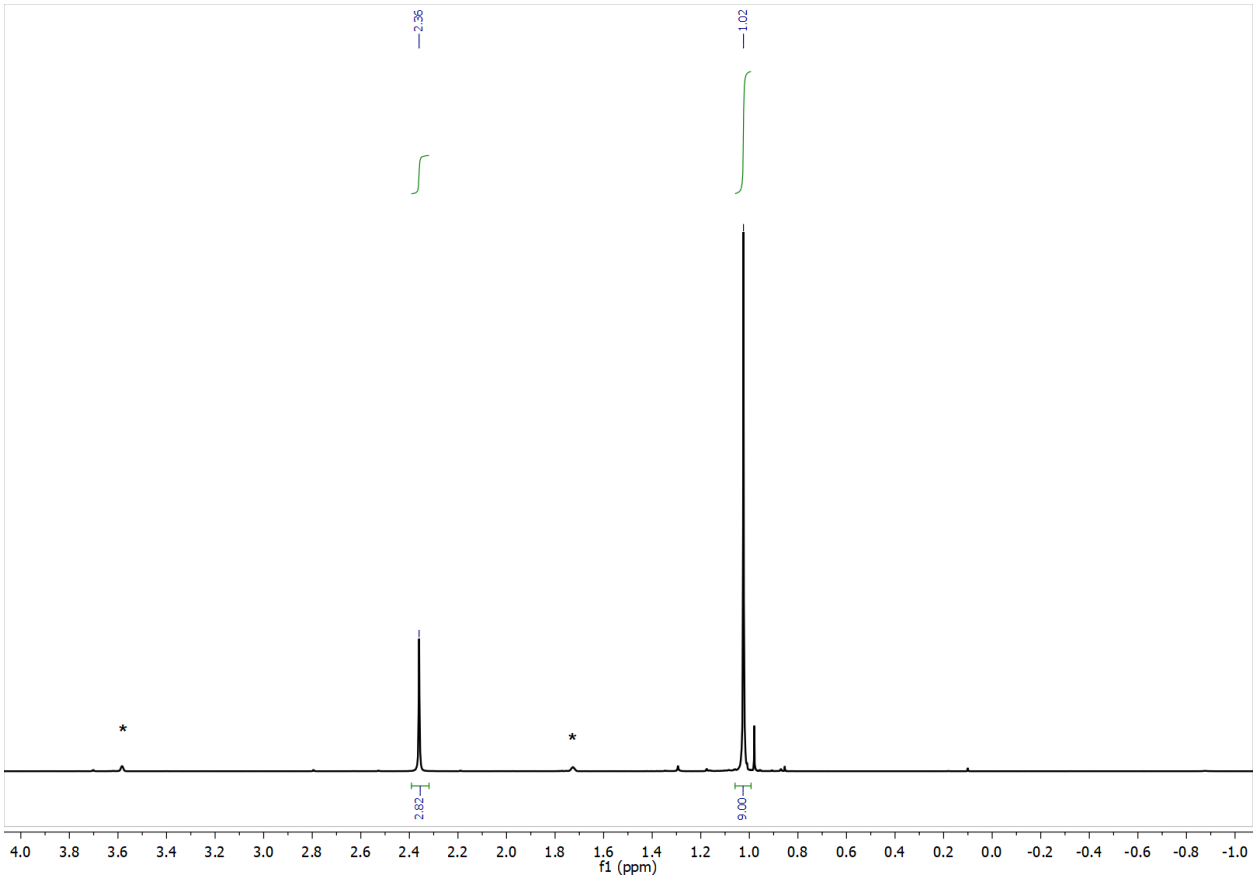

Figure S10. ^{1}H NMR (400 MHz, THF-d_8) spectrum of the equimolar mixture of **1** and ***t*Bu$_2$Zn**. * - THF-d_8.

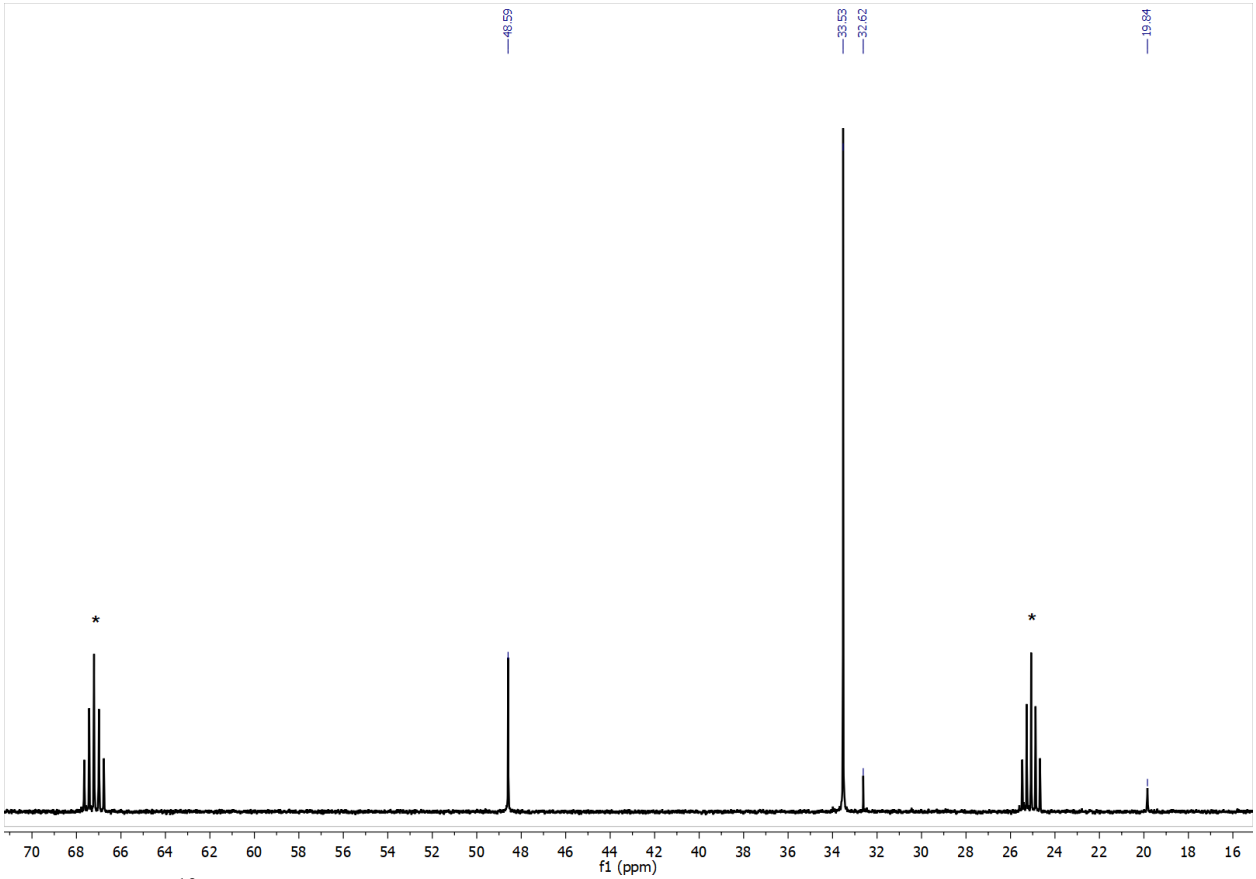

Figure S11. ^{13}C NMR (101 MHz, THF-d_8) spectrum of the equimolar mixture between **1** and ***t*Bu$_2$Zn**. * - THF-d_8.

