Supplemental Information for:

"Synthesis, structural studies and reactivity of vanadium complexes with tridentate (OSO) ligand"

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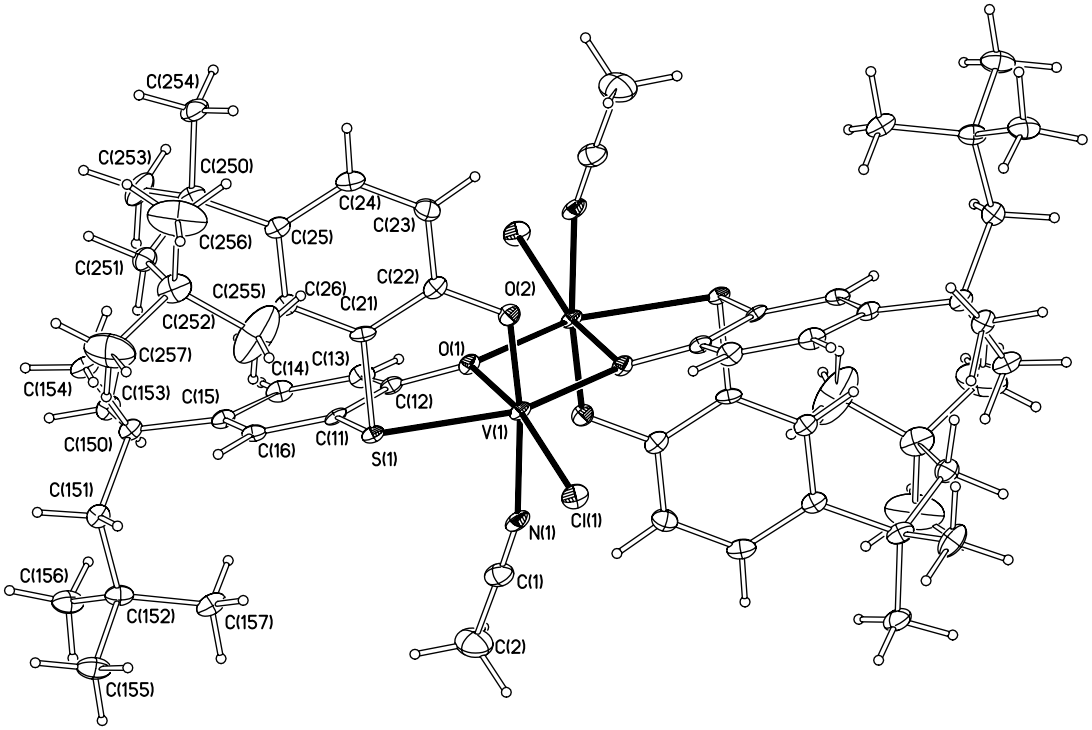
1. Details of the crystal structure determination for **1**·4CH_3CN.
2. Polymerisation data for **1** and **2**.

Details of the crystal structure determination for 1·4CH_3CN (CCDC 604895)



Symmetry transformations used to generate equivalent atoms: -x,-y+2,-z+1

Table S-1. Crystal data and structure refinement for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$.

Compund	$C_{60}H_{86}Cl_2N_2O_4S_2V_2 \cdot 4CH3CN$
Chemical formula	$C_{68}H_{98}Cl_2N_6O_4S_2V_2$
CCDC	604895
Formula weight	1300.44
λ (Å)	0.71073
T(K)	100(2)
Space group	P -1
Crystal system	Triclinic
Unit cell dimensions	
a(Å)	8.480(3)
b(Å)	14.312(5)
c(Å)	15.312(7)
alpha(°)	93.17(3)
Beta(°)	93.88(3)
gamma(°)	102.56(3)
V(Å^3)	1805.0(12)
Z	1
D_c(Mg/m^3)	1.196
F(000)	692
Habit	block
Crystal size (mm)	0.63 x 0.40 x 0.35
μ (mm^{-1})	0.438
Absorption correction	Empirical (SHELXA)
Max. and min.	transmission 0.833 and 0.483
Type of diffractometer	Kuma KM4 automatic diffractometer
Diffraction geometry	ω-2θ
Theta range (°)	2.05to 25.08
Number of reflections measured	6873
Number of unique reflections	6402
$R_{(int)}$	0.0409
Number of observed reflections	4695[I>2σ(I)]
Refinement method	least-squares on F^2
Number of parameters	392
Final R indices [I>2σ(I)]	R_1 = 0.0568, wR_2 =0.1552
Final R indices (all data)	R_1 =0.0846, wR_2 =0.1723
Goodness-of-fit (S)	1.043
Largest diff. peak and hole e.Å^{-3}	0.836 and -1.058

$R_1 = \Sigma||F_O| - |F_c|| / \Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table S-2. Bond lengths [Å] and angles [deg] for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$.

