Ligand Exchange Processes in Zirconocene Dichloride- Trimethylaluminum Bimetallic Systems and Their Catalytic Properties in Reaction with Alkenes

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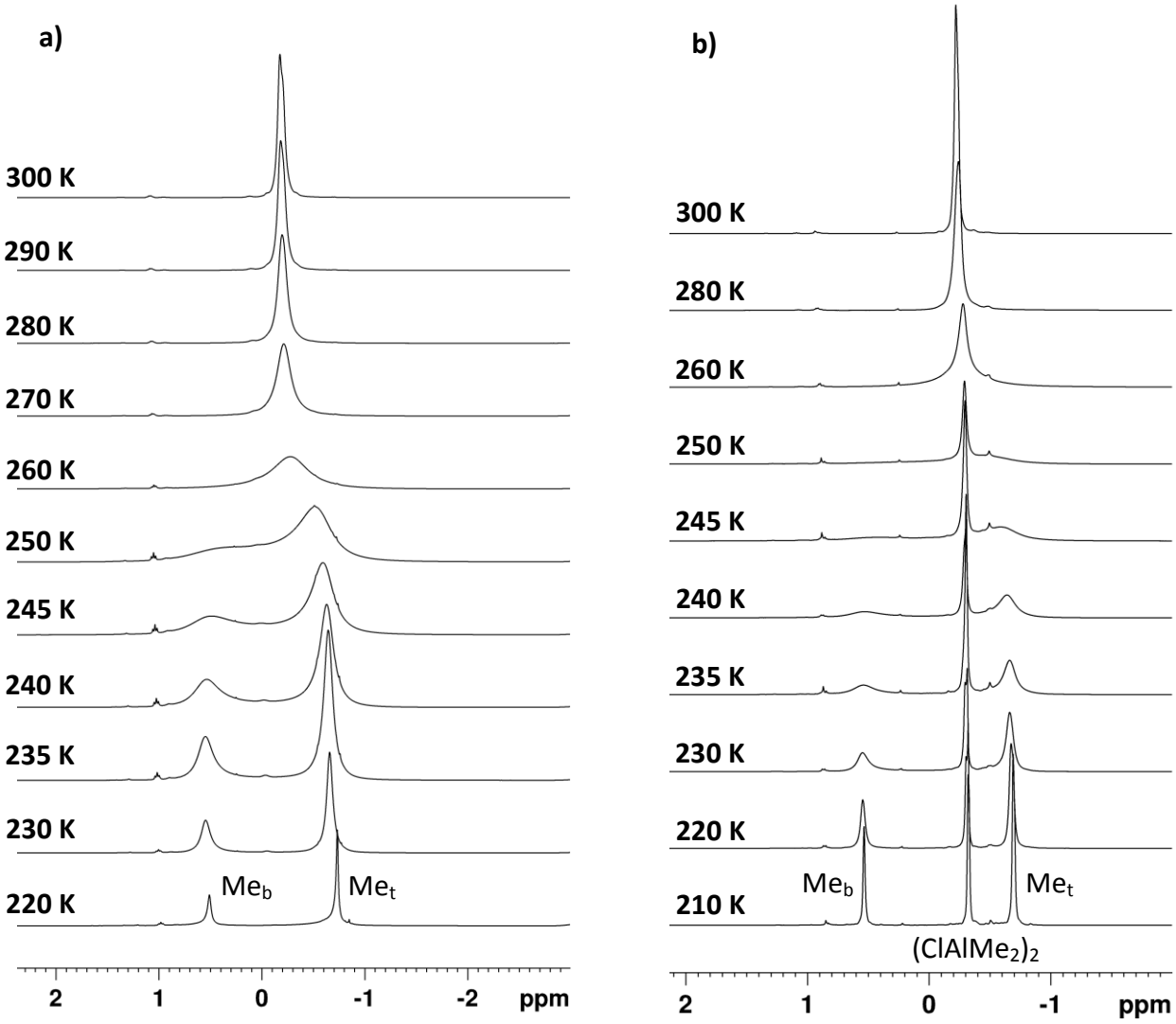
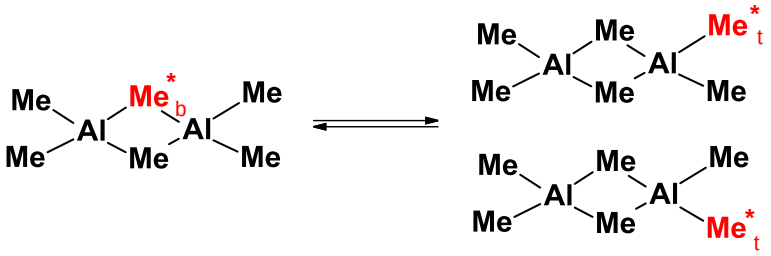
The procedure for the evaluation of the exchange constants using the line- shape analysis.
The procedure is considered on the example of a solution of trimethylaluminum in CD_2Cl_2. Thus, the ^{1}H NMR spectra in the temperature range 220-300 K were recorded (Fig. S1).

Figure S1. VT NMR of $(AlMe_3)_2$:
(a) 6.2 M/l in CD_2Cl_2; (b) 2.5 M/l in CD_2Cl_2+ $(ClAlMe_2)_2$.



Line-shape analyses were carried out using Dynamic NMR module (version 1.1.2) implemented into the Bruker Topspin 3.2 program, which simulate 1D temperature dependent NMR spectra of coupled half spin nuclei, interactively set up and iteratively refine the model parameters to get the best fit of the measured and simulated 1D NMR spectra and to obtain the reaction speed parameters of exchange processes. The theory of the calculation, special features of the DNMR module (chemical exchange operators, fitting quality, etc.) and detailed procedure are described in the software manual “DNMR Lineshape Analysis” written by Dr. János Rohonczy, 2007.

Exchange of methyl group in dimer $(AlMe_3)_2$ can be represented as follows:



1) The spectrum to fit was selected and the DNMR module of the Topspin was opened. The LB parameter from the solvent line shape simulation was found. Further, we fix this parameter when calculating exchange constants.
2) The interval (-1.5 - 1.5 ppm) and the initial values of the chemical shifts δMe_b and δMe_t in the spectra obtained at low temperatures, where the exchange is slow, were set. Since there is no scalar coupling between the Me- groups, they were fixed in the program as singlets with 0.5 (Nuc 1, Me_b) and 1 (Nuc 2, Me_t) pseudo spins within one molecule (molecule 1). In order to more accurately determine the chemical shifts the spectrum simulation was performed at all other fixed parameters. Further, these chemical shifts do not change.
3) Then we set the initial value of the exchange constant between Nuc 1 and Nuc 2 and the iteration step. The process of a line shape calculation was started, where the exchange constant value and signal intensity were automatically iterated until a satisfactory agreement between the calculated and experimental lines is reached (overlap> 90%, Fig. S2).

Figure S2. Result of spectrum simulation:
6.2 M/l $(AlMe_3)_2$ in CD_2Cl_2 at 240 K, blue line- original spectrum, green line- simulated spectrum.

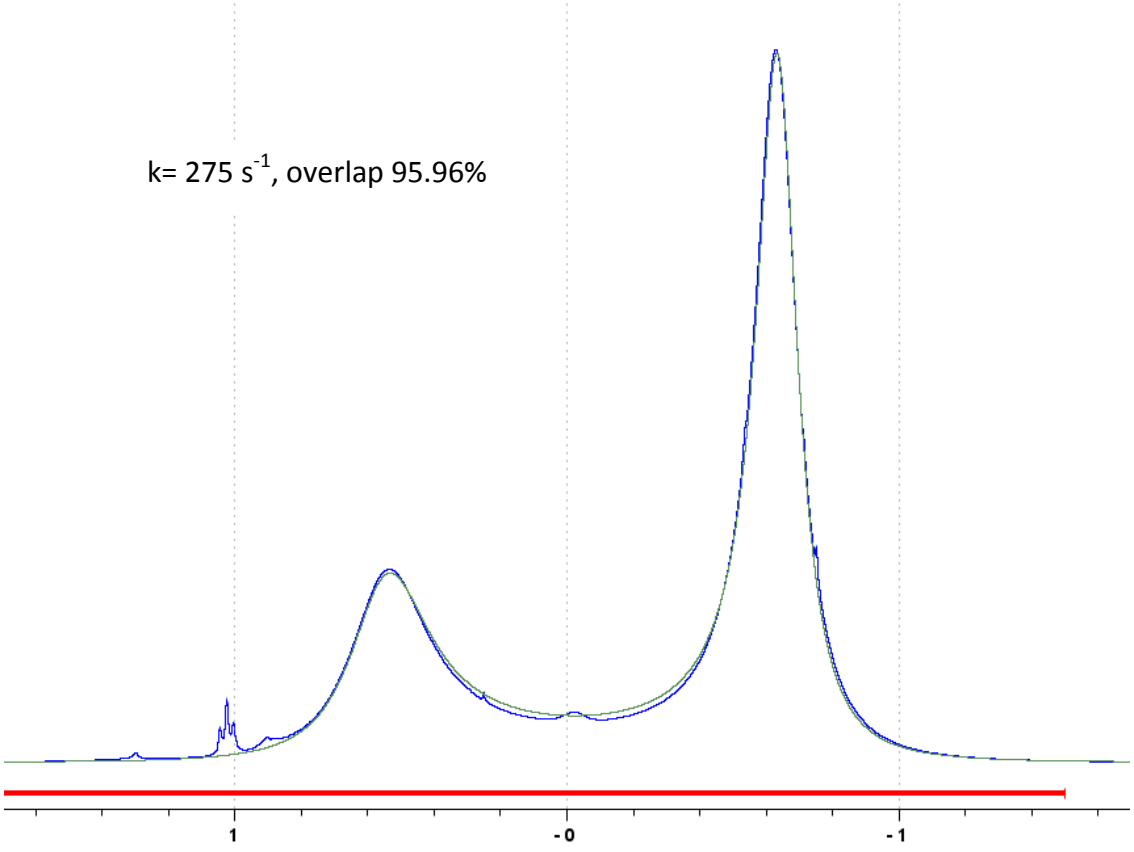
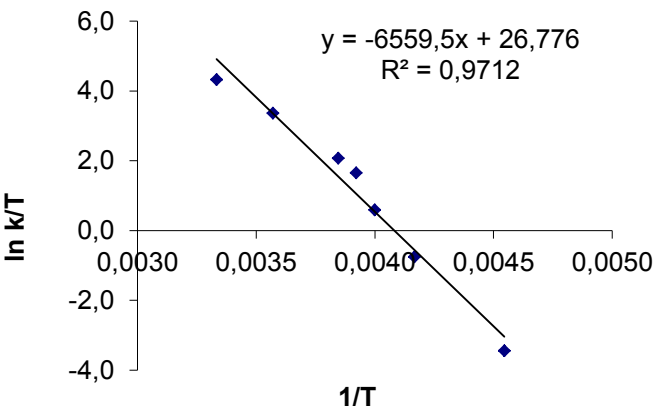
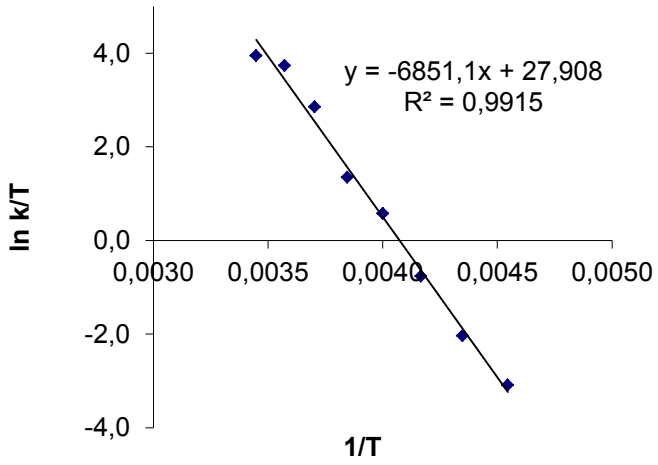
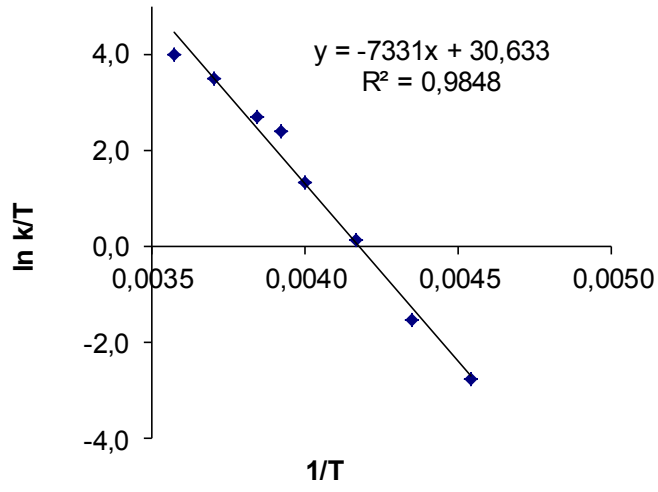
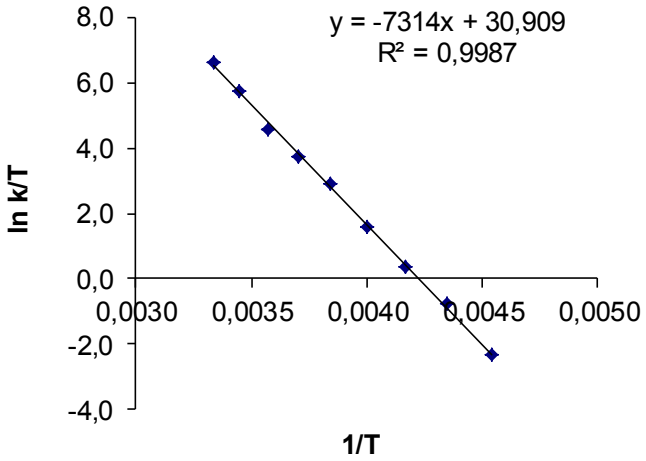


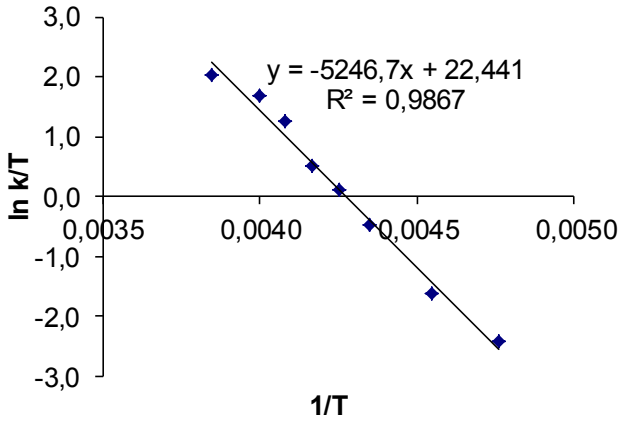
Table S1 Constants and plots of ln(k/T) vs 1/T for the methyl exchange in $(AlMe_3)_2$ obtained from line-shape analysis

Solvent	C, M/l	T, K	k, s^{-1}	
C_7D_8	4.9	220	7	
		240	113	
		250	451	
		255	1334	
		260	2059	
		280	8087	
		300	22730	
C_7D_8	0.3	220	10	
		230	30	
		240	112	
		250	444	
		260	1000	
		270	4667	
		280	11742	
		290	15000	
		300	22500	
CD_2Cl_2	6.2	220	14	
		230	50	
		240	275	
		250	955	
		255	2765	
		260	3786	
		270	8731	
		280	15005	
		290	19156	
		300	23182	

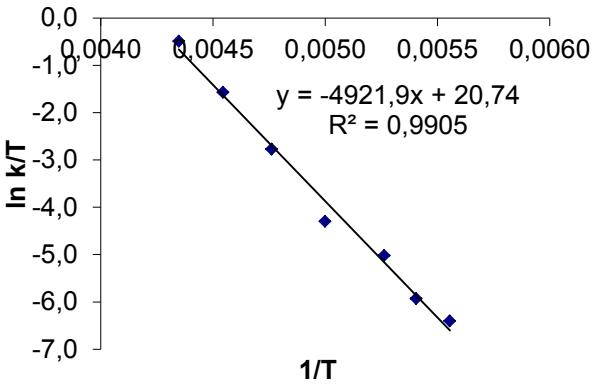
CD_2Cl_2	0.5	220	21
		230	105
		240	354
		250	1221
		260	4693
		270	11409
		280	27682
		290	90972
		300	230888



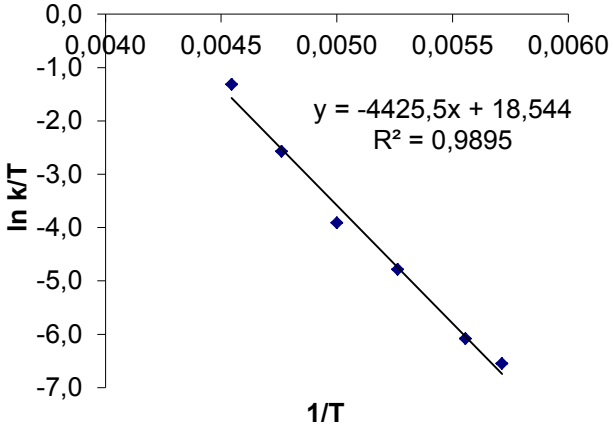
CD_2Cl_2 + $(ClAlMe_2)_2$	2.5 ($AlMe_3$) 1.1 ($ClAlMe_2$)	210	19
		220	44
		230	144
		235	263
		240	405
		245	858
		250	1349
		260	1975
		280	2021



CD_2Cl_2 + $Cp_2ZrMeCl$	0.4	180	0.3
		185	0.5
		190	1.3
		200	2.7
		210	13.2
		220	45.7
		230	140.8



C_7D_8 + $Cp_2ZrMeCl$	0.3	175	0.3
		180	0.4
		190	1.6
		200	4.0
		210	16.0
		220	59.0



The procedure for the evaluation of the constants of the methyl group exchange in $L_2ZrMeCl$ (5f, h, j-m) using 2D EXSY.

2D NMR EXSY (NOESY) spectra were recorded in the phase-sensitive mode using standard Bruker gradient pulse sequences with relaxation delay 1 s, 90º pulse - 8.0 μs, mixing time τ=0.01÷1 s. The mixing time was chosen in such a range that diagonal and cross- peaks were observed simultaneously. The areas of the diagonal and cross- peaks for the signals of the H^1 and H^3 atoms of the η^5- ligands in the 5–7 ppm region in the temperature range 230–310 K were determined. Despite the fact that this exchange is intermolecular, we considered it as a simple two-center exchange, without the participation of L_2ZrCl_2, the exchange with which for these complexes was not fixed (no corresponding cross- peaks were observed). Constants of the exchange were calculated by the formula[34]:

$$k = \frac{1}{\tau}\ln\frac{r+1}{r-1}, \quad \text{where} \quad r = \frac{I_{AA}+I_{BB}}{I_{AB}+I_{BA}}$$

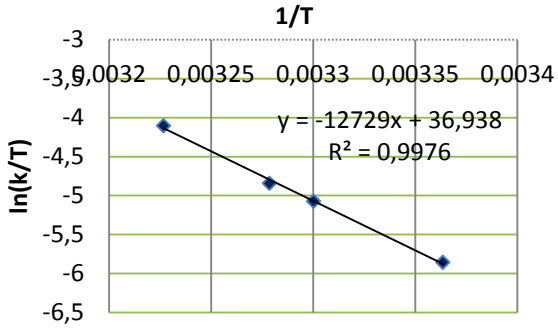
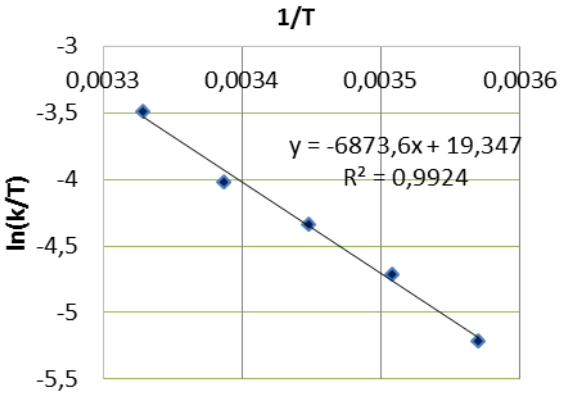
τ – mixing time, I_{AA}, I_{BB}- diagonal peak areas, I_{AB}, I_{BA}- cross-peak areas.