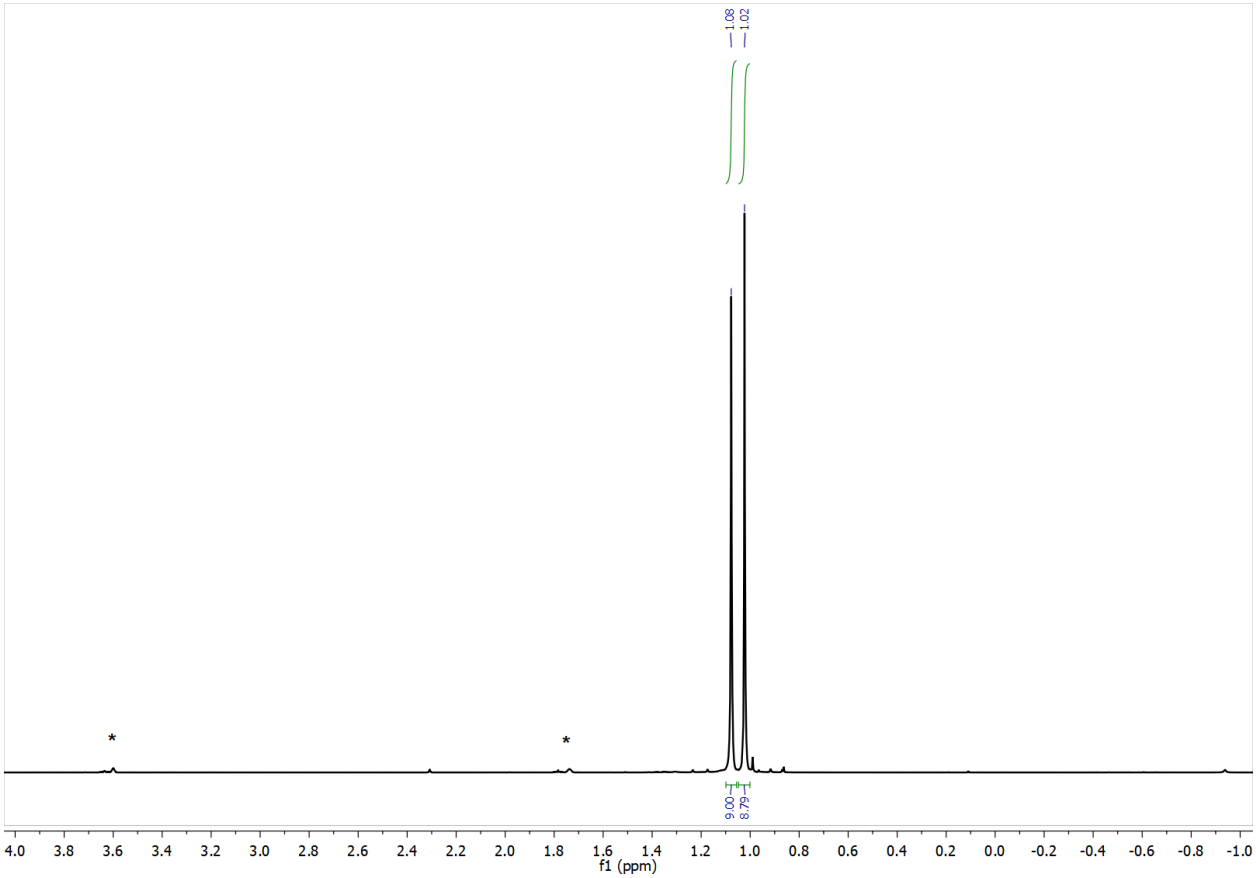

Figure S12. ^{1}H NMR (400 MHz, THF-d_8) spectrum of the equimolar mixture between **2** and **Me$_2$Zn**. * - THF-d_8.