V(1)-O(2)	1.873(2)
V(1)-O(1)	1.999(2)
V(1)-N(1)	2.163(3)
V(1)-Cl(1)	2.3148(12)
V(1)-S(1)	2.4741(13)
S(1)-C(11)	1.779(3)
S(1)-C(21)	1.788(3)
O(1)-C(12)	1.356(4)
O(2)-C(22)	1.345(4)
N(1)-C(1)	1.144(4)
N(2)-C(3)	1.132(5)
C(1)-C(2)	1.459(5)
C(3)-C(4)	1.457(5)
C(11)-C(16)	1.381(4)
C(11)-C(12)	1.408(4)
C(12)-C(13)	1.399(4)
C(13)-C(14)	1.380(5)
C(14)-C(15)	1.394(4)
C(15)-C(16)	1.402(4)
C(15)-C(150)	1.529(4)
C(21)-C(26)	1.385(4)
C(21)-C(22)	1.396(4)
C(22)-C(23)	1.401(4)
C(23)-C(24)	1.385(5)
C(24)-C(25)	1.406(5)
C(25)-C(26)	1.395(4)
C(25)-C(250)	1.526(4)
C(150)-C(153)	1.534(4)
C(150)-C(151)	1.546(4)
C(150)-C(154)	1.551(4)
C(151)-C(152)	1.548(4)
C(152)-C(157)	1.522(5)
C(152)-C(156)	1.538(4)
C(152)-C(155)	1.543(4)
C(250)-C(254)	1.540(4)
C(250)-C(253)	1.547(5)
C(250)-C(251)	1.548(5)
C(251)-C(252)	1.540(5)
C(252)-C(255)	1.519(6)
C(252)-C(256)	1.524(6)
C(252)-C(257)	1.528(6)
N(3)-C(5)	1.174(11)
C(5)-C(6)	1.466(12)
O(2)-V(1)-O(1)	96.21(9)
O(2)-V(1)-N(1)	173.34(10)
O(1)-V(1)-N(1)	80.13(9)
O(2)-V(1)-Cl(1)	98.05(8)
O(1)-V(1)-Cl(1)	165.39(7)
N(1)-V(1)-Cl(1)	85.37(8)
O(2)-V(1)-S(1)	84.69(8)
O(1)-V(1)-S(1)	81.63(7)
N(1)-V(1)-S(1)	89.25(8)
Cl(1)-V(1)-S(1)	96.51(4)
C(11)-S(1)-C(21)	101.86(13)
C(11)-S(1)-V(1)	94.88(10)
C(21)-S(1)-V(1)	92.49(11)