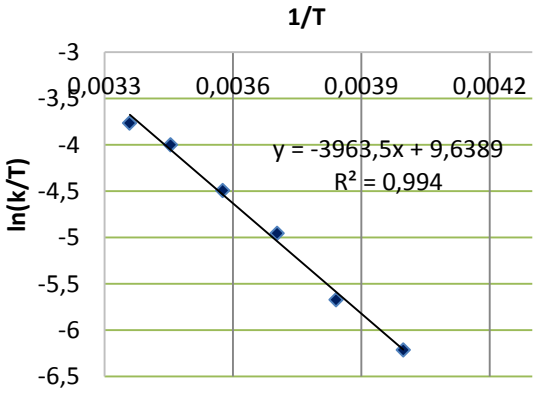
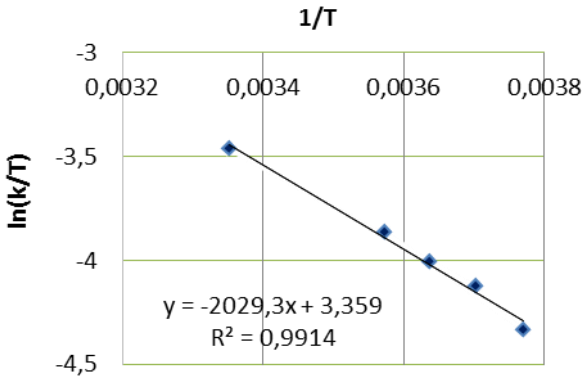
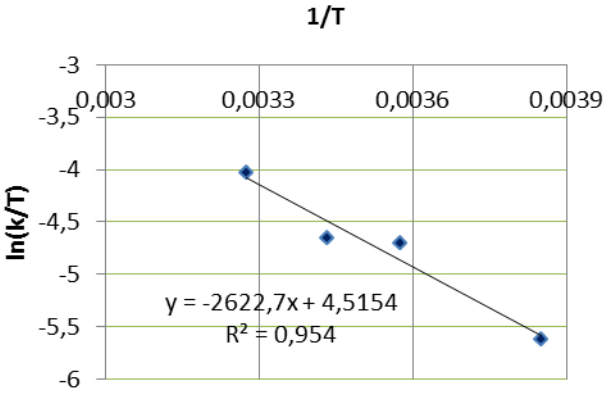
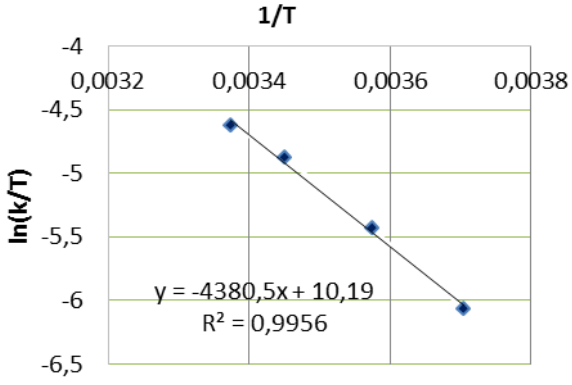
The values of $\Delta H^{\neq}$, $\Delta G^{\neq}$, $\Delta S^{\neq}$ were calculated according to the Eyring equation[11a]:

$$\mathbf{\ln(k/T) = -\Delta H^{\neq}/RT + \Delta S^{\neq}/R + \ln(k_b/h)},$$

where k_b – the Boltzmann constant, and h- the Planck constant.

Table S2 Constants and plots of ln(k/T) vs 1/T for the methyl group exchange in $L_2ZrMeCl$ (**5f, h, j-m**)

Complex	Solvent	T, K	k, s^{-1}	
5f	CD_2Cl_2	297.3	0.90	
		303.0	1.90	
		305.0	2.40	
		309.9	5.11	
5h	C_7D_8	280.1	1.52	
		285.0	2.54	
		290.0	3.78	
		295.2	5.45	
		300.4	9.17	

5j	CD_2Cl_2	250.1	0.50	
		260.3	0.90	
		270.0	1.90	
		279.6	3.13	
		289.5	5.30	
		297.7	6.90	
	C_7D_8	259.9	2.41	
		265.2	3.47	
		270.1	4.35	
		275.0	4.99	
		279.9	5.86	
		298.3	9.30	
5k	CD_2Cl_2	259.7	0.94	
		279.6	2.55	
		291.2	2.70	
		305.3	5.40	
	C_7D_8	270.0	0.63	
		279.8	1.22	
		289.9	2.20	
		296.5	2.90	

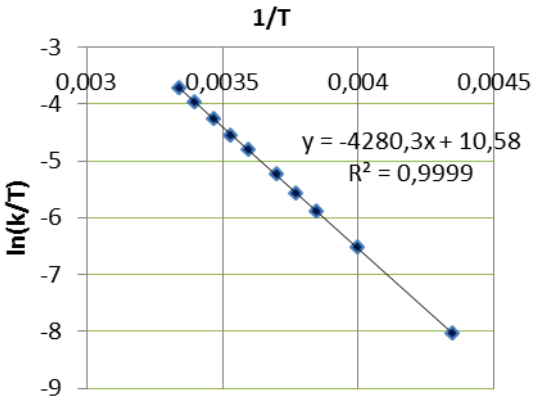
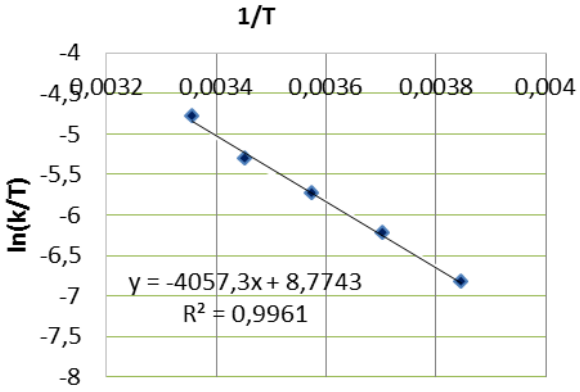
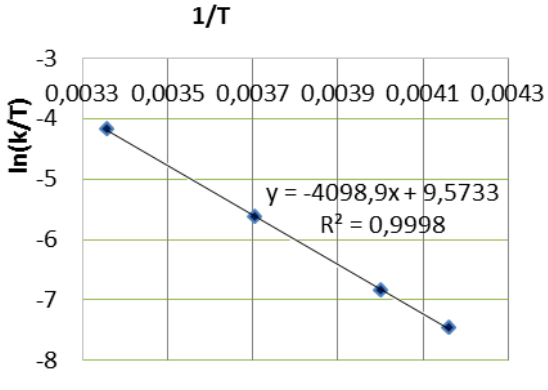
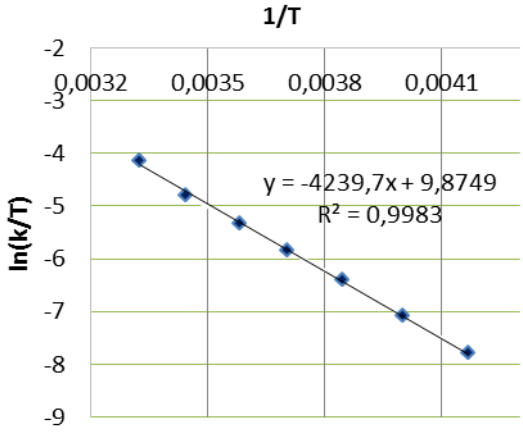
5l	CD_2Cl_2	230.0	0.07	
		250.2	0.37	
		259.9	0.71	
		265.1	1.00	
		270.1	1.44	
		278.0	2.28	
		283.2	2.99	
		288.1	4.03	
		294.1	5.50	
		299.4	7.20	
	C_7D_8	260	0.28	
		270	0.53	
		279.7	0.90	
		289.7	1.43	
		297.9	2.50	
5m	CD_2Cl_2	240.3	0.14	
		249.9	0.27	
		270	0.97	
		297.8	4.60	
	C_7D_8	239.9	0.10	
		250	0.21	
		260	0.43	
		270	0.78	
		279.3	1.35	
		290.3	2.37	
		300.7	4.80	

Figure S3. ^{1}H NMR of $Cp_2ZrMeCl$ in C_7D_8.

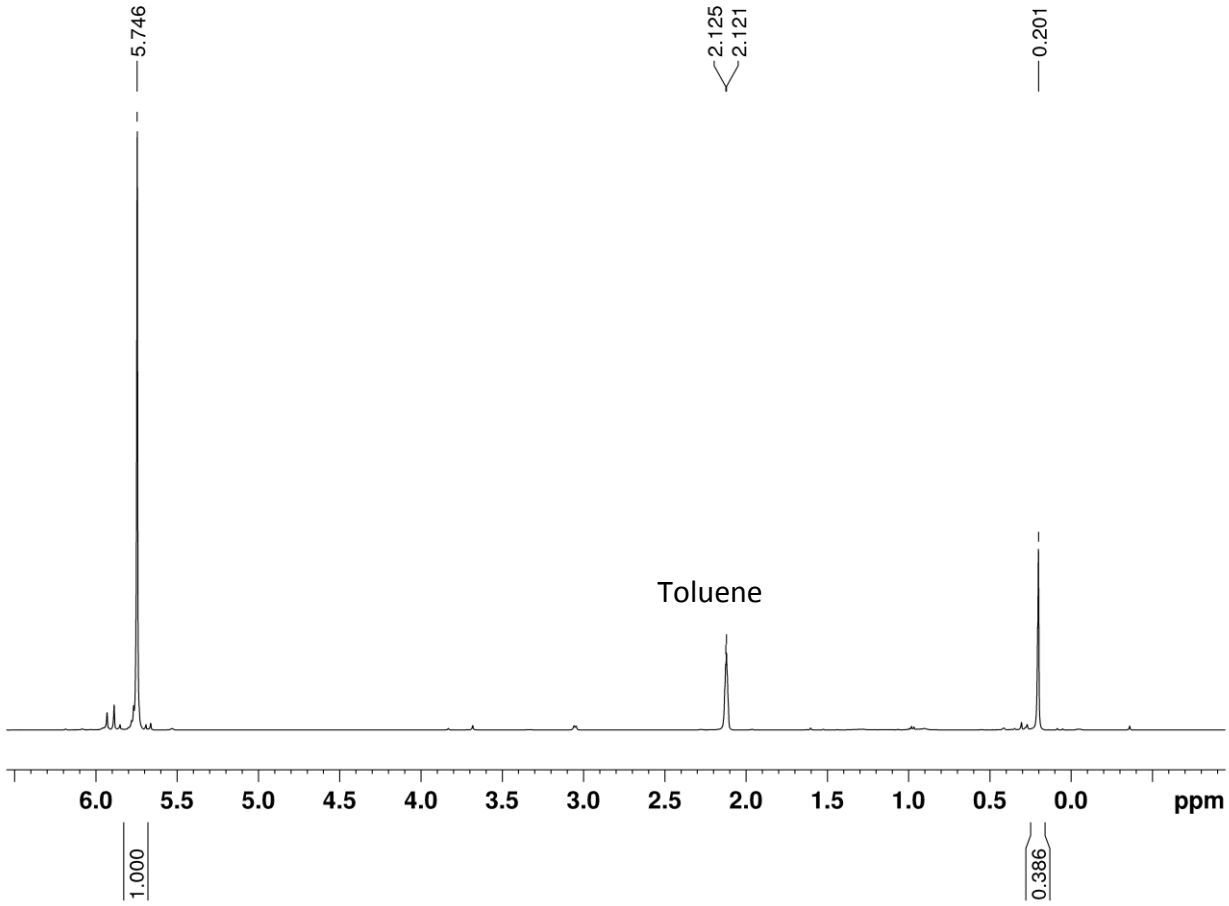


Figure S4. ^{1}H NMR of Cp_2ZrMe_2 in toluene + C_7D_8.

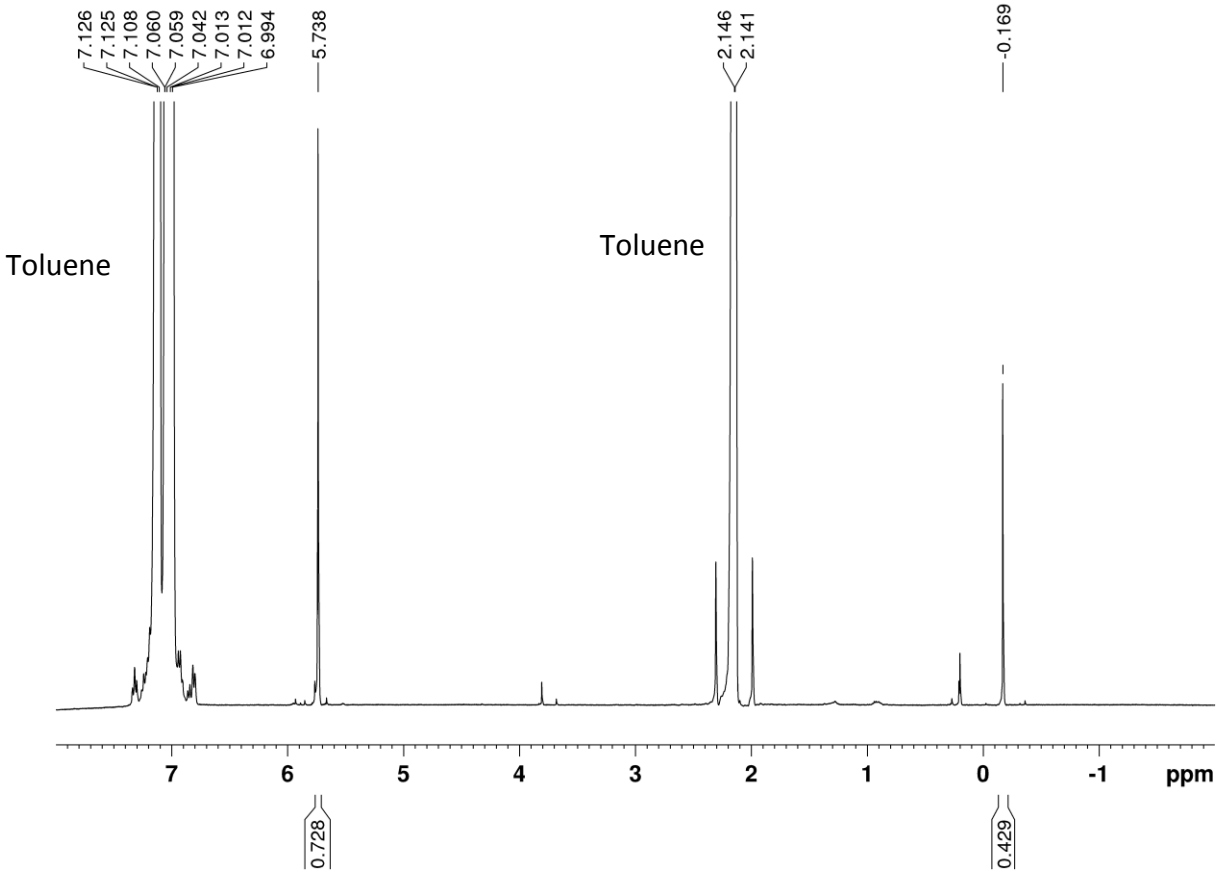


Figure S5. ^{1}H NMR of system Cp_2ZrMe_2+$(AlMe_3)_2$ in C_7D_8 at 298 K.

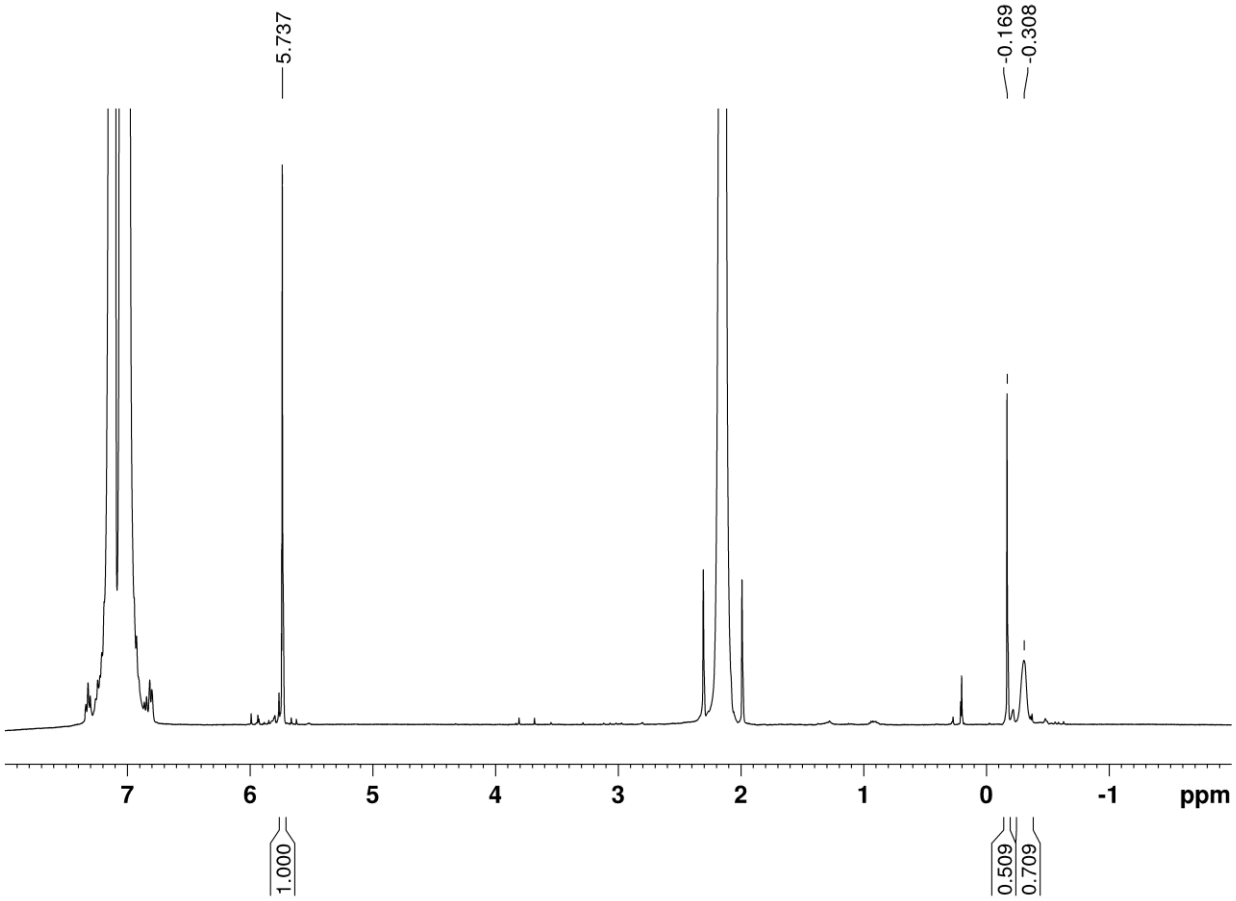


Figure S6. EXSY spectrum of system Cp_2ZrMe_2+$(AlMe_3)_2$ in C_7D_8 at 298 K (τ= 1 s).