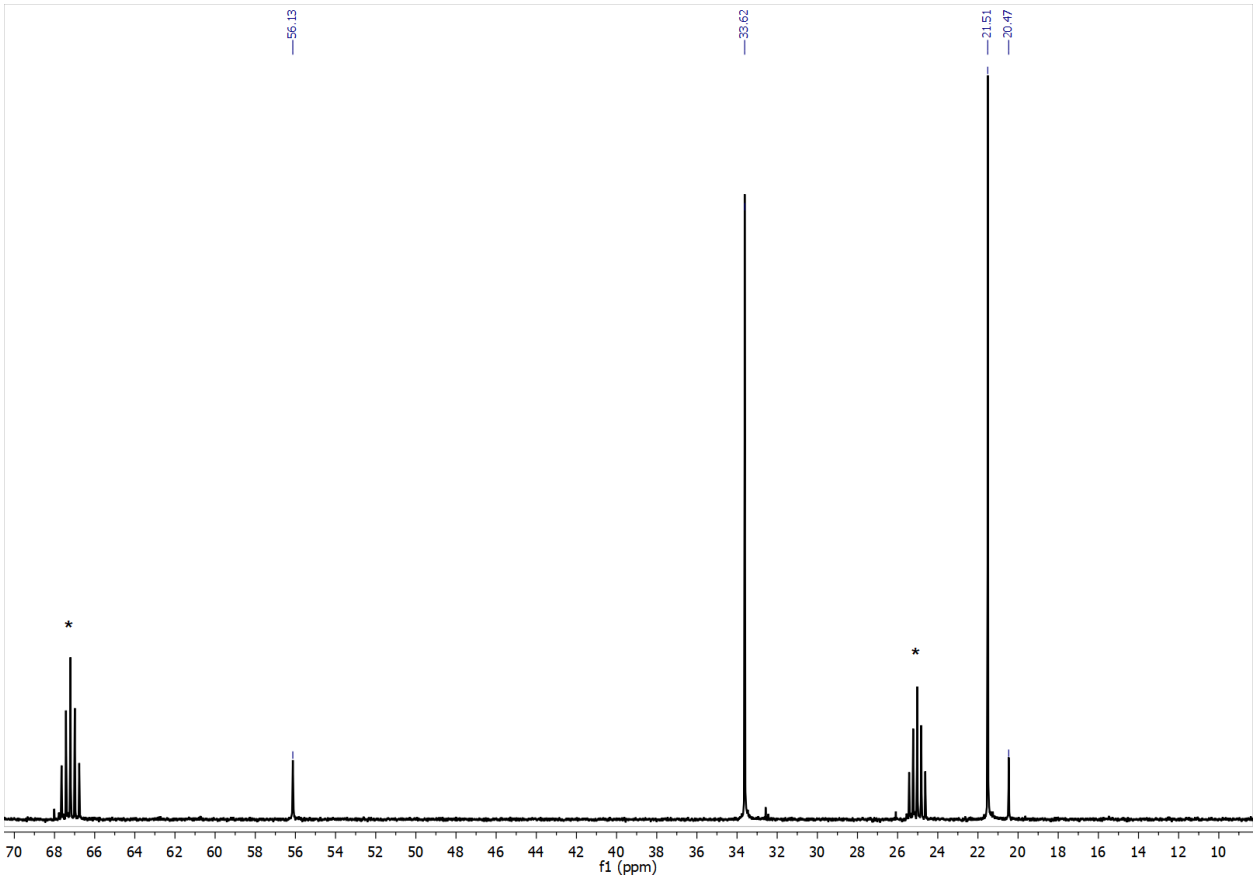

Figure S13. ^{13}C NMR (101 MHz, THF-d_8) spectrum of the equimolar mixture between **2** and **Me_2Zn**. * - THF-d_8.

II. Diffusivity measurement

The DOSY spectra were acquired on Bruker AVANCE II 300 MHz spectrometer at 298 K. Pulsed field gradient double stimulated echo convection-compensated (PFGSTE) sequence with total of 16 diffusion encoding bipolar gradients (ranging from 3 to 48 G/cm, smoothed-square shaped, equal steps in gradient squared) was used and the total width of the gradient pulse was optimized to achieve attenuation of about 90% of the initial intensity of the signals. Overall, the key acquisition parameters were as follows: total length of gradient encoding pulses gradient - 2ms, diffusion delay - 150ms, gradient recovery delay - 0.1ms, relaxation delay - 2.8s. Steady-state scans in number of 4 were performed prior to acquisition of the data. Raw data was processed with powerful DOSY Toolbox which is extensively described in its author's paper.[i] Samples were dissolved in dry and degassed THF-d_8 at concentration *ca.* 15mM. The molecular masses of analyzed compounds were estimated utilizing an external calibration curve (ECC) approach with normalized diffusion coefficients, with 9-methylanthracene (9-MeA; MW = 192) as an internal reference.[ii,iii] Moreover, we have applied the van-der-Waals radii-based correction in order to account for the underestimation of MW due to the presence of heavy atoms, according to the literature methods.[iv]

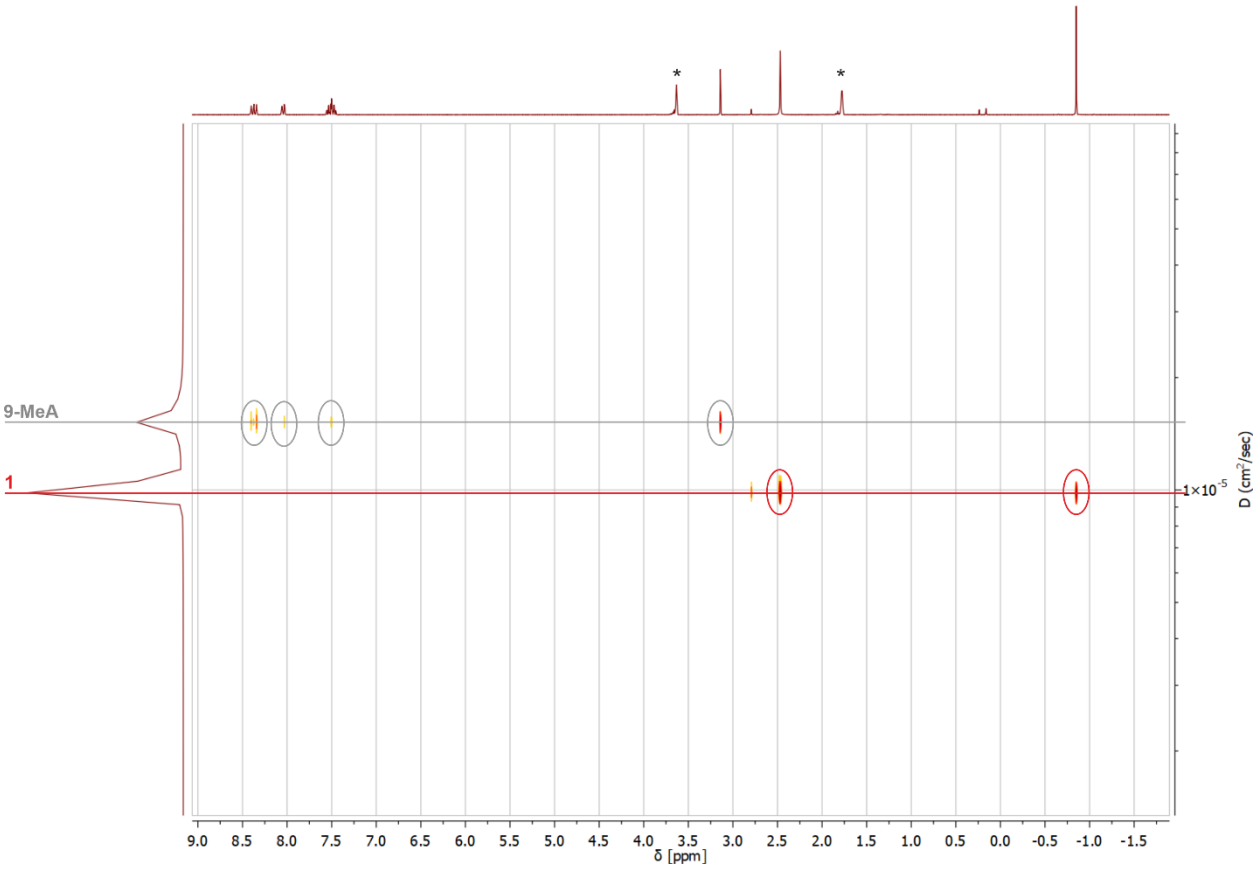

Figure S14. 2D DOSY-NMR spectrum of **1** in THF-d_8; * - residual solvent peaks.

Table S1. Diffusion coefficient of **1** and its estimated molecular weight.