C(12)-O(1)-V(1)	121.18(17)
C(22)-O(2)-V(1)	122.27(19)
C(1)-N(1)-V(1)	165.8(3)
N(1)-C(1)-C(2)	178.6(4)
N(2)-C(3)-C(4)	179.4(4)
C(16)-C(11)-C(12)	121.6(3)
C(16)-C(11)-S(1)	120.1(2)
C(12)-C(11)-S(1)	118.3(2)
O(1)-C(12)-C(13)	123.3(3)
O(1)-C(12)-C(11)	119.5(2)
C(13)-C(12)-C(11)	117.2(3)
C(14)-C(13)-C(12)	120.4(3)
C(13)-C(14)-C(15)	122.8(3)
C(14)-C(15)-C(16)	116.7(3)
C(14)-C(15)-C(150)	123.7(3)
C(16)-C(15)-C(150)	119.6(3)
C(11)-C(16)-C(15)	121.2(3)
C(26)-C(21)-C(22)	122.3(3)
C(26)-C(21)-S(1)	120.4(2)
C(22)-C(21)-S(1)	117.3(2)
O(2)-C(22)-C(21)	121.9(3)
O(2)-C(22)-C(23)	121.2(3)
C(21)-C(22)-C(23)	116.9(3)
C(24)-C(23)-C(22)	120.9(3)
C(23)-C(24)-C(25)	122.1(3)
C(26)-C(25)-C(24)	116.8(3)
C(26)-C(25)-C(250)	119.4(3)
C(24)-C(25)-C(250)	123.7(3)
C(21)-C(26)-C(25)	121.0(3)
C(15)-C(150)-C(153)	111.8(2)
C(15)-C(150)-C(151)	112.5(2)
C(153)-C(150)-C(151)	112.2(2)
C(15)-C(150)-C(154)	106.8(2)
C(153)-C(150)-C(154)	107.0(2)
C(151)-C(150)-C(154)	106.0(2)
C(150)-C(151)-C(152)	122.5(2)
C(157)-C(152)-C(156)	110.2(3)
C(157)-C(152)-C(155)	107.9(3)
C(156)-C(152)-C(155)	107.3(3)
C(157)-C(152)-C(151)	113.5(3)
C(156)-C(152)-C(151)	112.1(3)
C(155)-C(152)-C(151)	105.4(2)
C(25)-C(250)-C(254)	111.9(3)
C(25)-C(250)-C(253)	107.7(3)
C(254)-C(250)-C(253)	107.0(3)
C(25)-C(250)-C(251)	112.6(3)
C(254)-C(250)-C(251)	111.5(3)
C(253)-C(250)-C(251)	105.8(3)
C(252)-C(251)-C(250)	124.7(3)
C(255)-C(252)-C(256)	111.3(5)
C(255)-C(252)-C(257)	106.7(4)
C(256)-C(252)-C(257)	107.2(3)
C(255)-C(252)-C(251)	112.8(3)
C(256)-C(252)-C(251)	112.5(3)
C(257)-C(252)-C(251)	106.0(4)
N(3)-C(5)-C(6)	177.7(9)

Table S-3. Torsion angles [deg] for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$.

O(2)-V(1)-S(1)-C(11)	110.99(12)
O(1)-V(1)-S(1)-C(11)	13.90(11)
N(1)-V(1)-S(1)-C(11)	-66.24(12)
Cl(1)-V(1)-S(1)-C(11)	-151.49(10)
O(2)-V(1)-S(1)-C(21)	8.86(11)
O(1)-V(1)-S(1)-C(21)	-88.23(11)
N(1)-V(1)-S(1)-C(21)	-168.37(11)
Cl(1)-V(1)-S(1)-C(21)	106.38(10)
O(2)-V(1)-O(1)-C(12)	-104.9(2)
N(1)-V(1)-O(1)-C(12)	69.5(2)
Cl(1)-V(1)-O(1)-C(12)	62.4(3)
S(1)-V(1)-O(1)-C(12)	-21.24(19)
O(1)-V(1)-O(2)-C(22)	70.6(2)
N(1)-V(1)-O(2)-C(22)	14.3(9)
Cl(1)-V(1)-O(2)-C(22)	-106.2(2)
S(1)-V(1)-O(2)-C(22)	-10.4(2)
O(2)-V(1)-N(1)-C(1)	4.6(16)
O(1)-V(1)-N(1)-C(1)	-52.5(10)
Cl(1)-V(1)-N(1)-C(1)	125.7(10)
S(1)-V(1)-N(1)-C(1)	29.1(10)
V(1)-N(1)-C(1)-C(2)	10(16)
C(21)-S(1)-C(11)-C(16)	-95.4(3)
V(1)-S(1)-C(11)-C(16)	171.0(2)
C(21)-S(1)-C(11)-C(12)	84.5(2)
V(1)-S(1)-C(11)-C(12)	-9.1(2)
V(1)-O(1)-C(12)-C(13)	-160.0(2)
V(1)-O(1)-C(12)-C(11)	21.7(3)
C(16)-C(11)-C(12)-O(1)	175.1(3)
S(1)-C(11)-C(12)-O(1)	-4.8(4)
C(16)-C(11)-C(12)-C(13)	-3.3(4)
S(1)-C(11)-C(12)-C(13)	176.8(2)
O(1)-C(12)-C(13)-C(14)	-173.8(3)
C(11)-C(12)-C(13)-C(14)	4.5(4)
C(12)-C(13)-C(14)-C(15)	-2.2(5)
C(13)-C(14)-C(15)-C(16)	-1.5(4)
C(13)-C(14)-C(15)-C(150)	174.9(3)
C(12)-C(11)-C(16)-C(15)	-0.3(4)
S(1)-C(11)-C(16)-C(15)	179.6(2)
C(14)-C(15)-C(16)-C(11)	2.7(4)
C(150)-C(15)-C(16)-C(11)	-173.8(3)
C(11)-S(1)-C(21)-C(26)	76.7(2)
V(1)-S(1)-C(21)-C(26)	172.2(2)
C(11)-S(1)-C(21)-C(22)	-103.8(2)
V(1)-S(1)-C(21)-C(22)	-8.3(2)
V(1)-O(2)-C(22)-C(21)	7.7(4)
V(1)-O(2)-C(22)-C(23)	-170.9(2)
C(26)-C(21)-C(22)-O(2)	-177.6(3)
S(1)-C(21)-C(22)-O(2)	3.0(4)
C(26)-C(21)-C(22)-C(23)	1.1(4)
S(1)-C(21)-C(22)-C(23)	-178.4(2)
O(2)-C(22)-C(23)-C(24)	178.1(3)
C(21)-C(22)-C(23)-C(24)	-0.6(4)
C(22)-C(23)-C(24)-C(25)	-0.1(5)
C(23)-C(24)-C(25)-C(26)	0.4(4)
C(23)-C(24)-C(25)-C(250)	-178.0(3)
C(22)-C(21)-C(26)-C(25)	-0.8(4)
S(1)-C(21)-C(26)-C(25)	178.6(2)