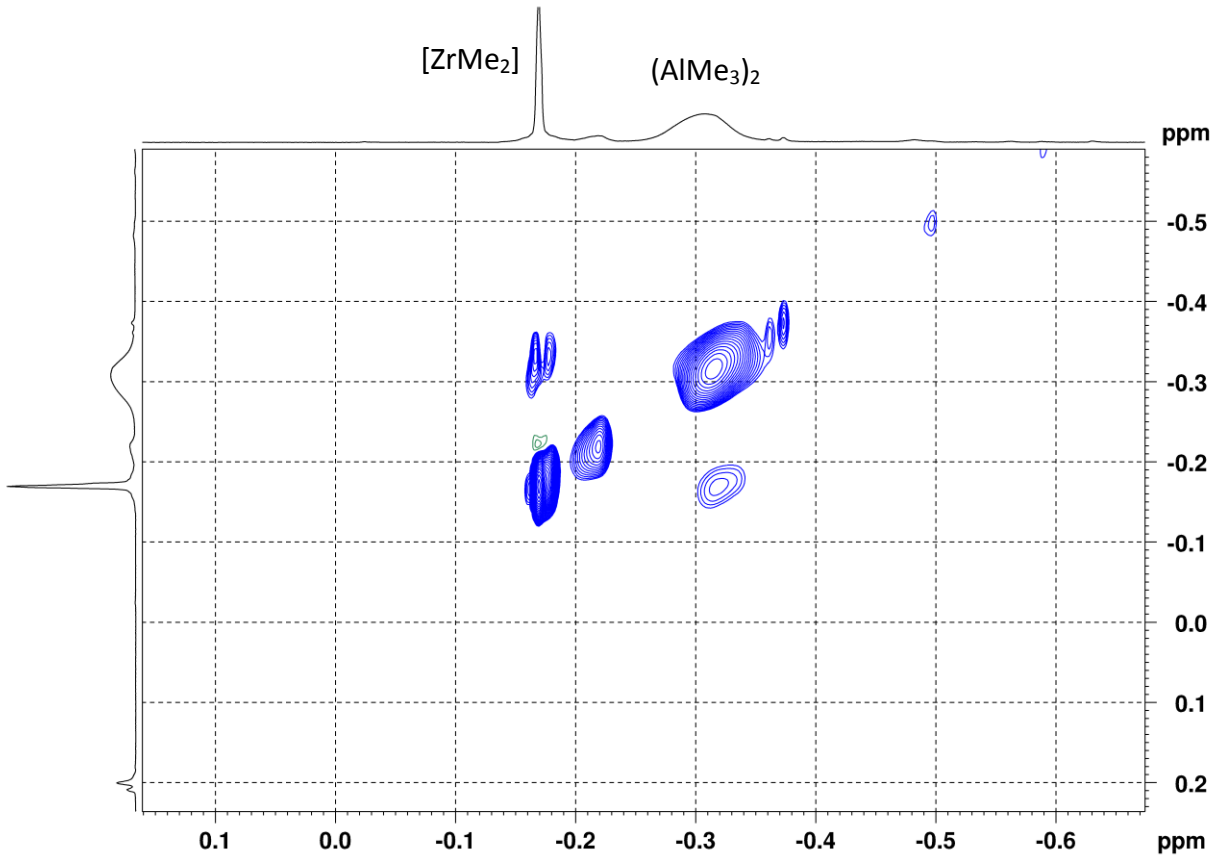


Figure S7. VT ^{1}H NMR study on system $Cp_2ZrMeCl$+$(AlMe_3)_2$ (1:3) in C_7D_8.

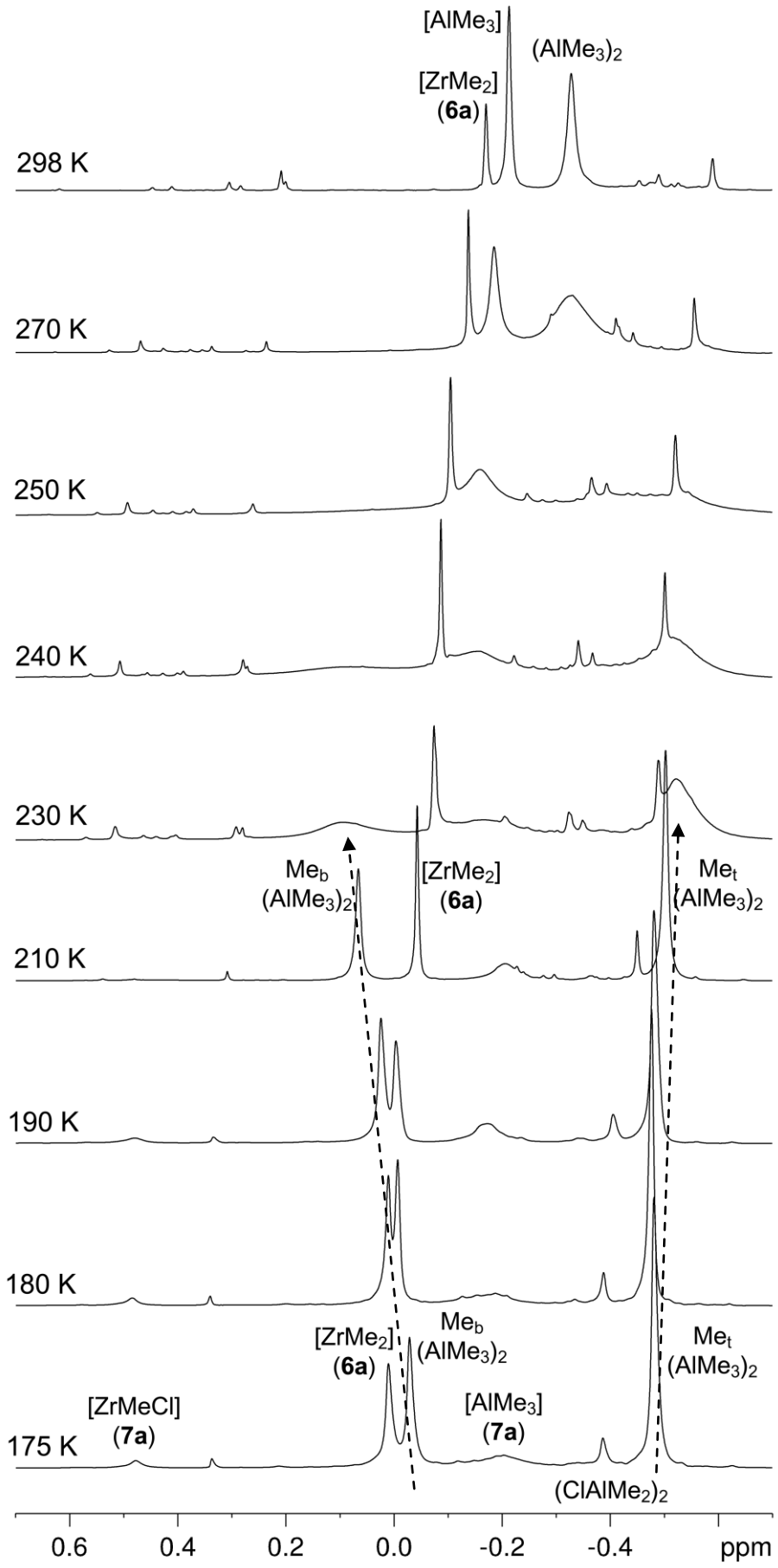


Figure S8. EXSY spectrum of system $Cp_2ZrMeCl$ (**5a**) + $(AlMe_3)_2$ (1:3) in C_7D_8 at 200 K (τ= 0.05 s).

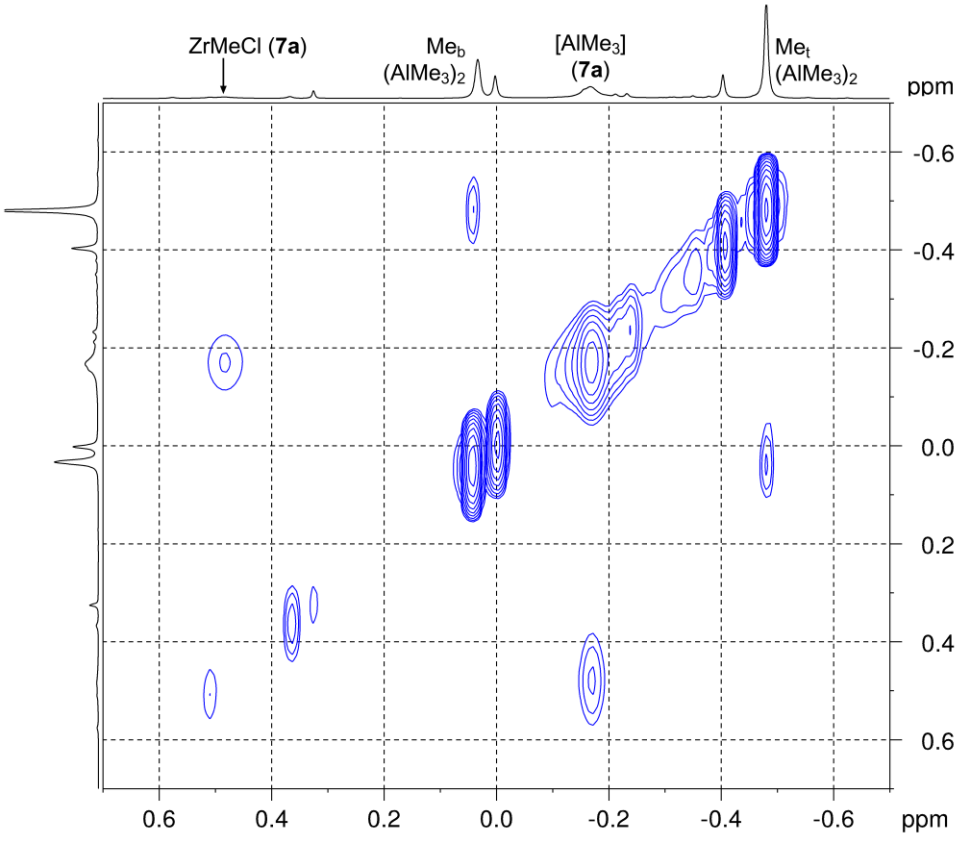


Figure S9. ^{1}H NMR of system Cp_2ZrCl_2 (**1a**) - $(AlMe_3)_2$ in CD_2Cl_2 at 297 K.

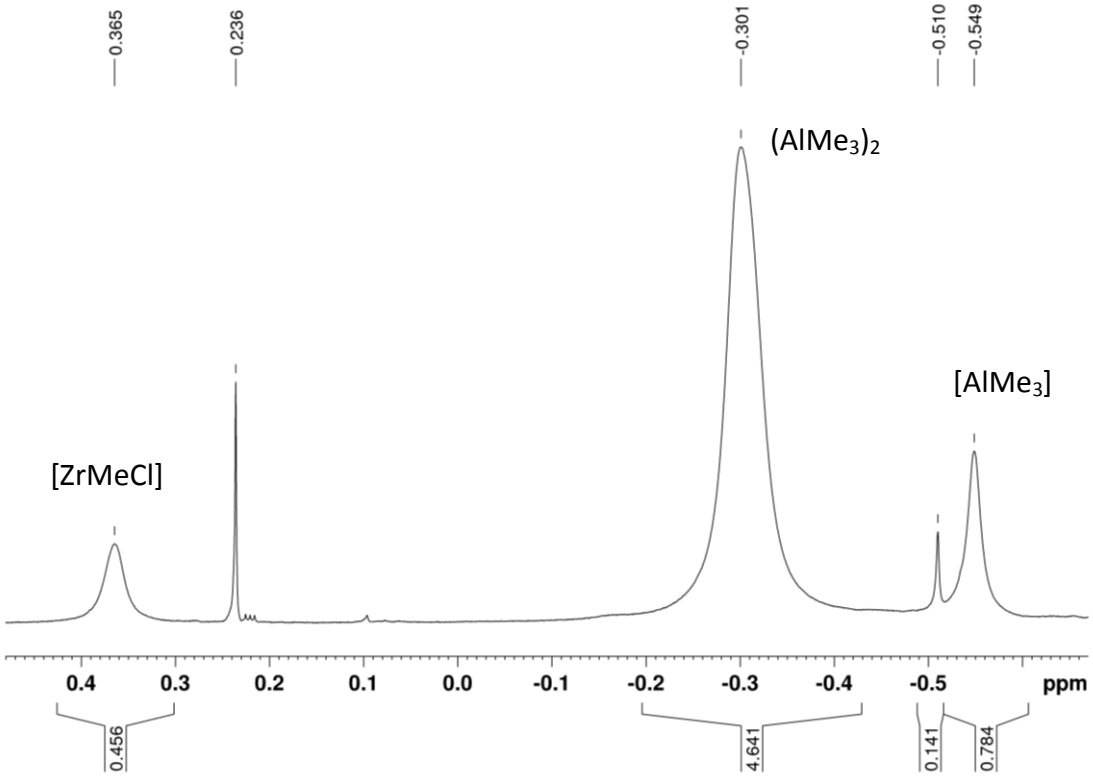


Figure S10. EXSY spectrum of system Cp_2ZrCl_2 (**1a**) -$(AlMe_3)_2$ in C_7D_8 at 297 K (τ= 0.05 s).

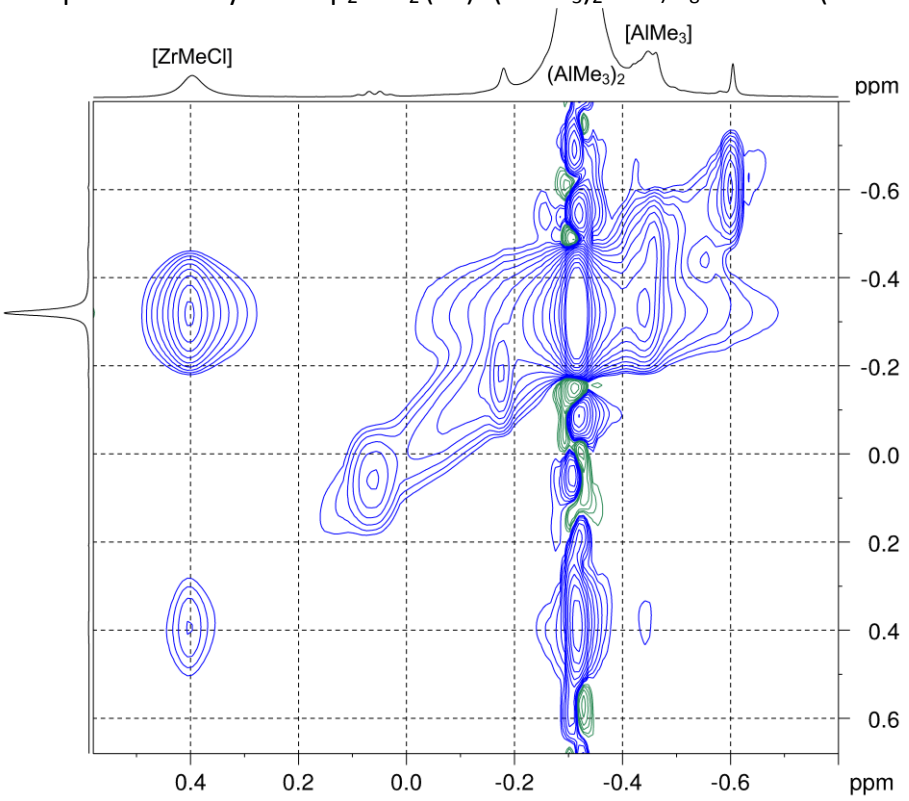


Figure S11. ^{1}H NMR of system $(CpMe)_2ZrCl_2$ (**1b**) - $(AlMe_3)_2$ in C_7D_8 at 300 K.

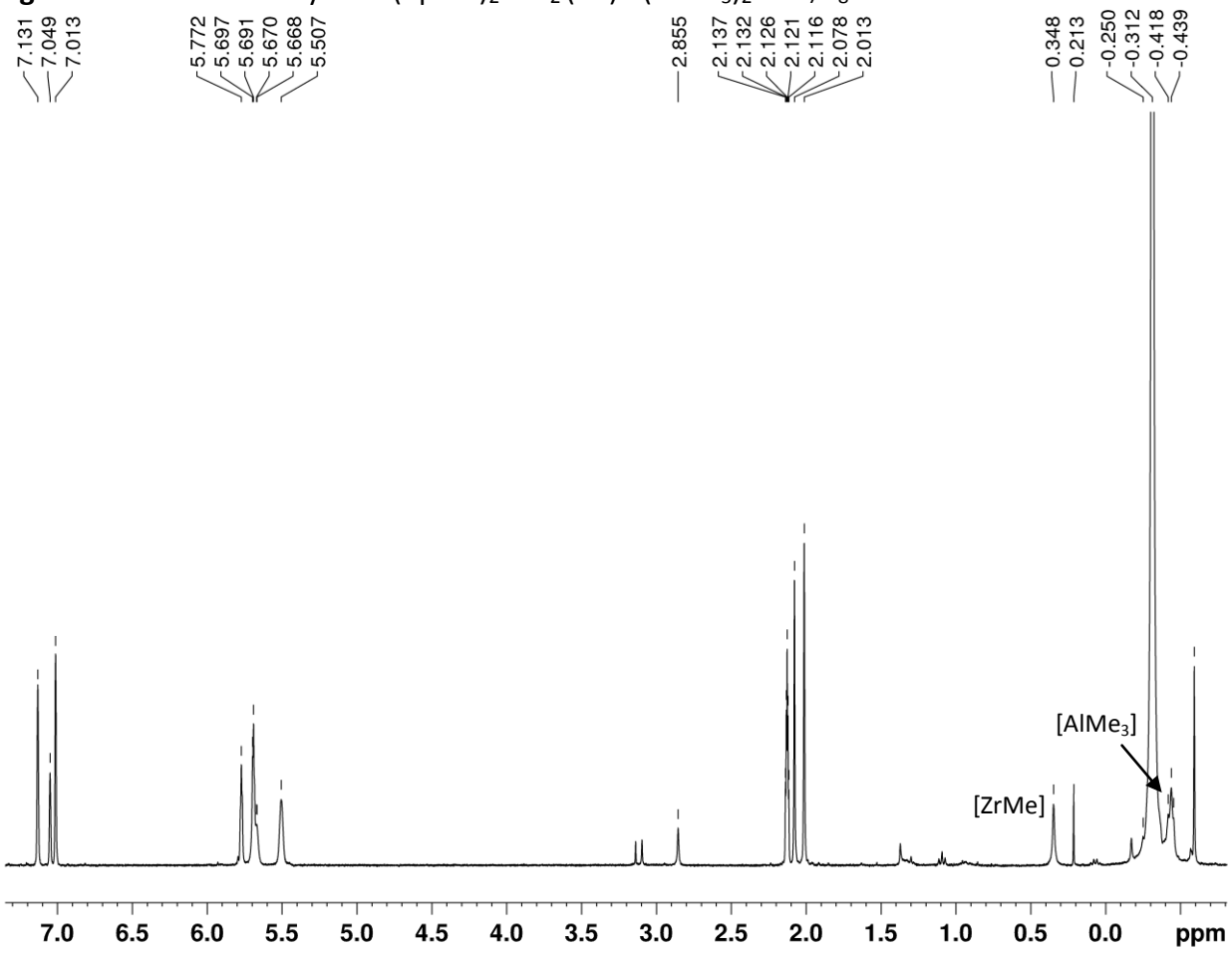


Figure S12. EXSY spectrum of system $(CpMe)_2ZrCl_2$ (**1b**) - $(AlMe_3)_2$ in C_7D_8 at 300 K (τ= 1 s).