D_{av} (9-MeA)·10^9 m^2/s	1.567
D_{av} (**1**)·10^9 m^2/s	1.012
MW_{calc} ({[$(MeSO_2)ZnMe$](THF-d_8)}/ Da	239.7
MW_{est} (**1**)/ Da	519
n	**2.2**

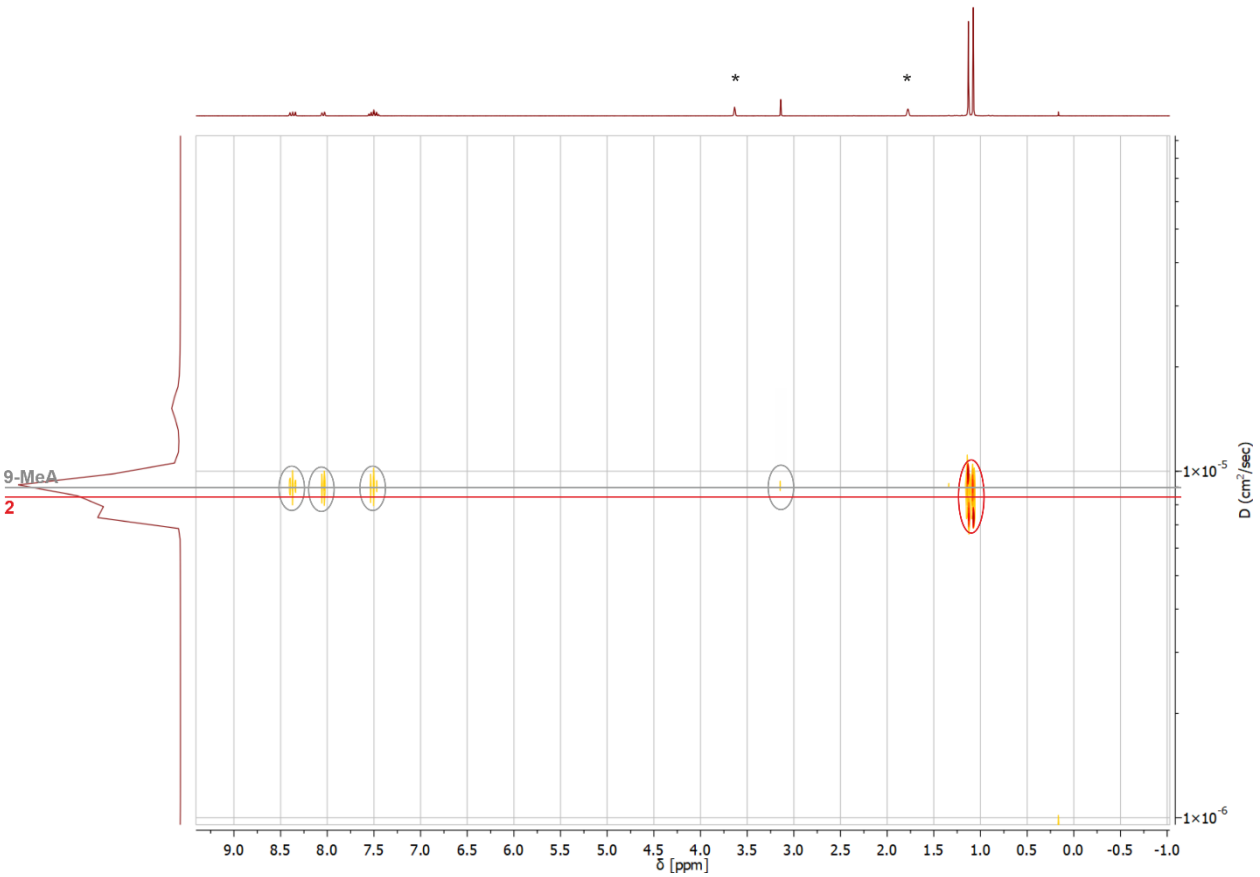

Figure S15. 2D DOSY-NMR spectrum of **2** in THF-d_8.

Table S2. Diffusion coefficient of **2** and its estimated molecular weight.

D_{av} (9-MeA)·10^9 m^2/s	1.577
D_{av} (**2**)·10^9 m^2/s	0.865
MW_{calc} ({[(*t*BuSO$_2$)Zn*t*Bu](THF-d_8)})/ Da	323.8
MW_{est} (**2**)/ Da	610
n	**1.9**

Figure S16. 2D DOSY-NMR spectrum of **3** in THF-d_8.

Table S3. Diffusion coefficient of **3** and its estimated molecular weight.

D_{av} (9-MeA)·10^9 m^2/s	1.567
D_{av} (**3**)·10^9 m^2/s	0.628
MW_{calc} ({[(PhSO$_2$)ZnPh](THF-d_8)})/ Da	363.8
MW_{est} (**3**)/ Da	821
n	**2.25**
D_{av} (**THF**)·10^9 m^2/s	2.090
MW_{calc} (**THF**)/ Da	72
MW_{est} (**THF**)/ Da	85

III. X-ray structure determination

Crystal data for 1

Table S4. Crystal data and structure refinement for **1**.

Empirical formula	$C_2H_6O_2SZn$	
Formula weight	159.50	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 4.5135(8) Å	a= 89.141(12)°.
	b = 7.7984(11) Å	b= 80.887(14)°.
	c = 7.8400(13) Å	g = 84.090(13)°.
Volume	271.02(8) $Å^3$	
Z	2	
Density (calculated)	1.954 Mg/m^3	
Absorption coefficient	4.785 mm^{-1}	
F(000)	160	
Crystal size	0.18 x 0.11 x 0.05 mm^3	
Theta range for data collection	2.626 to 26.500°.	
Index ranges	-5<=h<=5, -8<=k<=9, -9<=l<=9	
Reflections collected	2895	
Independent reflections	1117 [R(int) = 0.0810]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.787 and 0.537	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1117 / 0 / 57	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0632, wR2 = 0.1609	
R indices (all data)	R1 = 0.0701, wR2 = 0.1688	
Largest diff. peak and hole	1.568 and -1.647 e.$Å^{-3}$	

This compound crystallizes as twins. Component 2 rotated by 3.1089\% around [-0.20 -0.98 -0.08] (reciprocal) or [-0.39 -0.92 -0.02] (direct).