C(24)-C(25)-C(26)-C(21)	0.1(4)
C(250)-C(25)-C(26)-C(21)	178.6(3)
C(14)-C(15)-C(150)-C(153)	1.1(4)
C(16)-C(15)-C(150)-C(153)	177.4(3)
C(14)-C(15)-C(150)-C(151)	128.5(3)
C(16)-C(15)-C(150)-C(151)	-55.2(3)
C(14)-C(15)-C(150)-C(154)	-115.6(3)
C(16)-C(15)-C(150)-C(154)	60.6(3)
C(15)-C(150)-C(151)-C(152)	-72.6(3)
C(153)-C(150)-C(151)-C(152)	54.6(4)
C(154)-C(150)-C(151)-C(152)	171.1(3)
C(150)-C(151)-C(152)-C(157)	48.9(4)
C(150)-C(151)-C(152)-C(156)	-76.8(4)
C(150)-C(151)-C(152)-C(155)	166.8(3)
C(26)-C(25)-C(250)-C(254)	-179.6(3)
C(24)-C(25)-C(250)-C(254)	-1.3(4)
C(26)-C(25)-C(250)-C(253)	-62.3(4)
C(24)-C(25)-C(250)-C(253)	116.0(3)
C(26)-C(25)-C(250)-C(251)	53.9(4)
C(24)-C(25)-C(250)-C(251)	-127.7(3)
C(25)-C(250)-C(251)-C(252)	61.0(4)
C(254)-C(250)-C(251)-C(252)	-65.7(4)
C(253)-C(250)-C(251)-C(252)	178.4(3)
C(250)-C(251)-C(252)-C(255)	-62.5(5)
C(250)-C(251)-C(252)-C(256)	64.3(5)
C(250)-C(251)-C(252)-C(257)	-178.9(3)

Table S-4. Hydrogen bonds for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$ [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13)...Cl(1)$^{(i)}$	0.95	2.79	3.518(4)	134
C(6)-H(6A)...O(2)$^{(ii)}$	0.98	2.52	3.429(7)	155

Symmetry transformations used to generate equivalent atoms:
$^{(i)}$ -x,-y+2,-z+1; $^{(ii)}$ -x+1,-y+2,-z+1