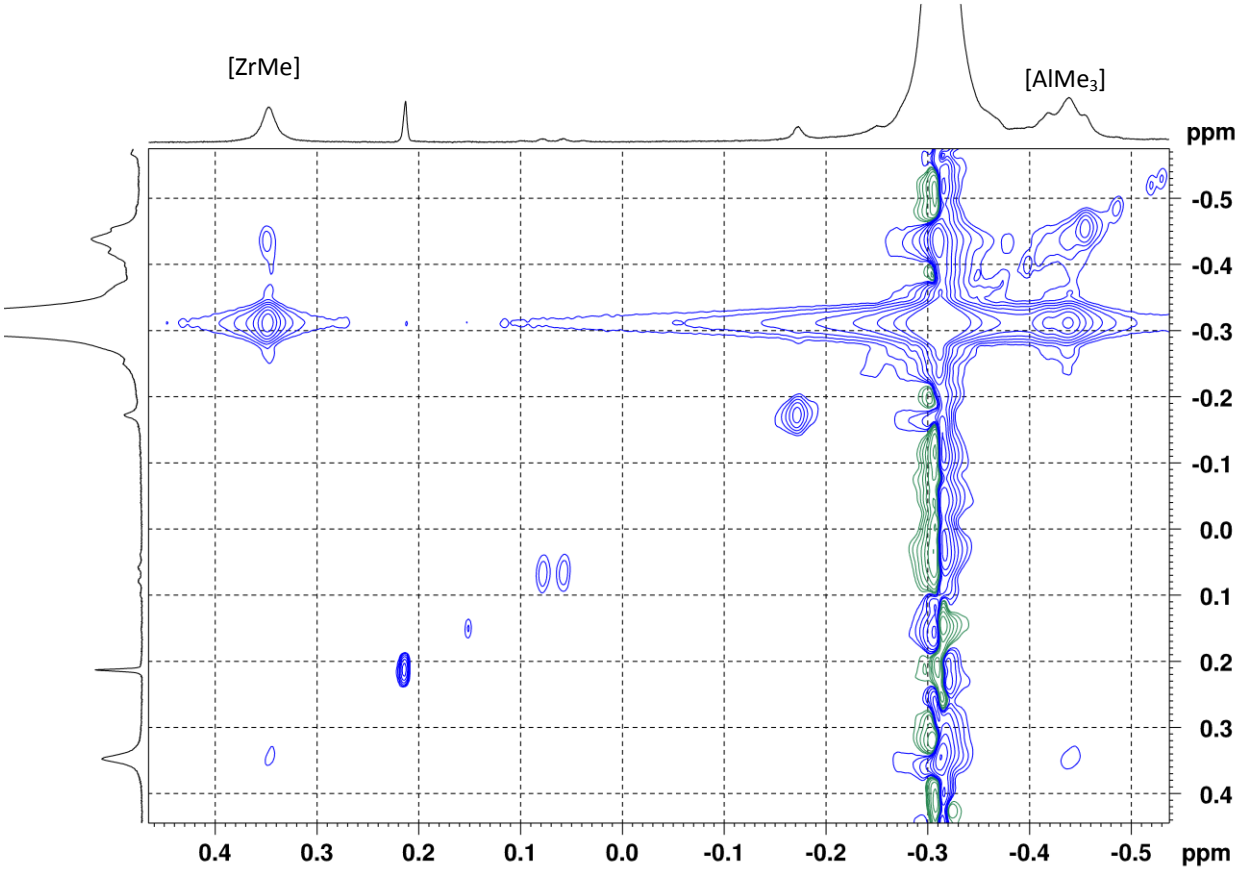


Figure S13. ^{1}H NMR of system $(C_5Me_5)_2ZrCl_2$ (**1c**) - $(AlMe_3)_2$ in CD_2Cl_2 at 298 K.

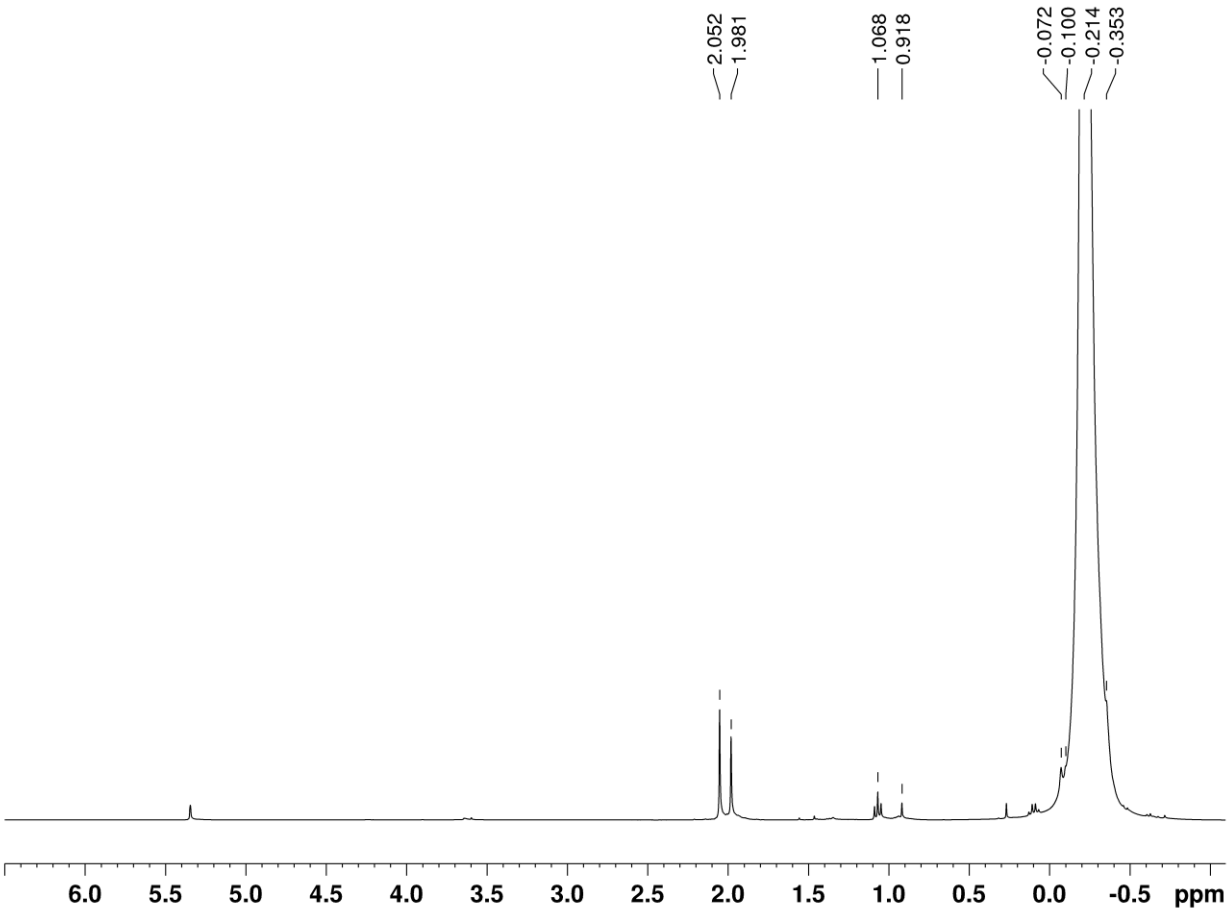


Figure S14. HSQC spectrum of system $(C_5Me_5)_2ZrCl_2$ (**1c**) - $(AlMe_3)_2$ in CD_2Cl_2 at 298 K.

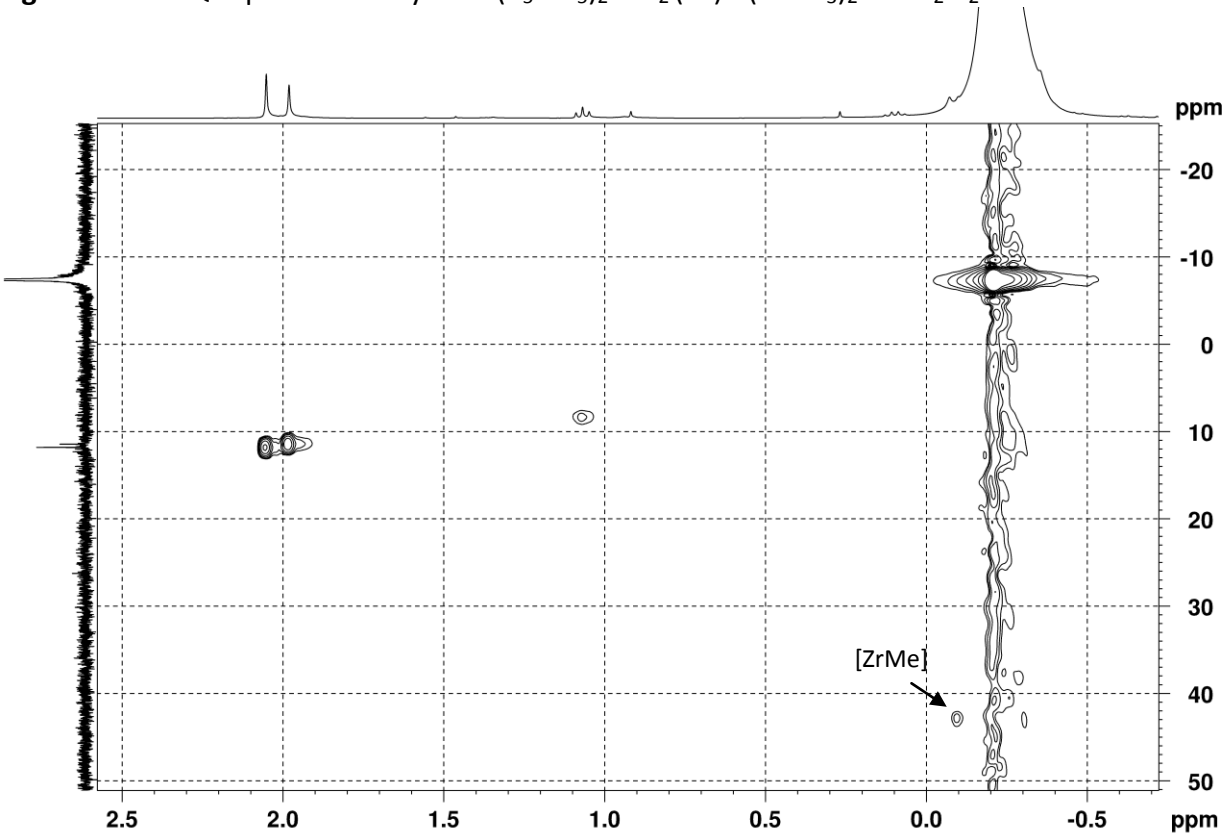


Figure S15. ^{1}H NMR of system $Me_2SiCp_2ZrCl_2$ (**1d**) - $(AlMe_3)_2$ in CD_2Cl_2 at 260 K.

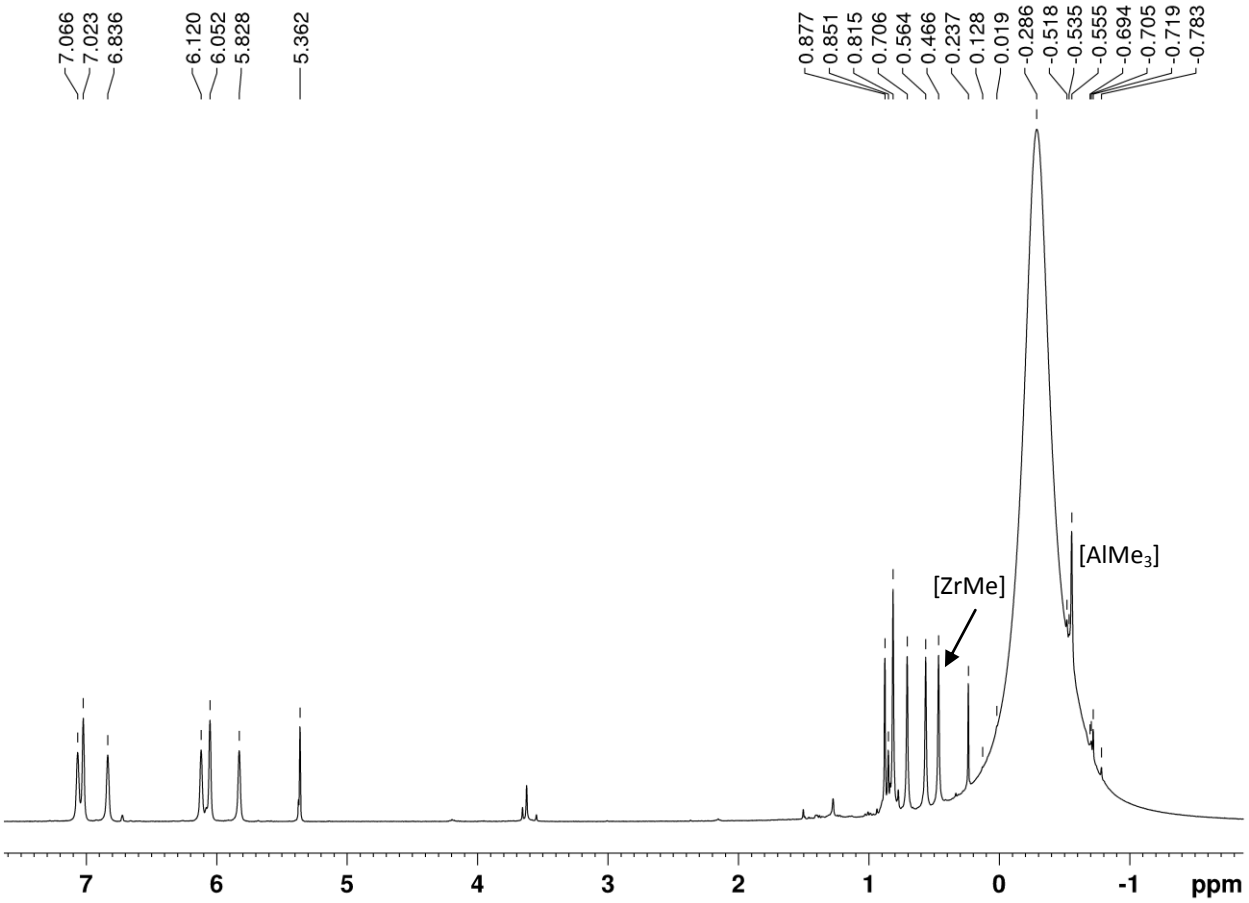


Figure S16. EXSY spectrum of system $Me_2SiCp_2ZrCl_2$ (**1d**) - $(AlMe_3)_2$ in CD_2Cl_2 at 300 K (τ= 0.3 s).

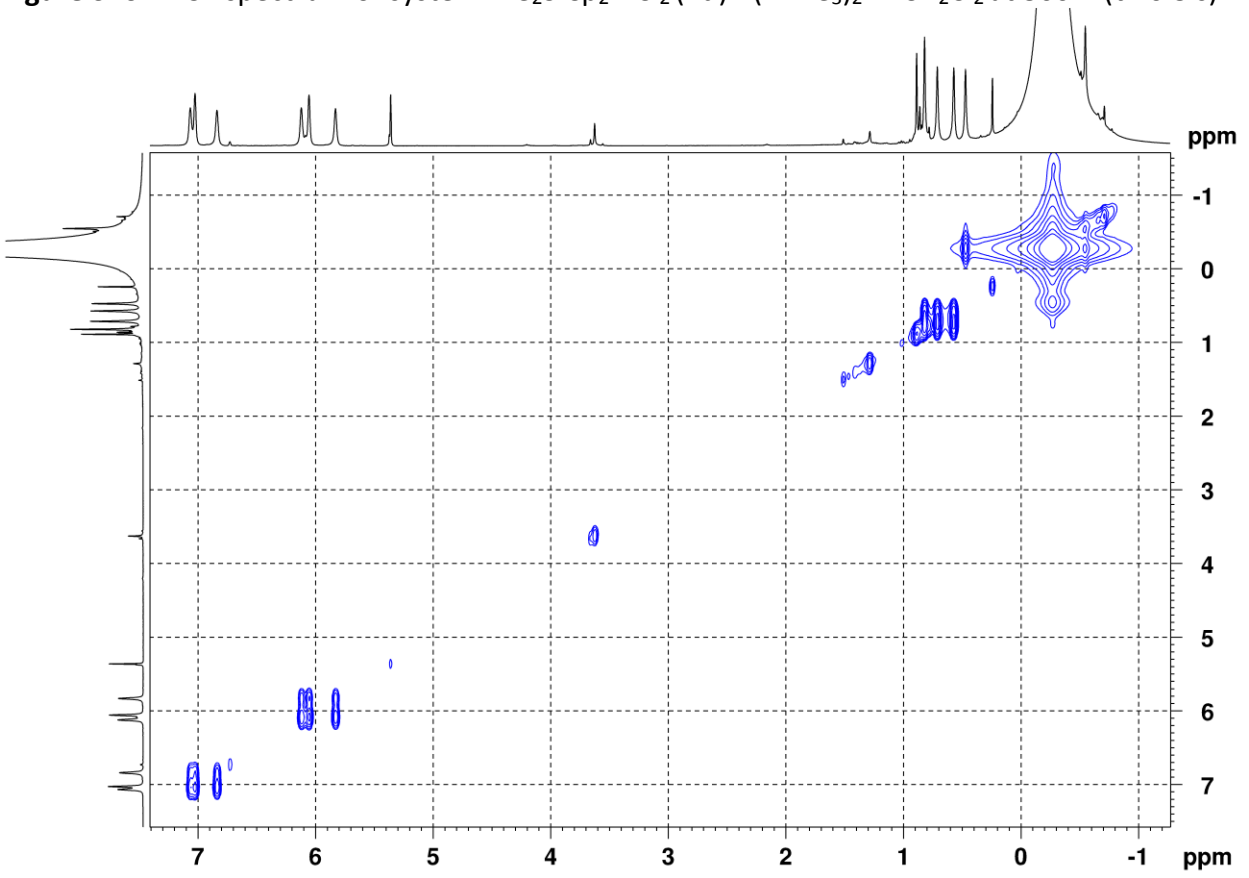


Figure S17. ^{1}H NMR of system $Me_2Si(C_5Me_4)_2ZrCl_2$ (**1e**) - $(AlMe_3)_2$ in C_7D_8 at 299 K.