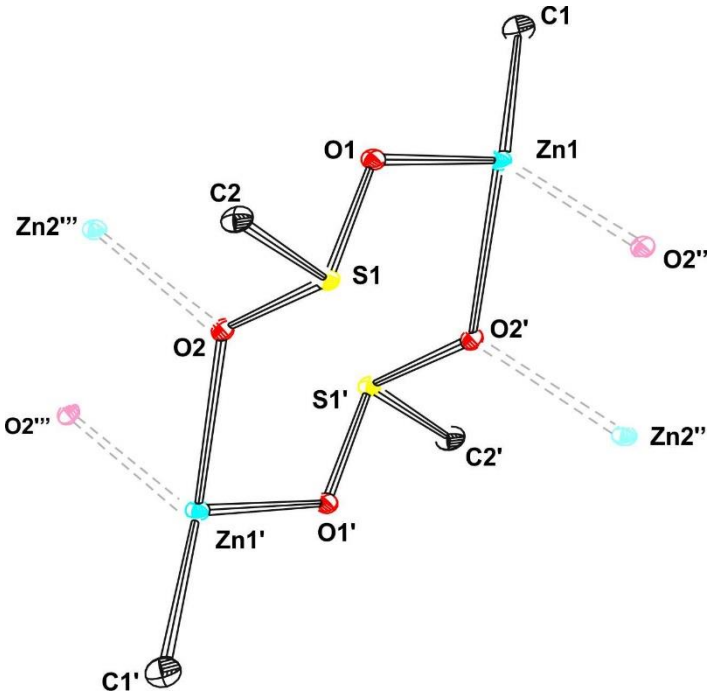

Figure S17. Molecular structure of **1** with thermal ellipsoids set at 40% probability**.** Hydrogen atoms have been omitted for clarity. Symmetry transformations used to generate equivalent atoms: (*x+1,y,z*); (*-x+1,-y+1,-z+1*); (3 x-1,y,z)

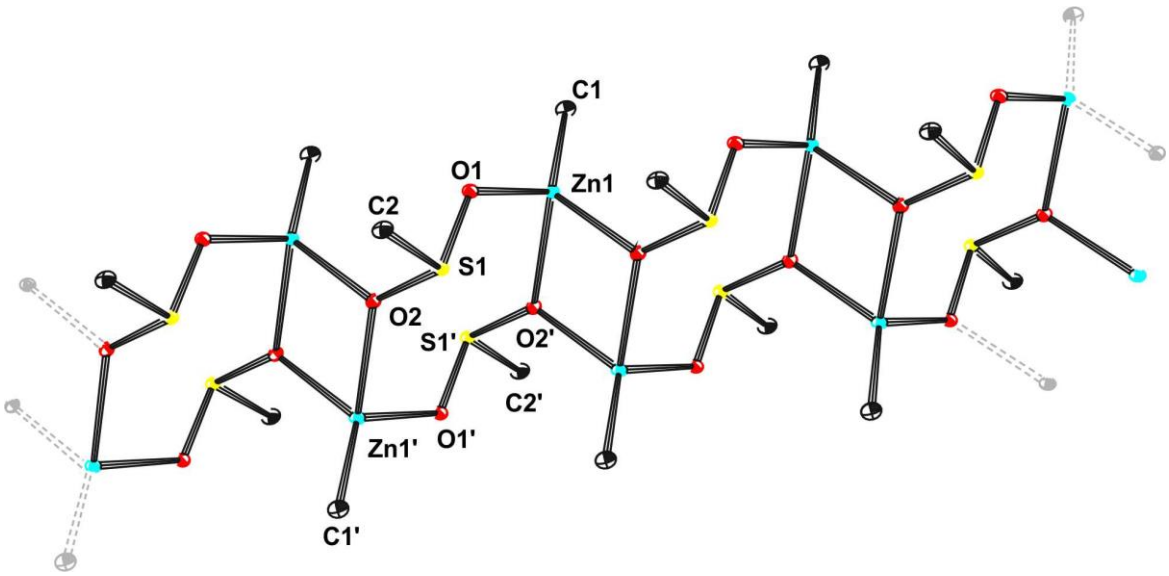

Figure S18. Chain structure of **1**.

Table S5. Selected intermolecular bond lengths [Å] and angles [°] for **1**.

Zn1 – O1	1.998(4)	O1 – Zn1 – C1	124.8(2)
Zn1 – O2’	2.096(4)	O1 – Zn1 – O2’	96.44(15)
Zn1 – O2’’	2.075(4)	O1 – Zn1 – O2’’	95.98(16)
Zn1 – C1	1.942(6)	O1 – S1 – O2	106.9(2)
S1 – O1	1.517(4)	O1 – S1 – C2	100.5(2)
S1 – O2	1.551(4)	O2 – S1 – C2	101.3(3)

Crystal data for 2

Table S6. Crystal data and structure refinement for **2**.

Empirical formula	$C_{32}H_{72}O_8S_4Zn_4$	
Formula weight	974.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.9492(3) Å	a= 86.157(3)°.
	b = 12.8183(7) Å	b= 78.812(2)°.
	c = 16.1223(5) Å	g = 75.515(3)°.
Volume	2345.05(16) $Å^3$	
Z	2	
Density (calculated)	1.380 Mg/m^3	
Absorption coefficient	2.238 mm^{-1}	
F(000)	1024	
Crystal size	0.24 x 0.17 x 0.08 mm^3	
Theta range for data collection	2.390 to 26.997°.	
Index ranges	-15<=h<=15, -16<=k<=16, -17<=l<=20	
Reflections collected	18888	
Independent reflections	10221 [R(int) = 0.0340]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10221 / 0 / 458	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.0646	
R indices (all data)	R1 = 0.0611, wR2 = 0.0720	
Largest diff. peak and hole	0.795 and -0.441 $e.Å^{-3}$	