Table S-5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
V(1)	1431(1)	9472(1)	5084(1)	12(1)
Cl(1)	3216(1)	9071(1)	6134(1)	21(1)
S(1)	2897(1)	9140(1)	3799(1)	11(1)
O(1)	306(2)	10135(1)	4201(1)	14(1)
O(2)	149(3)	8240(2)	4789(1)	16(1)
N(1)	2972(3)	10898(2)	5266(2)	18(1)
N(2)	4963(4)	1546(2)	8423(2)	32(1)
C(1)	3798(4)	11628(2)	5178(2)	24(1)
C(2)	4842(5)	12554(3)	5045(3)	41(1)
C(3)	3692(4)	1387(2)	8088(2)	23(1)
C(4)	2051(5)	1185(3)	7666(3)	41(1)
C(11)	2211(3)	9990(2)	3151(2)	11(1)
C(12)	997(3)	10424(2)	3460(2)	13(1)
C(13)	538(4)	11126(2)	2962(2)	17(1)
C(14)	1179(4)	11324(2)	2170(2)	16(1)
C(15)	2336(4)	10871(2)	1841(2)	14(1)
C(16)	2865(3)	10209(2)	2366(2)	13(1)
C(21)	1426(3)	8062(2)	3459(2)	13(1)
C(22)	240(4)	7741(2)	4030(2)	15(1)
C(23)	-883(4)	6882(2)	3768(2)	20(1)
C(24)	-812(4)	6387(2)	2974(2)	20(1)
C(25)	374(4)	6718(2)	2396(2)	16(1)
C(26)	1492(4)	7572(2)	2662(2)	14(1)
C(150)	2962(4)	11018(2)	934(2)	14(1)
C(151)	4834(4)	11283(2)	970(2)	15(1)
C(152)	5841(4)	12281(2)	1335(2)	18(1)
C(153)	2190(4)	11734(2)	445(2)	17(1)
C(154)	2430(4)	10036(2)	394(2)	21(1)
C(155)	7607(4)	12164(3)	1458(3)	28(1)
C(156)	5800(4)	13053(2)	679(2)	24(1)
C(157)	5364(4)	12610(2)	2222(2)	22(1)
C(250)	464(4)	6212(2)	1503(2)	19(1)
C(251)	2164(4)	6017(2)	1380(2)	21(1)
C(252)	3001(4)	5391(3)	1958(3)	30(1)
C(253)	170(5)	6896(3)	792(2)	29(1)
C(254)	-871(4)	5288(2)	1322(2)	24(1)
C(255)	3325(8)	5785(4)	2911(3)	73(2)
C(256)	2093(6)	4343(3)	1883(4)	62(2)
C(257)	4653(5)	5426(4)	1605(4)	58(1)
N(3)	7410(12)	14625(5)	4619(6)	130(3)
C(5)	8322(11)	14193(5)	4345(5)	86(2)
C(6)	9408(10)	13631(5)	3981(4)	84(2)

#1 -x,-y+2,-z+1 #2 -x+1,-y+2,-z+1

Table S-6. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{60}H_{86}Cl_2N_2O_4S_2V_2$ (**1**)·$4CH_3CN$.