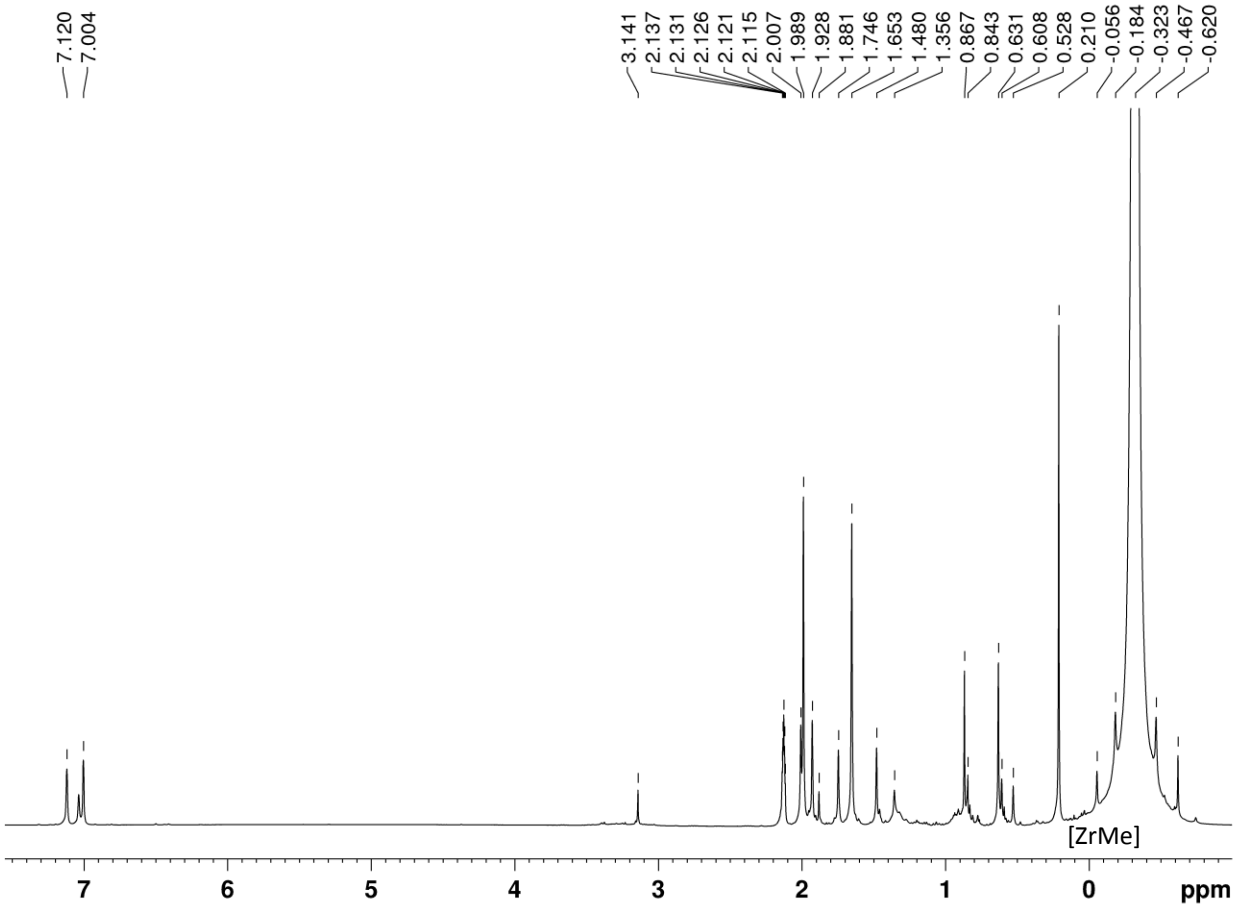


Figure S18. ^{1}H NMR of system *rac*- $Me_2C(2\text{-}Me\text{-}4\text{-}Bu^t\text{-}Cp)_2ZrCl_2$ (**1f**) - $(AlMe_3)_2$ in C_7D_8 at 298 K.

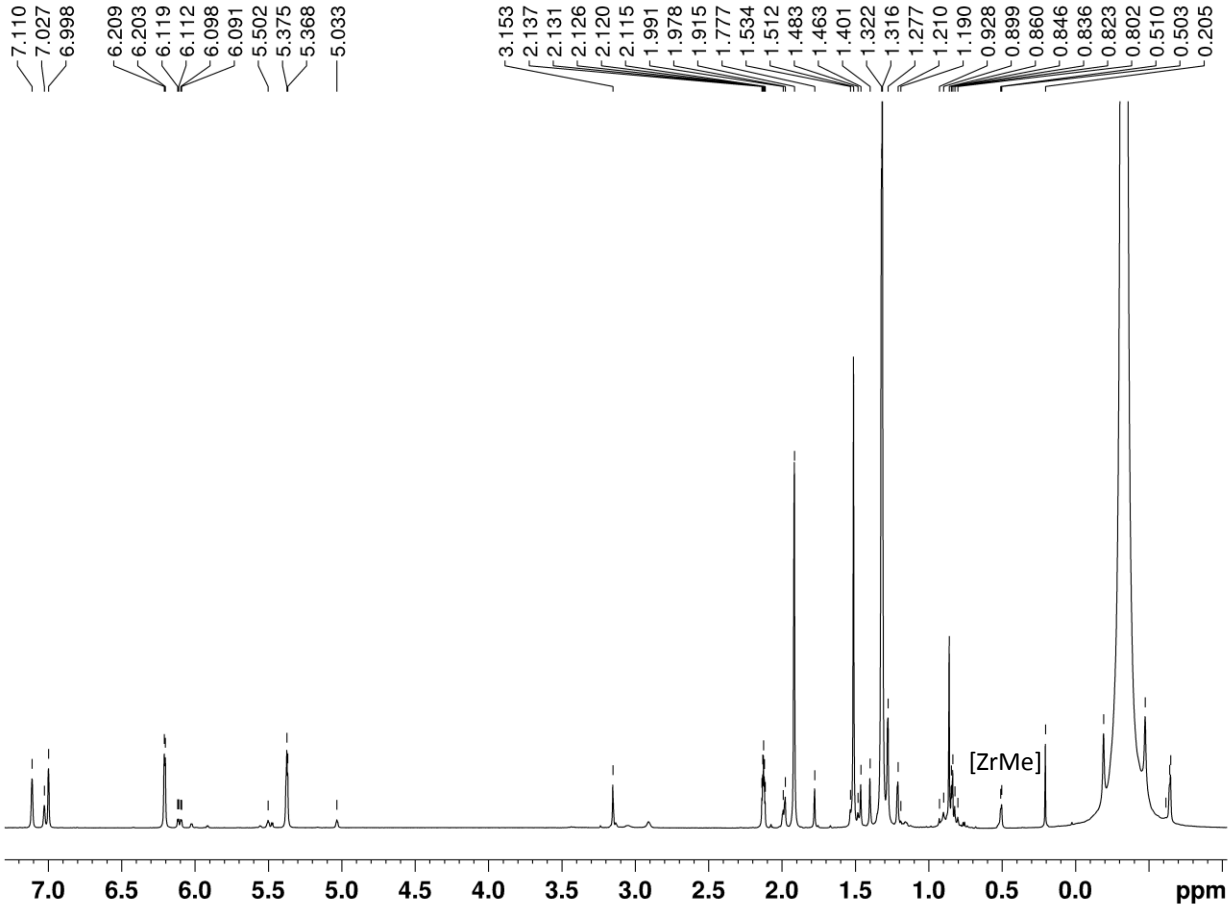


Figure S19. EXSY spectrum of system *rac*- $Me_2C(2\text{-}Me\text{-}4\text{-}Bu^t\text{-}Cp)_2ZrCl_2$ (**1f**) - $(AlMe_3)_2$ in C_7D_8 at 298 K (τ= 0.7 s).

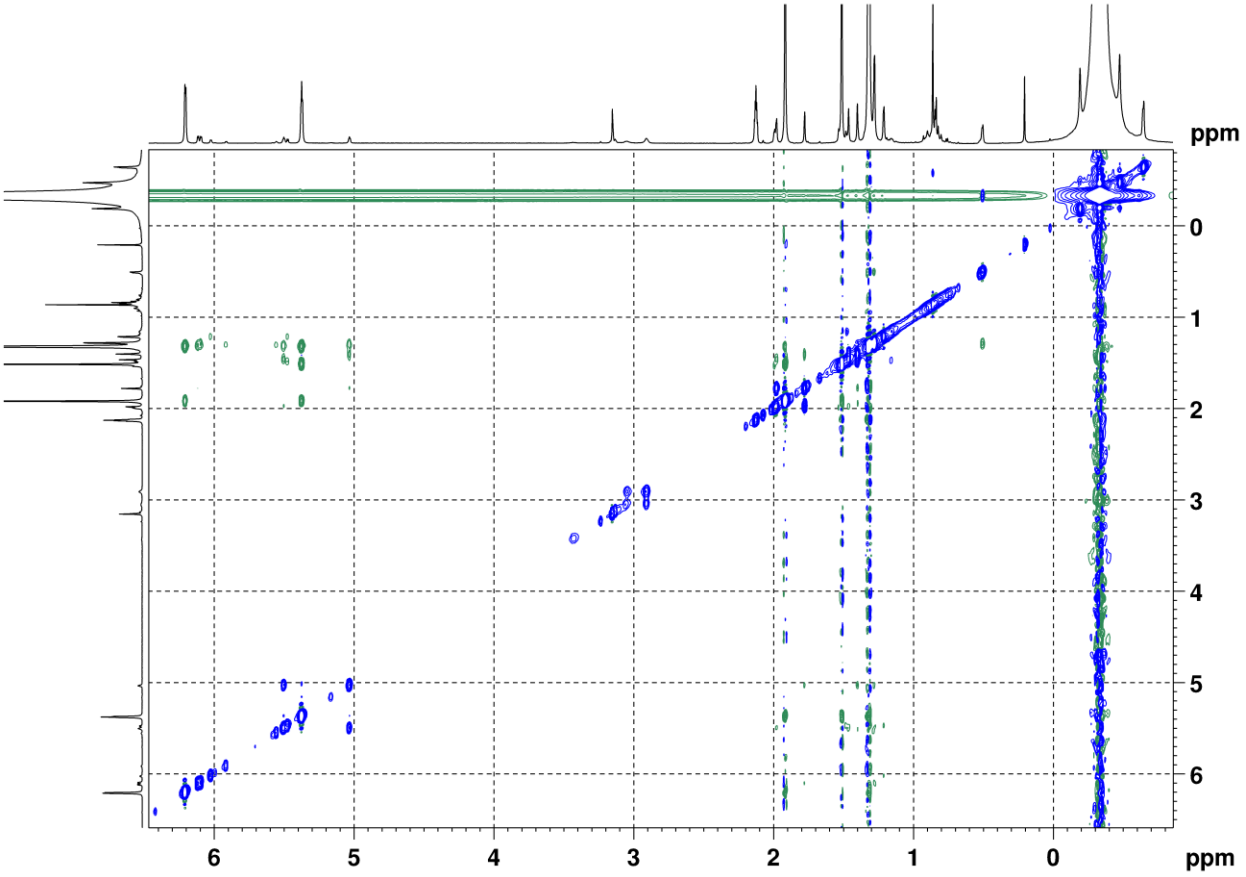


Figure S20. ^{1}H NMR of system *rac*- $Me_2C(3\text{-}Bu^t\text{-}Cp)_2ZrCl_2$ (**1h**) - $(AlMe_3)_2$ in C_7D_8 at 280 K.

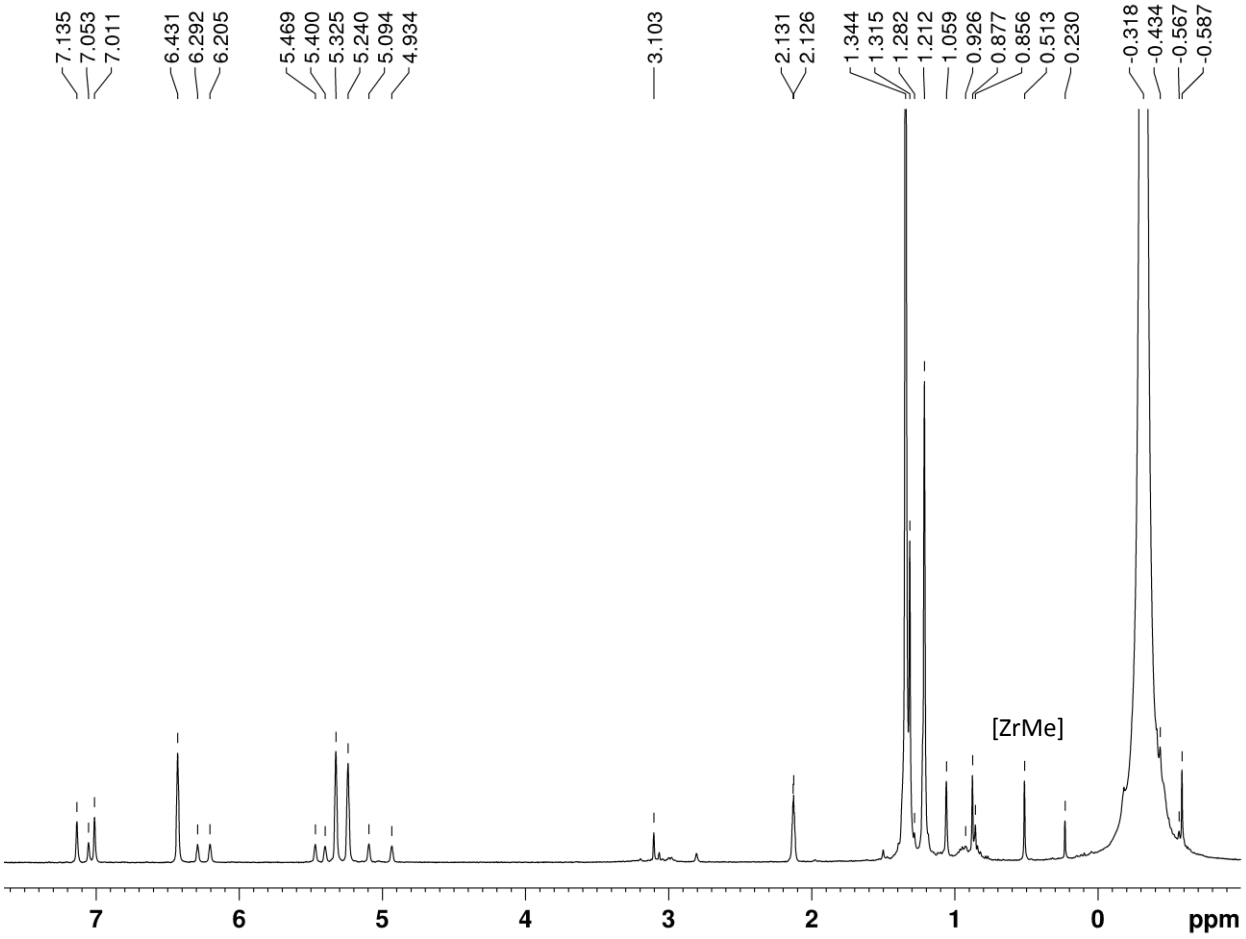


Figure S21. EXSY spectrum of system *rac*- $Me_2C(3\text{-}Bu^t\text{-}Cp)_2ZrCl_2$ (**1h**) - $(AlMe_3)_2$ in C_7D_8 at 280 K (τ= 0.3 s).

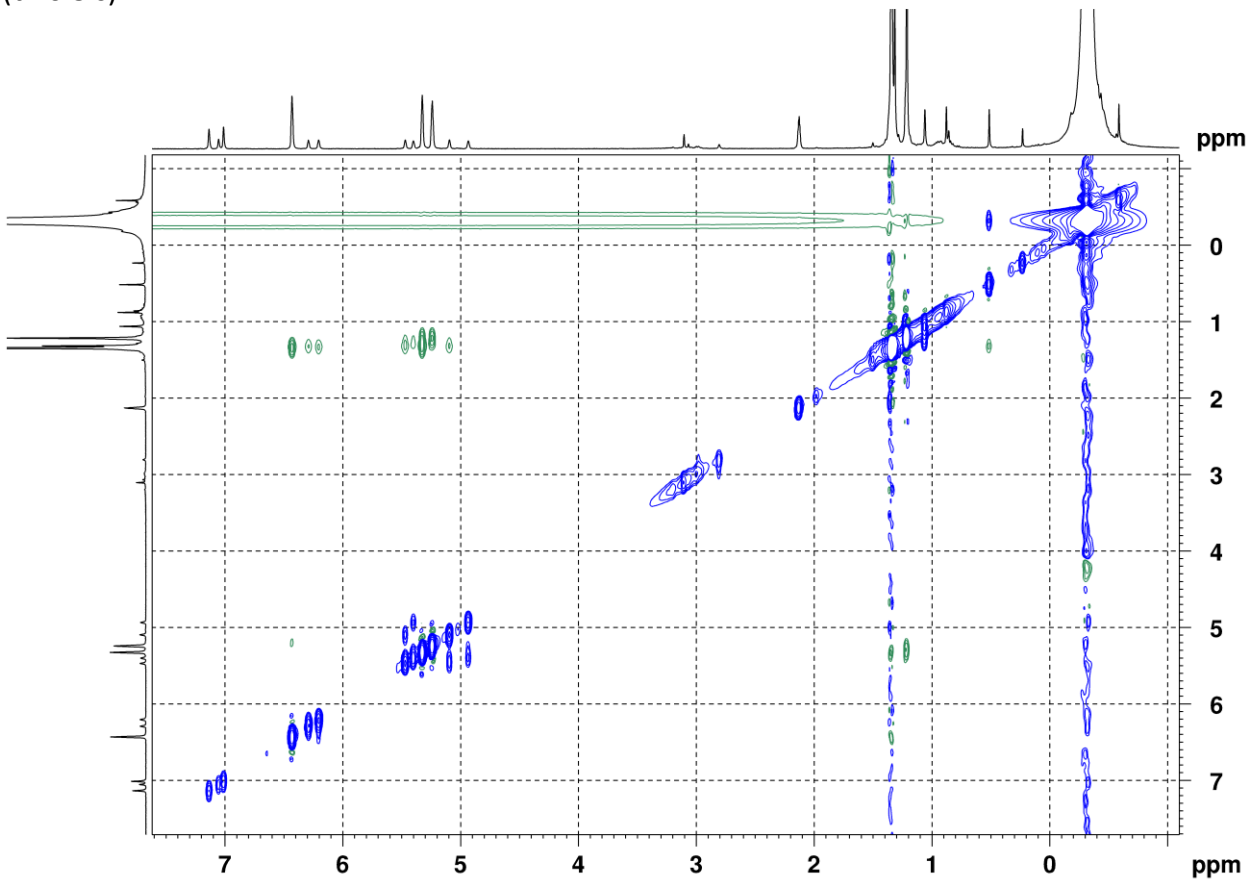


Figure S22. ^{1}H NMR of system Ind_2ZrCl_2 (**1i**) - $(AlMe_3)_2$ in CD_2Cl_2 at 300 K.