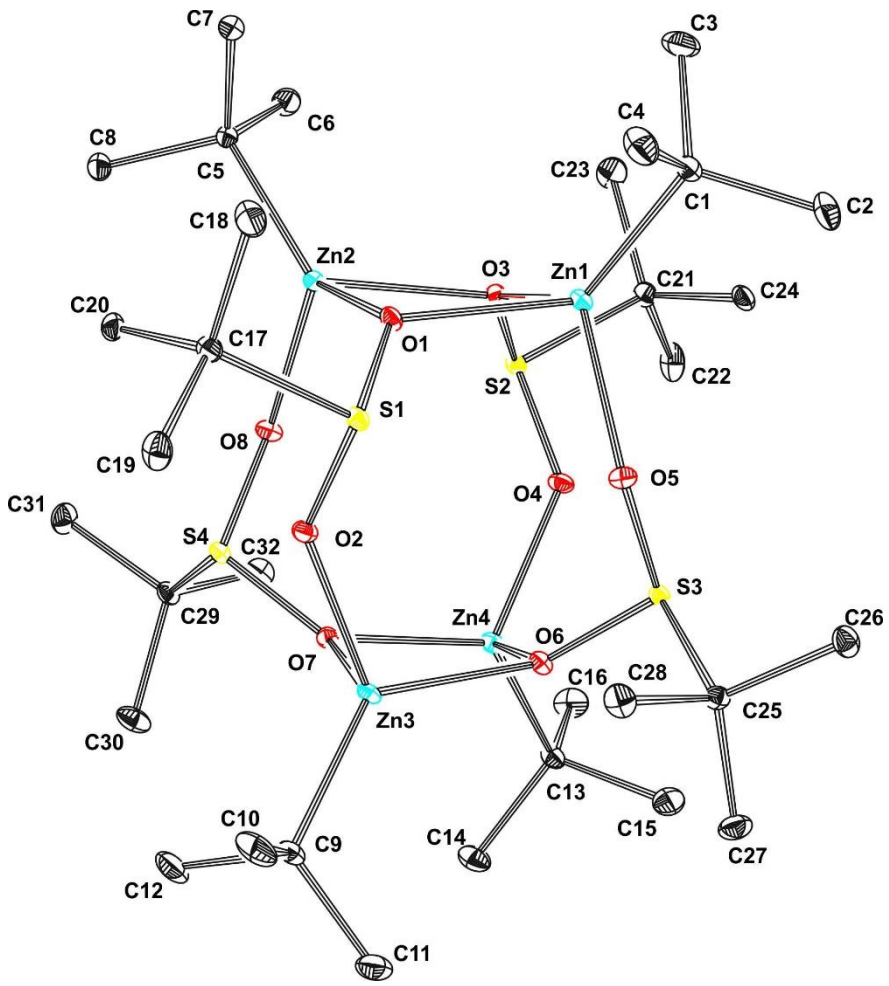

Figure S19. Molecular structure of **2** with thermal ellipsoids set at 34% probability**.** Hydrogen atoms have been omitted for clarity.

Table S7. Selected bond lengths [Å] and angles [°] for **2.**

Zn1 – C1	1.993(3)	C1 – Zn1 – O1	119.06(10)
Zn1 – O1	2.121(2)	C1 – Zn1– O3	129.44(10)
Zn1 – O3	2.074(2)	C1 – Zn1 – O5	114.55(11)
Zn1 – O5	2.0181(17)	O1 – Zn1– O3	78.64(8)
Zn2 – C5	1.993(3)	O1 – Zn1 – O5	92.89(8)
Zn2 – O1	2.066(2)	O3 – Zn1 – O5	110.87(7)
Zn2 – O3	2.107(2)	C5 – Zn2 – O1	129.46(10)
Zn2 – O8	2.0102(19)	C5 – Zn2 – O3	117.60(10)
Zn3– C9	1.990(3)	C5 – Zn2 – O8	114.74(11)
Zn3 – O2	2.0049(17)	O1 – Zn2 – O3	78.64(8)
Zn3 – O6	2.060(2)	O1 – Zn2 – O8	110.73(7)
Zn3 – O7	2.1170(18)	O3 – Zn2 – O8	93.90(8)
Zn4 – C13	1.991(3)	C9 – Zn3 – O2	116.90(10)
Zn4 – O4	2.0054(18)	C9 – Zn3 – O6	129.86(10)
Zn4 – O6	2.1164(19)	C9 – Zn3 – O7	117.97(11)
Zn4 – O7	2.068(2)	O2 – Zn3 – O6	108.48(8)
S1 – C17	1.830(3)	O2 – Zn3 – O7	91.85(7)
S1 – O1	1.5543(18)	O6 – Zn3 – O7	79.08(8)
S1 – O2	1.510(2)	C13 – Zn4 – O4	116.85(10)
S2 – C21	1.831(3)	C13 – Zn4 – O6	117.41(10)
S2 – O3	1.5552(19)	C13 – Zn4 – O7	128.59(11)
S2 – O4	1.5128(18)	O4 – Zn4 – O6	92.06(7)
S3 – C25	1.836(3)	O4 – Zn4 – O7	110.25(7)
S3 – O5	1.5119(18)	O6 – Zn4 – O7	78.94(8)
S3 – O6	1.548(2)	C17 – S1 – O1	101.78(12)
S4 – C29	1.831(3)	C17 – S1 – O2	101.58(13)
S4 – O7	1.551(2)	O1 – S1 – O2	107.10(11)
S4 – O8	1.5154(18)	C21 – S2 – O3	101.77(13)
		C21 – S2 – O4	101.72(13)
		O3 – S2 – O4	107.14(10)
		C25 – S3 – O5	102.15(12)
		C25 – S3 – O6	101.51(12)
		O5 – S3 – O6	108.24(12)
		C29 – S4 – O7	101.85(12)
		C29 – S4 – O8	102.11(12)
		O7 – S4 – O8	107.40(12)

Crystal data for 3

Table S8. Crystal data and structure refinement for **3**.

Empirical formula	$C_{32}H_{36}O_6S_2Zn_2$	
Formula weight	711.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.792(5) Å	α= 78.722(5)°.
	b = 9.326(5) Å	β= 74.655(5)°.
	c = 10.669(5) Å	γ = 67.772(5)°.
Volume	776.4(7) $Å^3$	
Z	1	
Density (calculated)	1.522 Mg/m^3	
Absorption coefficient	1.722 mm^{-1}	
F(000)	368	
Crystal size	0.21 x 0.16 x 0.07 mm^3	
Theta range for data collection	2.373 to 30.163°.	
Index ranges	-12<=h<=11, -12<=k<=12, -14<=l<=15	
Reflections collected	6161	
Independent reflections	3931 [R(int) = 0.0293]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.886 and 0.726	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3931 / 0 / 190	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0826	
R indices (all data)	R1 = 0.0449, wR2 = 0.0872	
Largest diff. peak and hole	0.652 and -0.495 e. $Å^{-3}$	