	U11	U22	U33	U23	U13	U12
V(1)	11(1)	14(1)	12(1)	0(1)	-5(1)	7(1)
Cl(1)	17(1)	29(1)	19(1)	6(1)	-6(1)	11(1)
S(1)	11(1)	11(1)	13(1)	1(1)	-5(1)	5(1)
O(1)	12(1)	18(1)	13(1)	-1(1)	-3(1)	8(1)
O(2)	17(1)	16(1)	15(1)	1(1)	0(1)	4(1)
N(1)	16(1)	23(2)	15(1)	-3(1)	-7(1)	7(1)
N(2)	24(2)	38(2)	35(2)	1(1)	-3(1)	9(1)
C(1)	19(2)	24(2)	28(2)	-4(1)	-3(1)	7(2)
C(2)	36(2)	27(2)	56(3)	-6(2)	6(2)	-3(2)
C(3)	26(2)	18(2)	23(2)	0(1)	-1(1)	7(1)
C(4)	29(2)	46(2)	43(2)	-9(2)	-17(2)	8(2)
C(11)	13(1)	9(1)	11(1)	-2(1)	-6(1)	4(1)
C(12)	12(1)	13(1)	13(1)	0(1)	-4(1)	4(1)
C(13)	16(2)	17(2)	21(2)	0(1)	-3(1)	12(1)
C(14)	16(2)	13(1)	20(2)	5(1)	-6(1)	8(1)
C(15)	15(1)	12(1)	14(2)	3(1)	-5(1)	3(1)
C(16)	9(1)	11(1)	19(2)	-1(1)	-4(1)	5(1)
C(21)	10(1)	10(1)	19(2)	0(1)	-6(1)	4(1)
C(22)	17(2)	14(1)	16(2)	1(1)	-4(1)	8(1)
C(23)	18(2)	17(2)	24(2)	4(1)	1(1)	2(1)
C(24)	17(2)	15(2)	26(2)	-1(1)	-4(1)	2(1)
C(25)	15(2)	14(1)	19(2)	0(1)	-4(1)	8(1)
C(26)	15(1)	14(1)	15(1)	3(1)	-3(1)	8(1)
C(150)	15(2)	14(2)	15(2)	2(1)	-4(1)	8(1)
C(151)	17(2)	14(1)	17(2)	4(1)	-1(1)	8(1)
C(152)	15(2)	15(2)	24(2)	5(1)	-5(1)	4(1)
C(153)	19(2)	20(2)	15(2)	5(1)	-4(1)	10(1)
C(154)	22(2)	16(2)	22(2)	-2(1)	-7(1)	4(1)
C(155)	15(2)	30(2)	39(2)	5(2)	-6(1)	4(1)
C(156)	22(2)	16(2)	31(2)	9(1)	-4(1)	-1(1)
C(157)	25(2)	17(2)	22(2)	-2(1)	-8(1)	4(1)
C(250)	20(2)	16(2)	21(2)	-1(1)	-6(1)	5(1)
C(251)	22(2)	18(2)	21(2)	-5(1)	2(1)	3(1)
C(252)	28(2)	24(2)	39(2)	-5(2)	-4(2)	15(2)
C(253)	44(2)	27(2)	18(2)	-1(1)	-9(2)	14(2)
C(254)	22(2)	23(2)	25(2)	-9(1)	-4(1)	3(1)
C(255)	106(5)	91(4)	44(3)	-13(3)	-32(3)	83(4)
C(256)	42(3)	30(2)	116(5)	22(3)	-13(3)	15(2)
C(257)	31(2)	46(3)	99(4)	-2(3)	1(2)	17(2)
N(3)	153(8)	71(4)	165(8)	42(5)	54(6)	6(5)
C(5)	109(6)	62(4)	72(4)	22(3)	-10(4)	-14(4)
C(6)	114(6)	66(4)	65(4)	20(3)	-12(4)	3(4)

``The anisotropic temperature factors are expressed as:
$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{23}klb^*c^* + 2U_{13}hla^*c^*)]$.

Tables of polymerisation data for 1·and 2.

Tabela S-7. Ethene Polymerizsation Catalyzed by **1**-Cocatalyst System Depending on Temperature[a]

Run no.	Cocatalyst.	[V] mmol/dm^3	Al:V	Activity kgPE/molVh	d_n, g/dm^3	M_w/M_n	T K
1	Al(i-Bu)$_3$	0,01	1000	1516	145	3,11	293
2	Al(i-Bu)$_3$	0,01	1000	2994	138	2,68	303
3	Al(i-Bu)$_3$	0,01	1000	6320	130	3,32	313
4	Al(i-Bu)$_3$	0,01	1000	10624	133	3,47	323
5	Al(i-Bu)$_3$	0,01	1000	9236	128	3,75	333
6	Al(i-Bu)$_3$	0,01	1000	4288	116	4,16	343

[a] Polymerisation conditions: P_{ethene} = 0,5 MPa, time = 30 min, V_{hexane} = 1 L

Tabela S-8. Ethene Polymerisation Catalyzed by **2**-Cocatalyst System Depending on Temperature[a]

Run no.	Cocatalyst	[V] mmol/dm^3	Al:V	Activity kgPE/molVh	d_n, g/dm^3	M_w/M_n	T_p K
1	Al(i-Bu)$_3$	0,01	1000	974	123	3,22	293
2	Al(i-Bu)$_3$	0,01	1000	1590	134	3,17	303
3	Al(i-Bu)$_3$	0,01	1000	2416	129	3,51	313
4	Al(i-Bu)$_3$	0,01	1000	3068	133	3,74	323
5	Al(i-Bu)$_3$	0,01	1000	3632	125	3,65	333
6	Al(i-Bu)$_3$	0,01	1000	2906	127	3,98	343

[a] Polymerisation conditions: P_{ethene} = 0,5 MPa, time = 30 min, V_{hexane} = 1 L