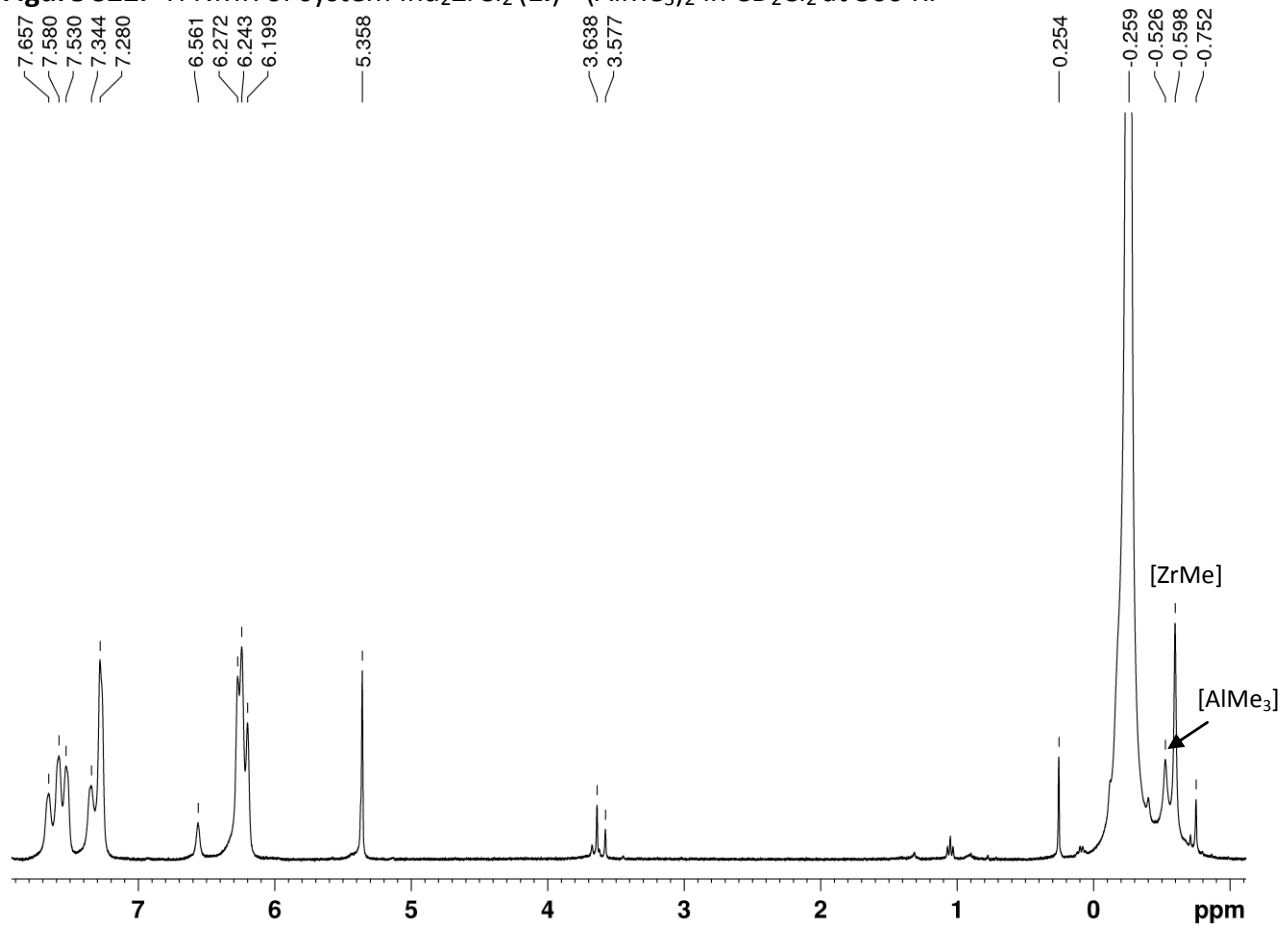


Figure S23. EXSY spectrum of system Ind_2ZrCl_2 (**1i**) - $(AlMe_3)_2$ in CD_2Cl_2 at 300 K (τ= 0.3 s).

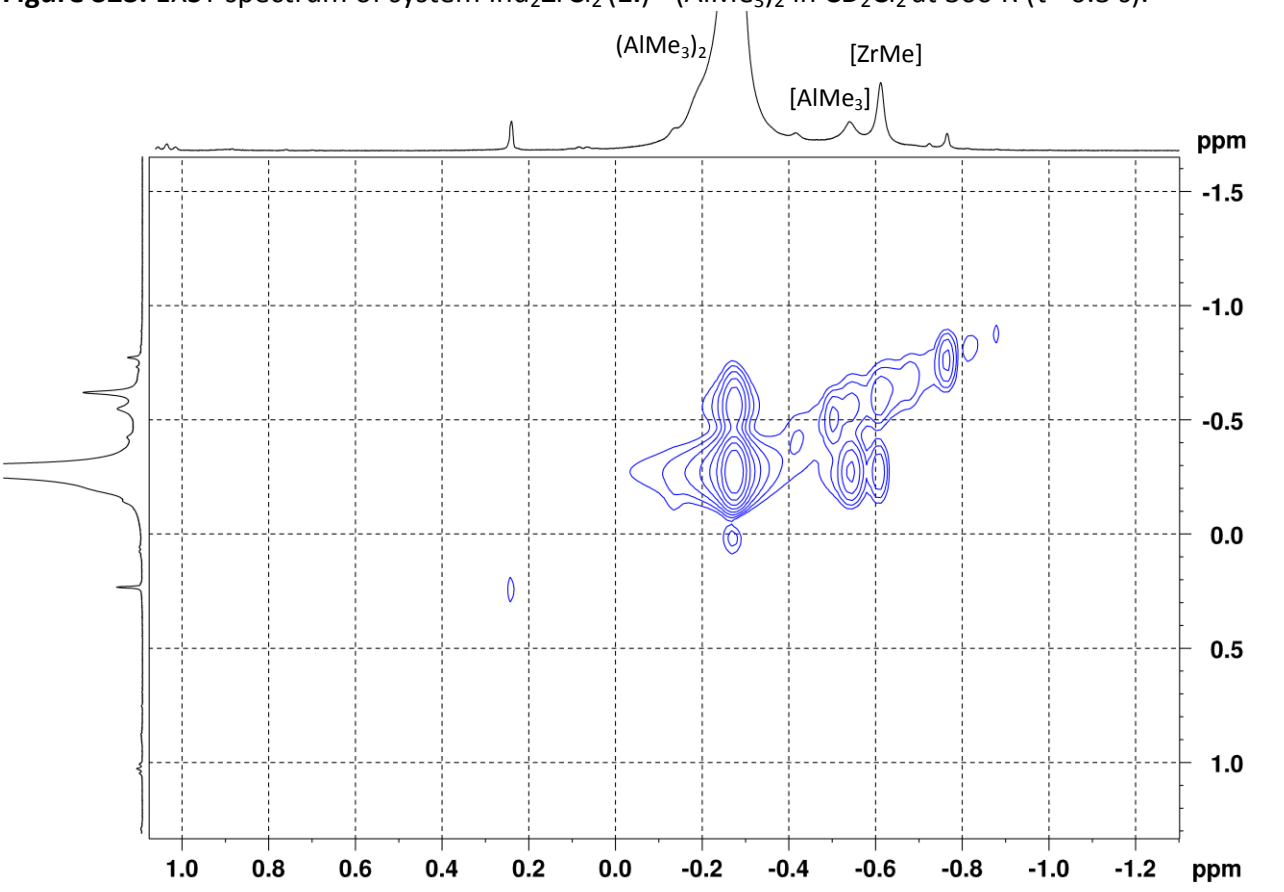


Figure S24. ^{1}H NMR of system *rac*- $H_2C(Ind)_2ZrCl_2$ (**1j**) - $(AlMe_3)_2$ in CD_2Cl_2 at 290 K.

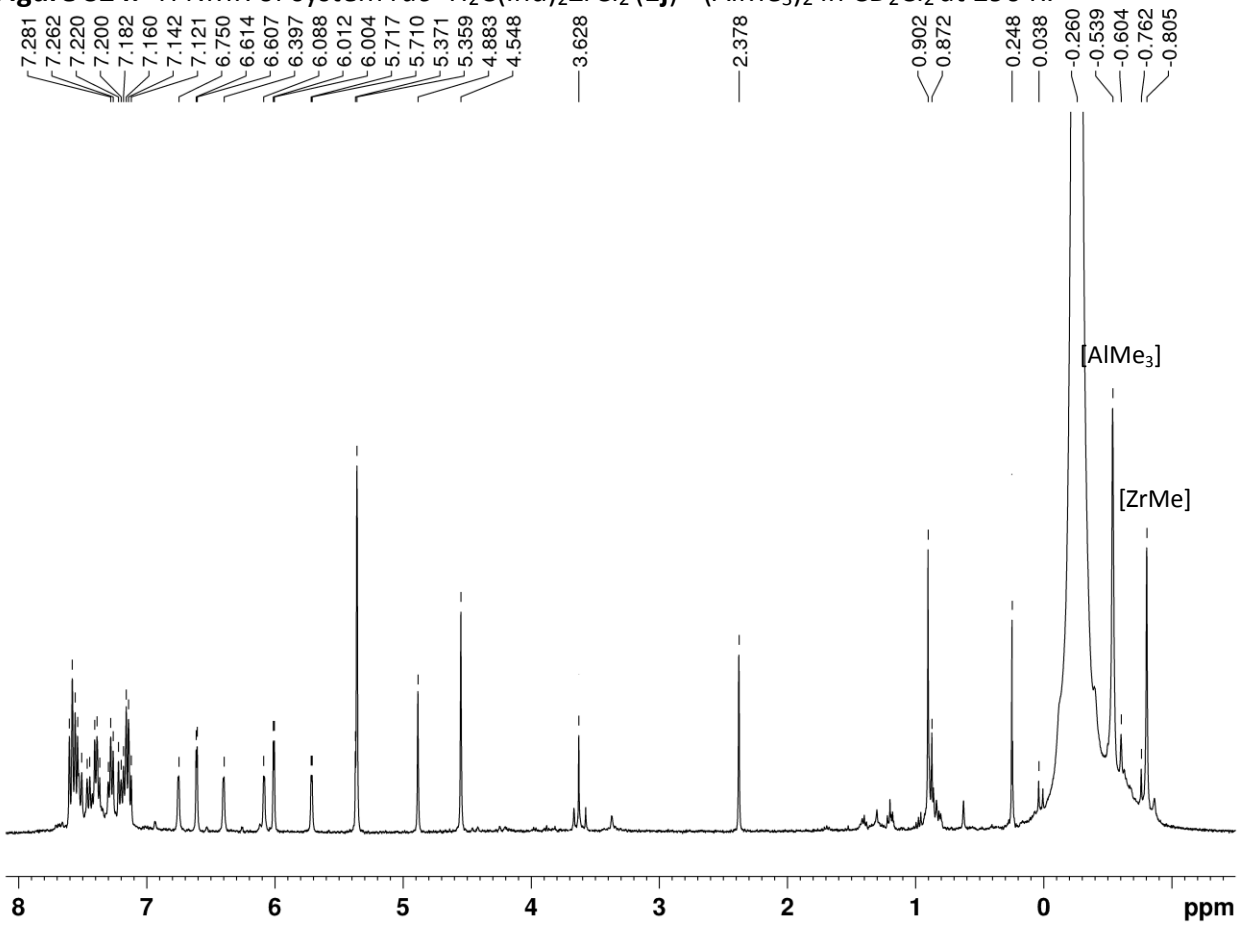


Figure S25. EXSY spectrum of system *rac*- $H_2C(Ind)_2ZrCl_2$ (**1j**) - $(AlMe_3)_2$ in CD_2Cl_2 at 290 K (τ= 0.3 s).

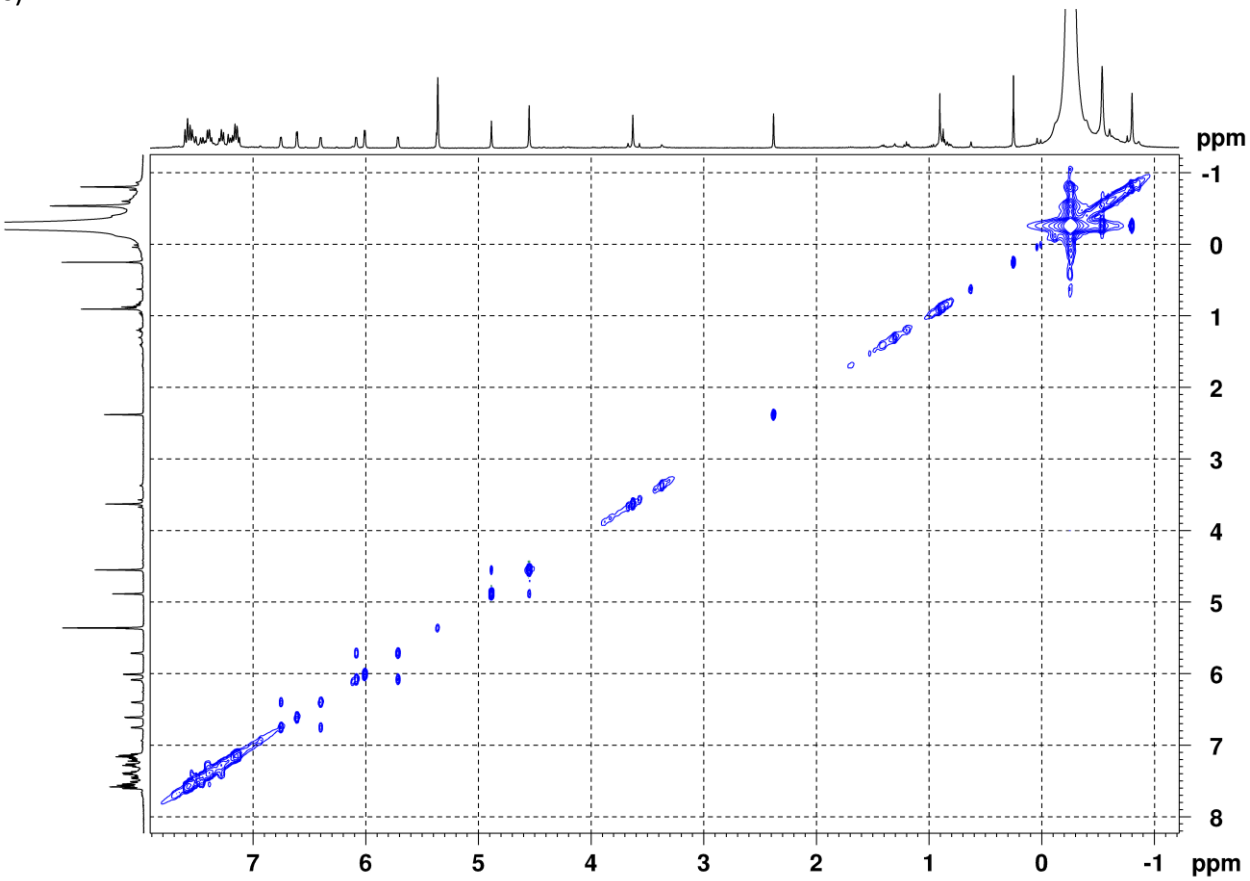


Figure S26. ^{1}H NMR of system *rac*- $Me_2C(Ind)_2ZrCl_2$ (**1k**) - $(AlMe_3)_2$ in CD_2Cl_2 at 300 K.

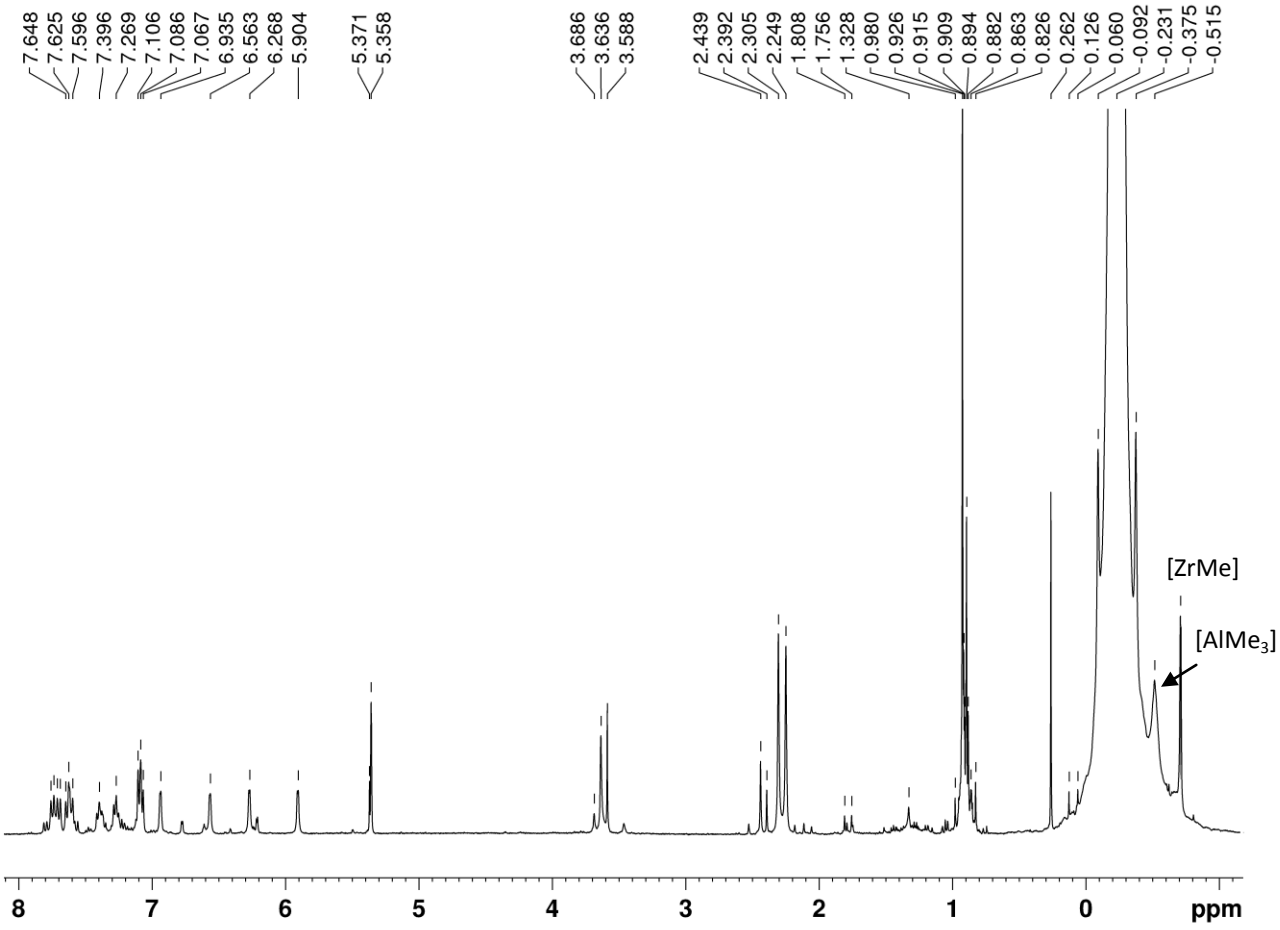


Figure S27. EXSY spectrum of system *rac*- $Me_2C(Ind)_2ZrCl_2$ (**1k**) - $(AlMe_3)_2$ in CD_2Cl_2 at 280 K (τ= 0.3 s).