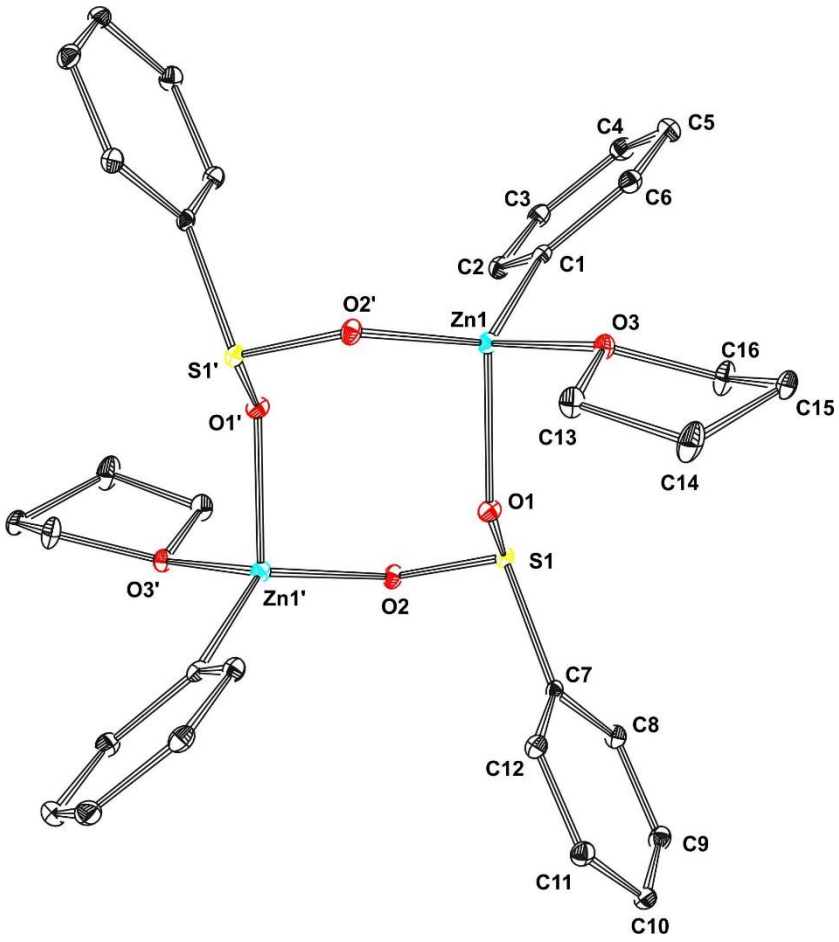

Figure. S20. Molecular structure of **3** with thermal ellipsoids set at 40% probability**.** Hydrogen atoms have been omitted for clarity. Symmetry transformations used to generate equivalent atoms: (*-x,-y+1,-z+2*)

Table S9. Selected bond lengths [Å] and angles [°] for **3.**

Zn1 – C1	1.960(2)	C1 – Zn1 – O1	118.20(8)
Zn1 – O1	2.0264(16)	C1 – Zn1 – O2’	133.46(8)
Zn1 – O3	2.0881(17)	C1 – Zn1 – O3	112.11(8)
Zn1 – O2’	1.9869(17)	O1 – Zn1 – O2’	97.77(7)
S1 – C7	1.788(2)	O1 – Zn1 – O3	92.88(7)
S1 – O1	1.5273(17)	C7 – S1 – O1	100.93(10)
S1 – O2	1.5281(18)	C7 – S1– O2	103.94(9)
		O1 – S1 – O2	107.37(9)
		S1 – O1 – Zn1	120.52(10)
		S1 – O2 – Zn1’	119.74(9)

III. Theoretical section

Coordinates of the calculated molecular systems

1. Me_2Zn/SO_2

Zn	-1.29130800	0.16562900	0.00016900
C	-2.01222400	-1.64583500	0.00124700
H	-3.10654100	-1.64681600	0.00588600
H	-1.67680900	-2.19276000	-0.88570400
S	2.29682700	-0.11423300	-0.00136000
O	1.60358500	-0.40075900	-1.24175900
O	1.60957800	-0.39735700	1.24311800
C	-0.62167200	2.00501900	-0.00062100
H	-0.00861400	2.19552600	0.88657400
H	-0.01085500	2.19551100	-0.88936600
H	-1.43979700	2.73174700	0.00042100
H	-1.66931600	-2.19452000	0.88424100

2. $Me_2Zn\text{--}SO_2$*

Zn	-0.94452000	-0.00229200	-0.02893400
C	-2.86143700	-0.24567400	0.23190300
H	-3.04776100	-1.15745900	0.80286400
H	-3.28642700	0.60637000	0.76664200
S	1.66835600	-0.23587000	-0.35902100
O	2.52429200	-0.03249800	0.80344100
O	0.60865400	-1.31685100	-0.13564200
C	0.37286400	1.76213200	-0.12119800
H	0.39794200	1.97815800	0.95167400
H	1.27474600	2.17549800	-0.56934000
H	-0.47179000	2.26809400	-0.60773400
H	-3.35691800	-0.33195000	-0.73836100

3. $(MeSO_2)ZnMe$

Zn	-1.02223400	-0.00797400	-0.00814600
C	-2.93418400	0.01613100	0.34482500
H	-3.25768700	1.02119100	0.62519300
H	-3.48740000	-0.29193400	-0.54598400
S	1.58748700	0.00010100	-0.51449300
O	0.61048400	1.20092900	-0.33193200
O	0.61214100	-1.20197500	-0.31564400
C	2.50167700	0.00956500	1.05374600
H	3.11993500	-0.88877400	1.09113300
H	3.12162800	0.90717100	1.07901500
H	1.76481800	0.01586600	1.85855700
H	-3.18002600	-0.67170500	1.15752800

4. $^tBu_2Zn/SO_2$

Zn	-0.24793000	-0.61336200	-0.01597700
C	-2.20665700	-0.24406400	-0.02142400
S	1.14543500	2.57578000	0.16347900

O	0.47234500	1.71866500	1.12838500
O	0.73193600	2.47588800	-1.22147500
C	1.62391400	-1.33862600	-0.02804000
C	1.59833200	-2.59414300	-0.91890200
H	1.35506300	-2.35674600	-1.95984900
H	2.58419200	-3.08659100	-0.91992100
H	0.87085500	-3.33375100	-0.56833100
C	-2.51638100	1.06015800	-0.76824600
H	-2.18423100	1.03160000	-1.81084800
H	-3.60235900	1.24836700	-0.77594900
H	-2.04233100	1.92477500	-0.29502500
C	2.00184000	-1.74151000	1.40527700
H	2.99576200	-2.21781000	1.42511400
H	2.04158700	-0.87743500	2.07624000
H	1.29470700	-2.46057400	1.83256600
C	-2.69319300	-0.11730900	1.43047800
H	-3.77610400	0.08708400	1.45769400
H	-2.52604800	-1.03543300	2.00422000
H	-2.19525700	0.70175800	1.95908600
C	2.67794000	-0.37358400	-0.57152400
H	3.67028500	-0.85231000	-0.58693800
H	2.45941100	-0.04074500	-1.59045100
H	2.79082700	0.51730100	0.05982900
C	-2.95060500	-1.40293100	-0.70367300
H	-4.03795100	-1.22276100	-0.69444500
H	-2.65352500	-1.52367400	-1.75083100
H	-2.77931300	-2.35903500	-0.19746500

5. $^{t}Bu_2Zn$--SO_2*

Zn	-0.40137400	-0.25040200	-0.16399800
C	-2.36573400	-0.01529700	0.09251800
S	1.91482300	-1.26337300	-0.33883800
O	2.51231600	-1.46704100	0.98782200
O	0.57217700	-2.00453800	-0.50073700
C	1.36359700	1.26611200	-0.02227100
C	0.48719300	2.25222000	-0.81057100
H	0.46113800	2.01858600	-1.87922900
H	-0.54049500	2.31292000	-0.44681600
H	0.91885600	3.26178500	-0.71898300
C	2.80156400	1.42246000	-0.49876500
H	3.50504000	0.80481900	0.06266400
H	2.91192800	1.19588200	-1.56308000
H	3.10578200	2.46919800	-0.35497200
C	-2.98379100	0.51448700	-1.20855200
H	-4.07331100	0.61880300	-1.08922500
H	-2.59451300	1.49935800	-1.48387800
H	-2.81503400	-0.16271000	-2.05143600
C	-2.65725900	0.96048900	1.23779700
H	-3.74484700	1.06691900	1.37053000
H	-2.24778000	0.61273500	2.19091500
H	-2.25921600	1.96163400	1.04612700