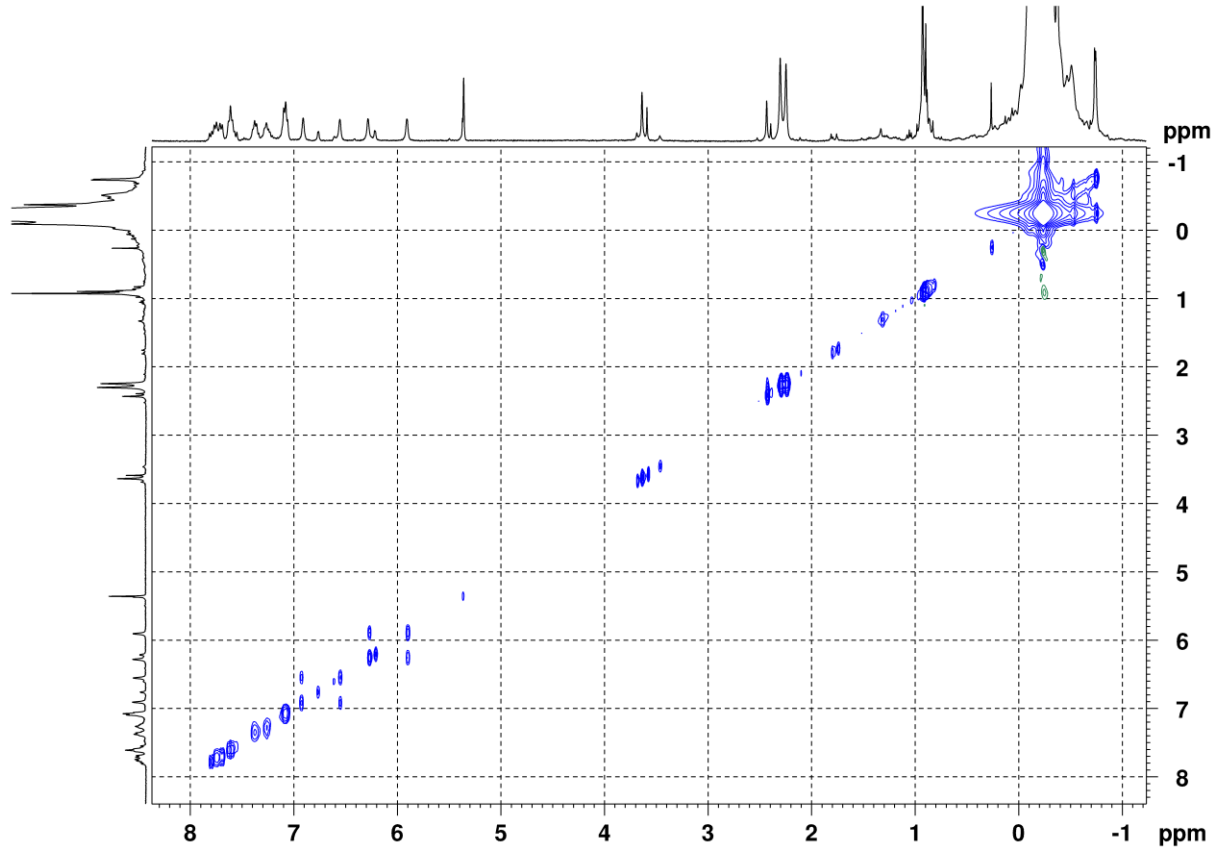


Figure S28. ^1H NMR of system *rac*- $Me_2Si(Ind)_2ZrCl_2$ (**1l**) - $(AlMe_3)_2$ in CD_2Cl_2 at 283 K.

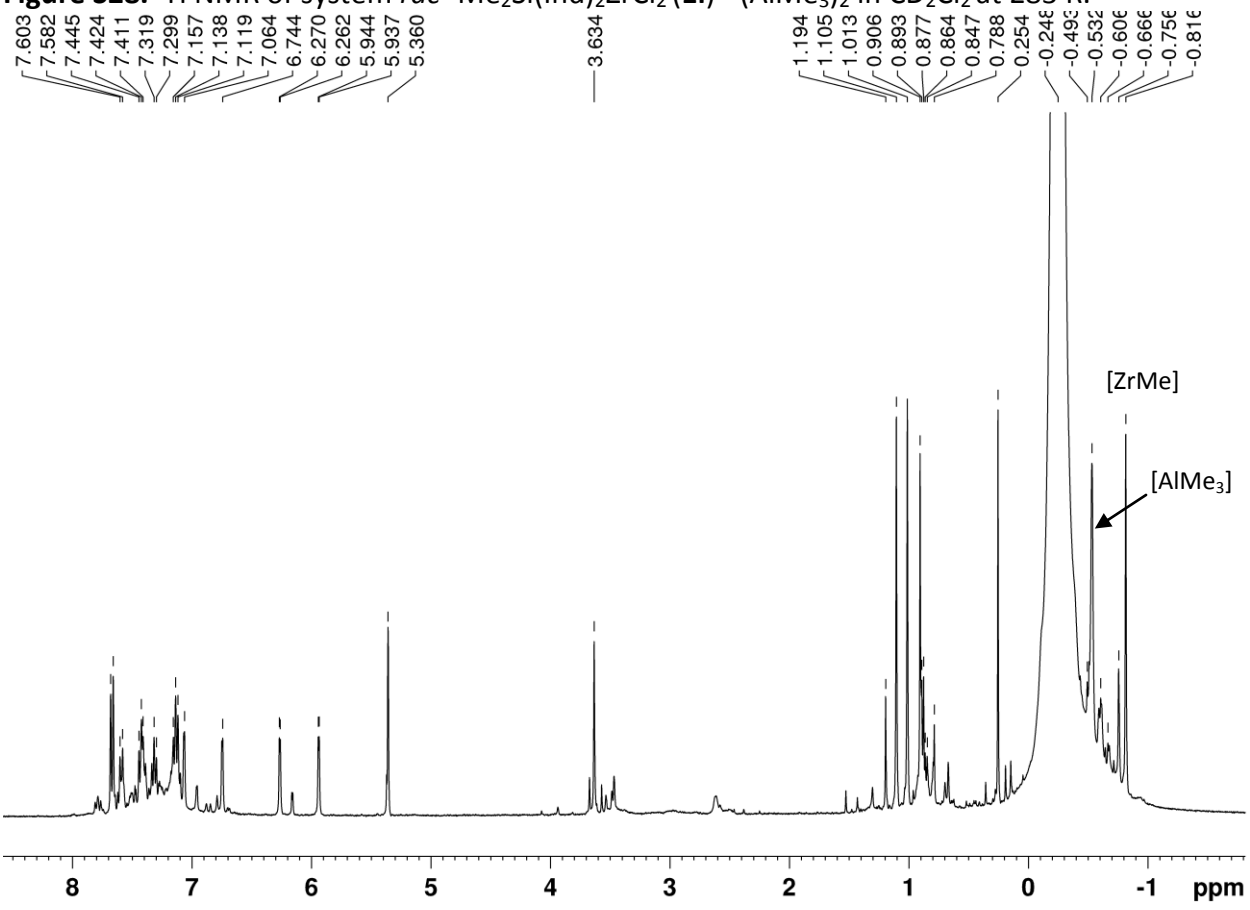


Figure S29. EXSY spectrum of system *rac*- $Me_2Si(Ind)_2ZrCl_2$ (**1l**) - $(AlMe_3)_2$ in CD_2Cl_2 at 283 K (τ= 0.3 s).

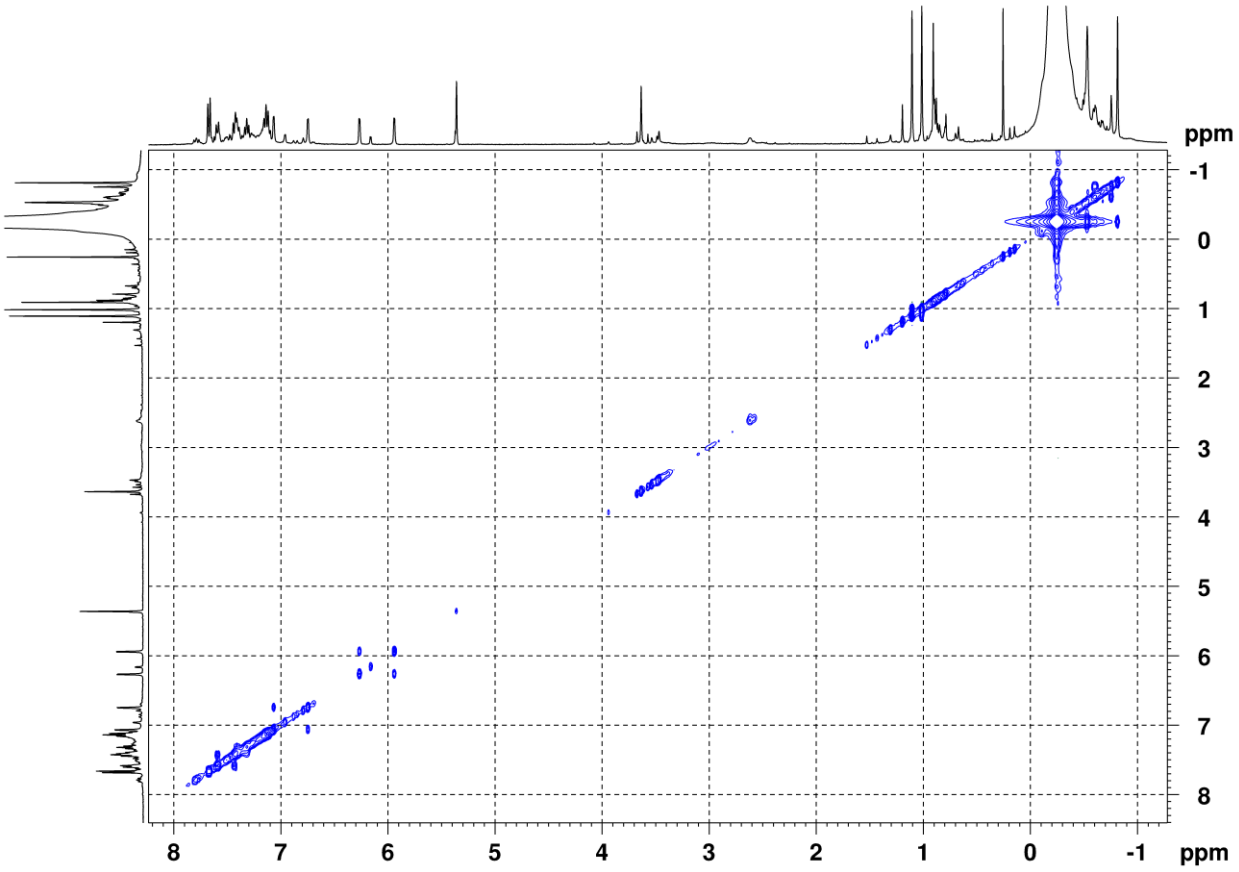


Figure S30. ^{1}H NMR of system *rac*- $C_2H_4(Ind)_2ZrCl_2$ (**1m**) - $(AlMe_3)_2$ in CD_2Cl_2 at 298 K.

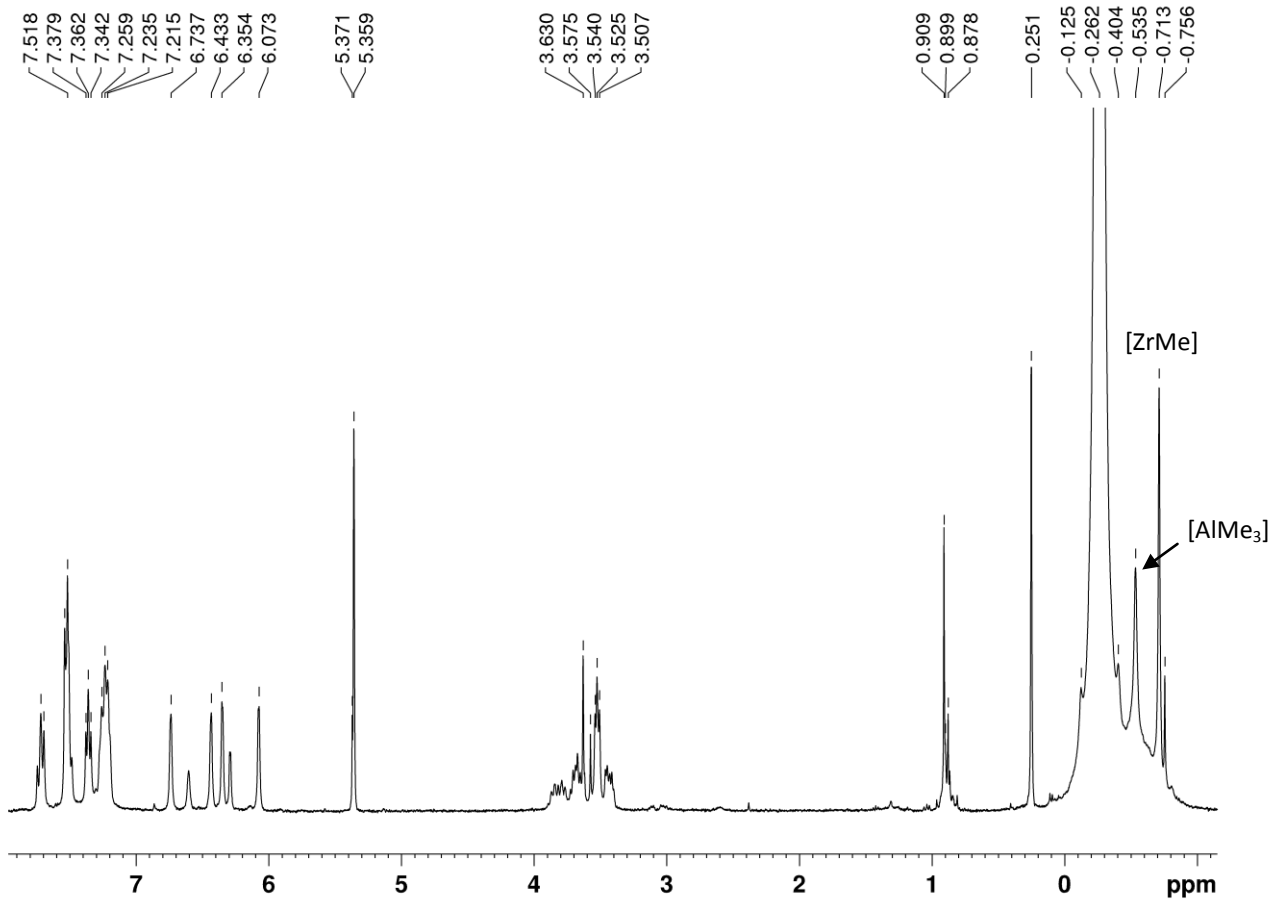


Figure S31. EXSY spectrum of system *rac*- $C_2H_4(Ind)_2ZrCl_2$ (**1m**) - $(AlMe_3)_2$ in CD_2Cl_2 at 298 K (τ= 0.3 s).

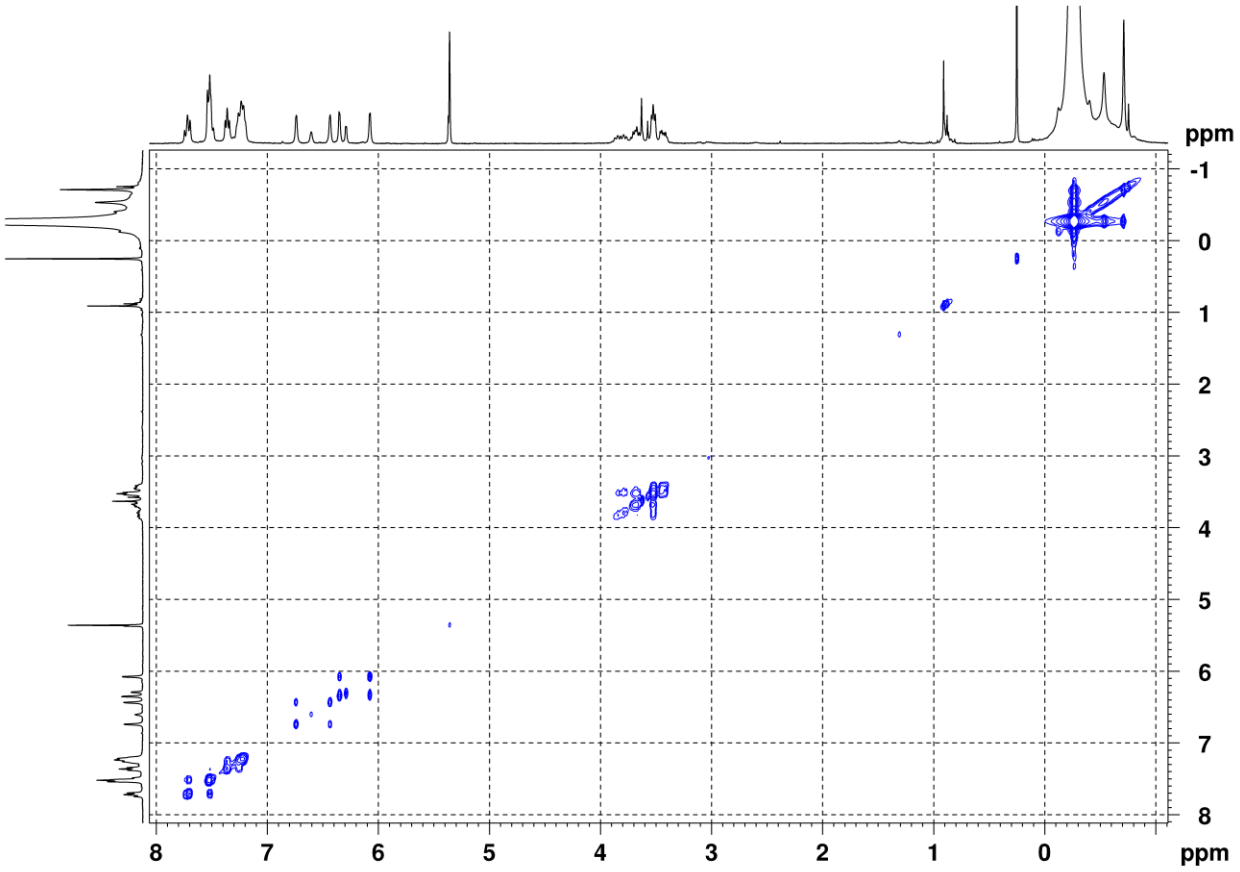


Figure S32. ^{1}H NMR of system *rac*- $Me_2Si(THInd)_2ZrCl_2$ (**1n**) - $(AlMe_3)_2$ in CD_2Cl_2 at 280 K.

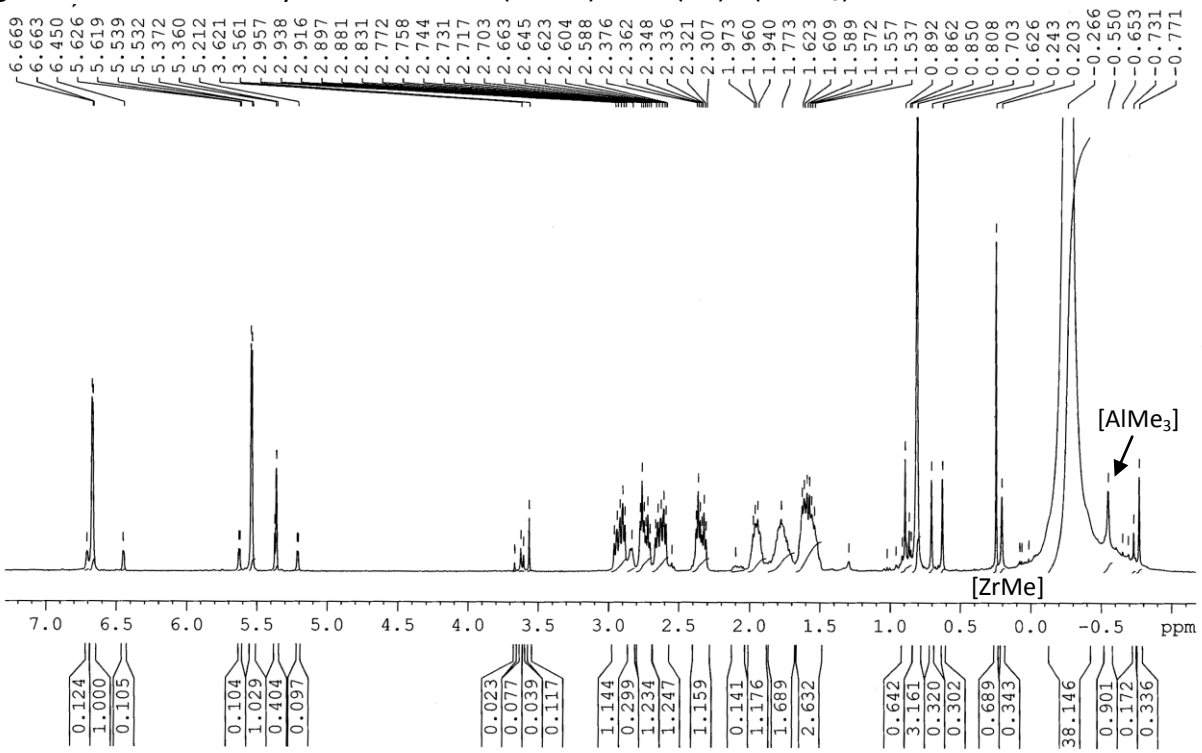


Figure S33. ^{1}H NMR of system *rac*- $C_2H_4(THInd)_2ZrCl_2$ (**1o**) - $(AlMe_3)_2$ in CD_2Cl_2 at 280 K.

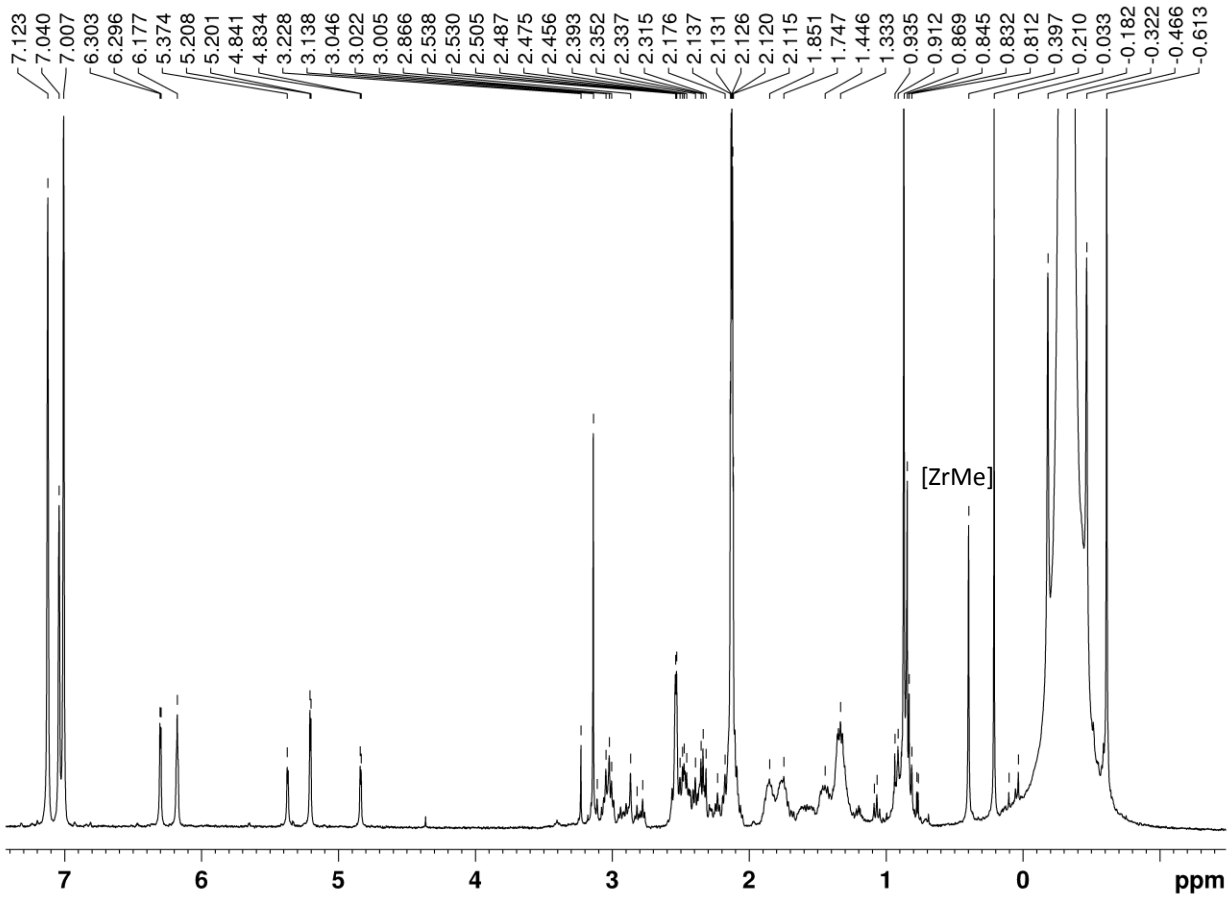


Figure S34. EXSY spectrum of system *rac*- $C_2H_4(THInd)_2ZrCl_2$ (**1o**) - $(AlMe_3)_2$ in CD_2Cl_2 at 298 K (τ= 0.3 s).

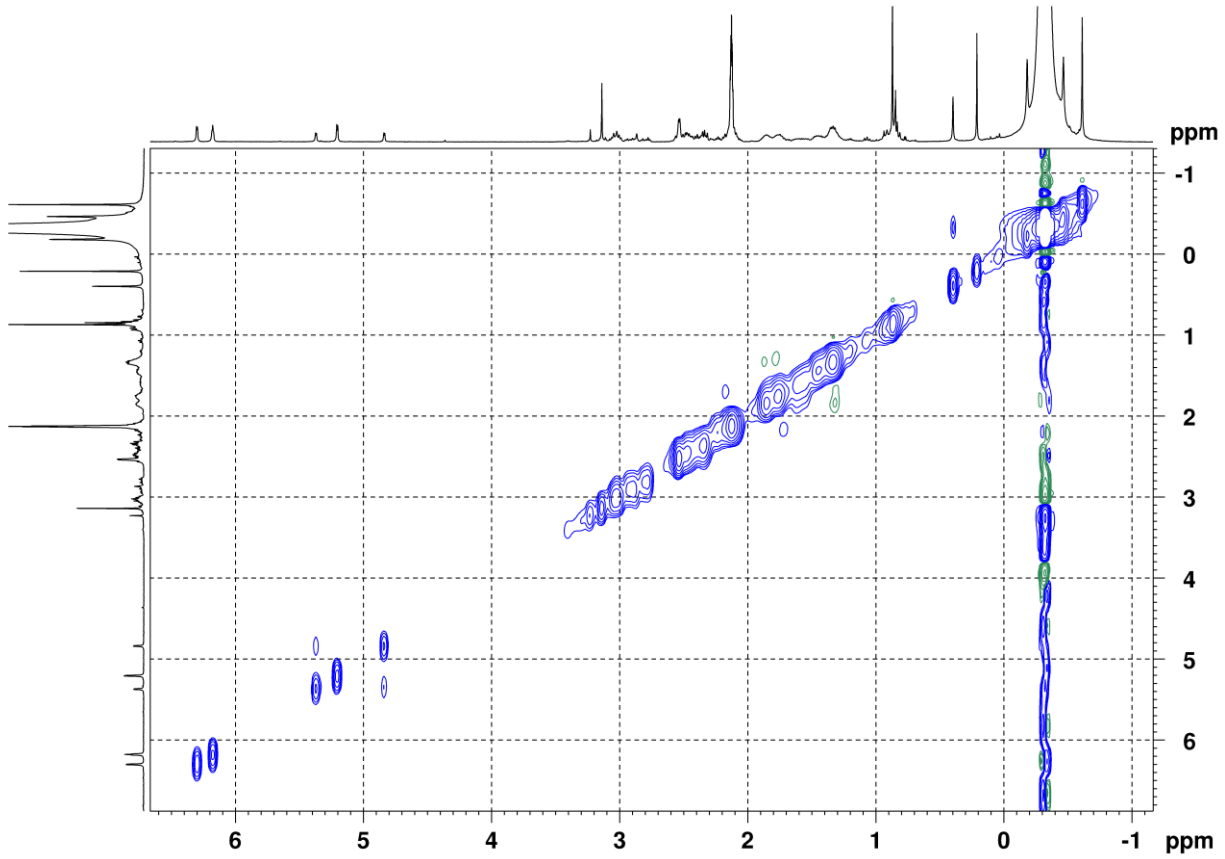
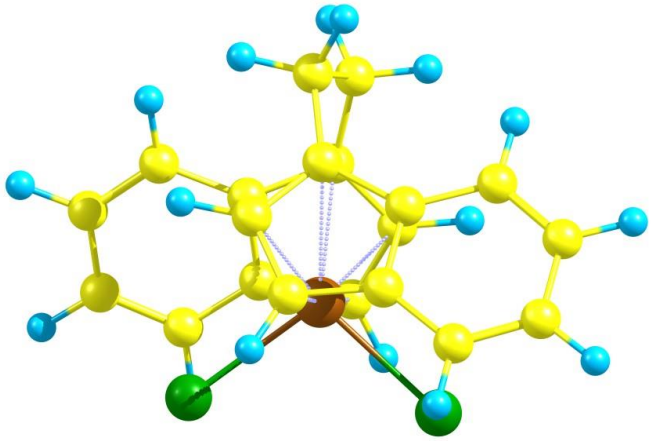


Table S3. Calculated thermodynamic parameters (298.15 K, 1 atm, [S] = cal/(mol*K); [H] = [G] = kcal/mol) for conformers of complexes **1m** and **5m**.

Conformer	H^0	G^0	S^0
1m-a	-1091010.3	-1091050.6	135.2
1m-b	-1091009.3	-1091051.9	142.8
5m-a	-827199.7	-827242.4	143.2
5m-b	-827200.1	-827242.2	141.2

Cartesian coordinates

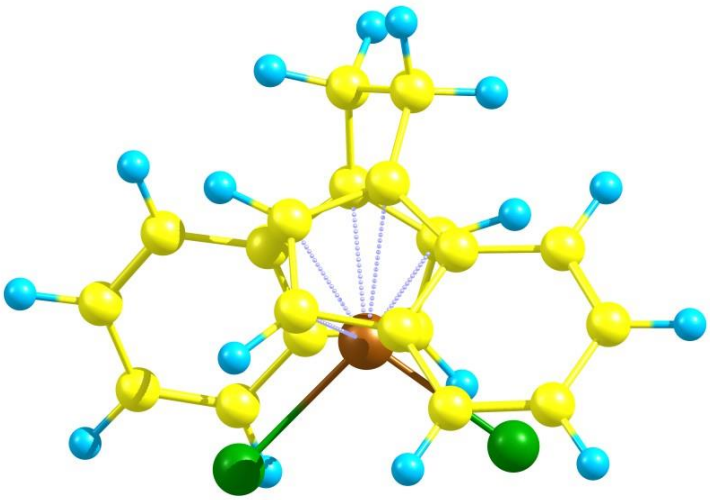
Conformer 1m-a



40	0.000007000	-0.483960000	0.000031000
6	-2.044984000	1.010879000	-0.499507000
6	-2.341418000	-0.212938000	-1.200033000
6	-1.330957000	-0.405328000	-2.186284000
6	-0.475153000	0.721411000	-2.144901000
6	-0.877834000	1.594084000	-1.099828000
1	-1.240637000	-1.252574000	-2.860286000
1	0.400343000	0.871753000	-2.776608000
6	1.331090000	-0.405336000	2.186238000
6	0.475318000	0.721441000	2.144939000
6	0.877930000	1.594100000	1.099841000
6	2.045026000	1.010861000	0.499426000
6	2.341480000	-0.212968000	1.199917000
1	1.240791000	-1.252575000	2.860253000
1	-0.400124000	0.871764000	2.776723000
17	1.325085000	-2.019787000	-1.317803000
6	2.894469000	1.434270000	-0.569605000
6	3.487978000	-0.978199000	0.841680000
6	3.985573000	0.669352000	-0.886759000
6	4.285281000	-0.534524000	-0.177315000
1	2.698847000	2.369032000	-1.096681000
1	4.650487000	0.986675000	-1.690583000
1	5.166733000	-1.108464000	-0.463795000
1	3.710300000	-1.903795000	1.373006000
6	-3.487950000	-0.978150000	-0.841890000
6	-2.894460000	1.434260000	0.569501000
6	-3.985599000	0.669352000	0.886575000
6	-4.285302000	-0.534489000	0.177079000
1	-3.710267000	-1.903723000	-1.373259000
1	-5.166782000	-1.108419000	0.463491000

1	-4.650533000	0.986665000	1.690386000
1	-2.698857000	2.369004000	1.096620000
6	-0.241144000	2.906509000	-0.729882000
6	0.241250000	2.906526000	0.729884000
1	0.604392000	3.082556000	-1.409876000
1	-0.950033000	3.733244000	-0.895230000
1	-0.604286000	3.082597000	1.409873000
1	0.950153000	3.733255000	0.895207000
17	-1.325343000	-2.019346000	1.318099000

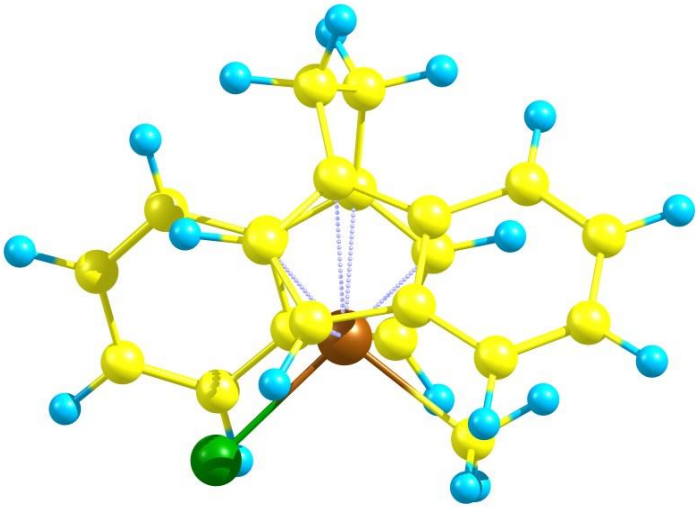
Conformer 1m-b



40	-0.001353000	-0.317782000	0.094278000
6	2.276766000	0.918210000	0.202608000
6	2.426413000	-0.179594000	1.125980000
6	1.466143000	-0.005466000	2.162412000
6	0.778044000	1.207021000	1.911891000
6	1.252654000	1.785735000	0.702534000
1	1.293441000	-0.675401000	2.999882000
1	-0.020938000	1.609674000	2.534705000
6	-1.131789000	-0.098445000	-2.182833000
6	-0.492531000	1.123114000	-1.873648000
6	-1.149146000	1.741877000	-0.769205000
6	-2.254549000	0.902694000	-0.422853000
6	-2.236667000	-0.246440000	-1.294105000
1	-0.827924000	-0.803043000	-2.951141000
1	0.393478000	1.506682000	-2.378921000
17	-1.307660000	-1.549778000	1.712281000
6	-3.281293000	1.030348000	0.560199000
6	-3.229400000	-1.260401000	-1.154643000
6	-4.224312000	0.043713000	0.653658000
6	-4.195942000	-1.104538000	-0.199356000
1	-3.316907000	1.904246000	1.212305000
1	-5.019262000	0.126547000	1.395398000
1	-4.965222000	-1.867521000	-0.078734000
1	-3.208264000	-2.135589000	-1.804552000
6	3.414822000	-1.178932000	0.888987000
6	3.101716000	0.977136000	-0.963870000
6	4.034475000	-0.005028000	-1.159062000
6	4.196233000	-1.079686000	-0.228383000
1	3.529149000	-2.006752000	1.589060000
1	4.956529000	-1.835496000	-0.426009000

1	4.677740000	0.030115000	-2.038782000
1	3.007562000	1.805982000	-1.667842000
6	0.773161000	3.068142000	0.076081000
6	-0.748650000	3.034623000	-0.112184000
1	1.068974000	3.933474000	0.687986000
1	1.264464000	3.195305000	-0.900166000
1	-1.085726000	3.901236000	-0.701858000
1	-1.245241000	3.109243000	0.867502000
17	1.007389000	-2.163866000	-1.103763000

Conformer 5m-a



40	0.006571000	-0.547729000	0.100062000
6	-2.152373000	0.748415000	-0.547341000
6	-2.425258000	-0.609946000	-0.945153000
6	-1.472832000	-0.970495000	-1.943585000
6	-0.680716000	0.172885000	-2.204631000
6	-1.058020000	1.231884000	-1.339113000
1	-1.386396000	-1.935431000	-2.435647000
1	0.143545000	0.219392000	-2.916712000
6	1.273828000	0.064770000	2.261264000
6	0.377977000	1.120469000	1.971221000
6	0.766801000	1.767988000	0.769434000
6	1.961652000	1.116908000	0.316976000
6	2.288045000	0.075621000	1.259226000
1	1.221641000	-0.604687000	3.115057000
1	-0.508758000	1.374545000	2.552292000
17	1.334693000	-2.340656000	-0.843460000
6	2.806677000	1.332746000	-0.815299000
6	3.461382000	-0.710462000	1.069352000
6	3.923923000	0.553436000	-0.964159000
6	4.254305000	-0.465450000	-0.018439000
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1	4.584032000	0.715361000	-1.816898000
1	5.153922000	-1.060211000	-0.177423000
1	3.709138000	-1.497178000	1.782600000
6	-3.515571000	-1.315718000	-0.360894000
6	-2.957155000	1.357690000	0.464285000
6	-3.990672000	0.642639000	1.011715000
6	-4.275298000	-0.693862000	0.593238000
1	-3.734488000	-2.335754000	-0.679542000
1	-5.116867000	-1.220338000	1.044418000
1	-4.623254000	1.104615000	1.770472000
1	-2.778955000	2.390822000	0.765812000

6	-0.441982000	2.604370000	-1.285140000
6	0.082801000	2.942556000	0.121530000
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1	-1.171127000	3.365198000	-1.607101000
1	-0.747309000	3.256375000	0.770295000
1	0.771679000	3.800505000	0.067145000
6	-1.134868000	-1.752368000	1.600003000
1	-1.623885000	-2.596977000	1.087864000
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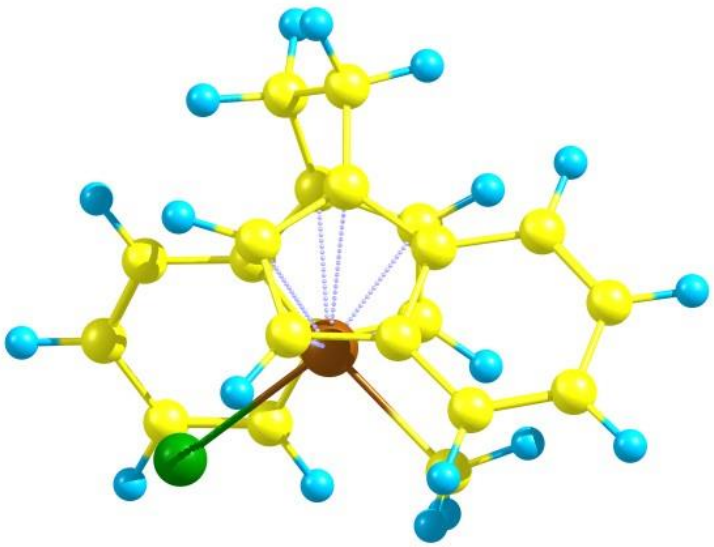
1	-1.917862000	-1.163723000	2.109712000

Conformer 5m-b



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6	-0.988859000	0.741013000	-2.071492000
6	-1.406729000	1.516041000	-0.957439000
1	-1.465889000	-1.334967000	-2.750163000
1	-0.258825000	1.054795000	-2.818112000
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6	0.350482000	1.378005000	1.663224000
6	1.028185000	1.818826000	0.492314000
6	2.175534000	0.974125000	0.338933000
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6	4.201525000	-0.003439000	-0.514220000
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