C	1.26340700	1.42956500	1.48587000
H	0.22896300	1.49094100	1.83742300
H	1.76176100	0.60552400	2.00752100
H	1.76671600	2.35729300	1.79908900
C	-2.95700000	-1.39297500	0.42236100
H	-4.04815600	-1.31293200	0.54530500
H	-2.76822600	-2.12237800	-0.37015100
H	-2.55233600	-1.80207600	1.35254100

6. (^{t}BuSO$_2$)Zn^{t}Bu

Zn	0.91662600	-0.31419100	0.01647200
C	2.81288900	0.26283900	0.00417100
S	-1.63732900	-1.04983500	-0.04680400
O	-0.68018600	-0.85655100	1.17382600
O	-0.66472700	-0.75471900	-1.23057600
C	-2.71940800	0.47540200	0.01319600
C	-1.84181500	1.71952300	0.07429300
H	-1.22072000	1.72046200	0.97293000
H	-1.20148400	1.79467700	-0.80759300
H	-2.47692900	2.60981400	0.10457300
C	2.94340700	1.53853400	-0.84203200
H	2.35555800	2.36672000	-0.43347800
H	3.99407400	1.86792800	-0.86841400
H	2.62642000	1.38091900	-1.87759800
C	3.28316300	0.54992200	1.43717100
H	3.21906000	-0.33524200	2.07728600
H	4.33564300	0.87447200	1.43160400
H	2.70062400	1.34647000	1.91052100
C	-3.56237800	0.43108000	-1.26325600
H	-4.13874400	-0.49658300	-1.33041600
H	-4.27174900	1.26414700	-1.26205700
H	-2.93430600	0.51278700	-2.15249300
C	-3.58117900	0.31928100	1.26809800
H	-4.28959300	1.15073700	1.33115900
H	-4.15937600	-0.60933300	1.24364300
H	-2.96631000	0.31972500	2.17016400
C	3.68428700	-0.84375800	-0.60863200
H	3.39287800	-1.07635100	-1.63749200
H	4.73793900	-0.52356700	-0.63206300
H	3.64100900	-1.77146000	-0.02965700

7. Ph$_2$Zn/SO$_2$

Zn	-0.51942600	-0.67374800	0.07201200
S	1.95022200	1.96726400	-0.40469400
O	0.49430500	2.01898400	-0.34109300
O	2.67899300	2.87266600	0.46174100
C	-2.41406900	-0.31200200	0.04308000
C	-3.36803500	-1.33023400	0.22227300
C	-2.89293500	0.99549300	-0.15891600
C	-4.73718800	-1.05968300	0.20050900

H	-3.04798300	-2.35555200	0.38283500
C	-4.26061100	1.27332000	-0.18154900
H	-2.19240400	1.81184400	-0.29946400
C	-5.18610700	0.24525700	-0.00206200
H	-5.45083000	-1.86425900	0.34141600
H	-4.60293600	2.29053500	-0.33834100
H	-6.24891200	0.45919700	-0.01915200
C	3.42855500	-1.78349200	-1.04182900
C	2.03930000	-1.65041700	-1.00046100
C	1.38589700	-1.06343500	0.09743300
C	2.19850600	-0.62970400	1.16589500
C	3.59006100	-0.76300500	1.13550500
C	4.20846000	-1.33525100	0.02561800
H	3.90320600	-2.23279100	-1.90738700
H	1.46311900	-2.00298300	-1.85054600
H	1.74601100	-0.17629600	2.04325100
H	4.18524700	-0.41422000	1.97190300
H	5.28732800	-1.43352200	-0.00794300

8. Ph_2Zn--SO_2*

Zn	-0.29207100	0.22254900	-0.10350800
S	1.70151600	2.06268700	-0.20540900
O	0.24524300	2.23200900	-0.59317000
O	1.97359500	2.44137200	1.18067100
C	-2.16855300	-0.22096700	0.00530900
C	-2.61594600	-1.52811300	0.25642800
C	-3.13253100	0.78539600	-0.17026500
C	-3.97872200	-1.82207200	0.32926600
H	-1.90133600	-2.33255900	0.39866300
C	-4.49620600	0.49587400	-0.09803400
H	-2.82109900	1.80649100	-0.36402800
C	-4.92099700	-0.80906300	0.15183900
H	-4.30335700	-2.83836800	0.52440300
H	-5.22452500	1.28757400	-0.23577300
H	-5.97983800	-1.03517400	0.20864600
C	3.06741800	-1.94013000	-1.23152200
C	2.15364100	-0.89033200	-1.25930400
C	1.73621600	-0.25552600	-0.06873700
C	2.32262600	-0.67037700	1.14267800
C	3.23273000	-1.72248000	1.17667400
C	3.60314700	-2.35941700	-0.01115500
H	3.36922500	-2.42482700	-2.15292700
H	1.75930800	-0.56025000	-2.21643400
H	2.07924000	-0.14228300	2.05940500
H	3.66771600	-2.03606400	2.11870300
H	4.32490100	-3.16779900	0.01204700

9. $(PhSO_2)ZnPh$

Zn	-0.82077500	-0.64417400	-0.01431400
S	1.64757000	-1.51345700	-0.41743500

O	0.64331000	-0.94776900	-1.45858700
O	0.76143600	-1.49528100	0.87793200
C	2.76996200	-0.12607300	-0.13374600
C	3.86350100	-0.33959200	0.70424500
C	2.54814700	1.10785000	-0.73778600
C	4.73755800	0.71394200	0.96248900
H	4.02392600	-1.31194700	1.15701300
C	3.42874500	2.15702200	-0.47539700
H	1.70485800	1.23103700	-1.40560500
C	4.51857600	1.96127500	0.37395200
H	5.58687900	0.56243500	1.61795900
H	3.26732200	3.12324200	-0.93867200
H	5.20210000	2.77840300	0.57241100
C	-2.61887000	0.04361200	0.09369500
C	-3.28241400	0.49071400	-1.06199800
C	-3.30933300	0.12481400	1.31517100
C	-4.58159300	0.99771600	-1.00214600
H	-2.78675200	0.44521100	-2.02650700
C	-4.60847200	0.63095900	1.38132900
H	-2.83556500	-0.20904500	2.23268200
C	-5.24739200	1.06865300	0.22125400
H	-5.07231600	1.33538500	-1.90844300
H	-5.12021200	0.68290600	2.33608800
H	-6.25655600	1.46193400	0.27031000

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