Supporting Information

Micellization and Adsorption Properties of New Cationic Gemini Surfactants Having Hydroxyisopropyl Group

Ziyafaddin H. Asadov[a], Gulnara A. Ahmadova[a], Ravan A. Rahimov[a,b*], Seyid-Zeynab F. Hashimzade[a], Etibar H. Ismailov[a], Nahida Z. Asadova[c], Samira A. Suleymanova[a], Fedor I. Zubkov[d], Ayaz M. Mammadov[a], Durna B. Agamaliyeva[a]

[a]*Institute of Petrochemical Processes of Azerbaijan National Academy of Sciences, Hojaly ave. 30, AZ 1025, Baku, Azerbaijan*

[b]*Department of Chemical Engineering, Baku Engineering University, Hasan Aliyev str. 120, Baku, Absheron, AZ0101, Azerbaijan*

[c]*Faculty of Biology, Baku State University, Z. Xalilov str. 23, Az 1148 Baku, Azerbaijan*

[d]*Organic Chemistry Department, Faculty of Science, Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya St., Moscow, 117198, Russian Federation*

***Corresponding author:**

Dr. Ravan A. Rahimov

Institute of Petrochemical Processes of Azerbaijan National Academy of Sciences, Hojaly ave. 30, Az 1025, Baku, Azerbaijan

Tel.: +99450 545 20 48 Fax: +99412 490 24 76

e-mail: revan_chem@mail.ru

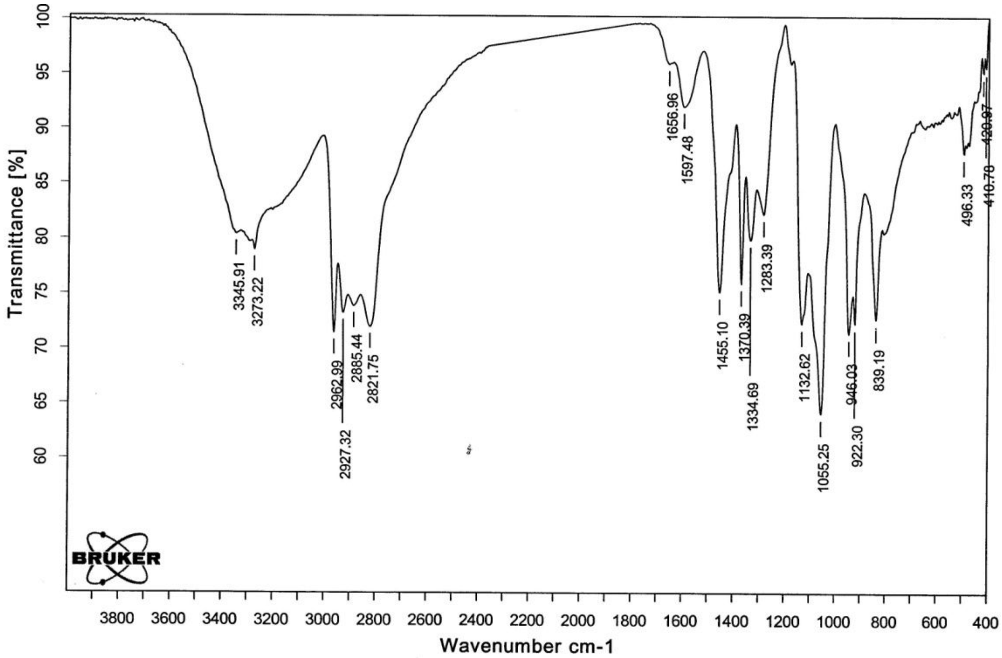

Fig. S1. IR spectrum of N,N'-Bis(2-hydroxypropyl)ethylenediamine

IR-spectrum ν, cm^{-1}: 3345 ν (NH), 3273 ν (OH), 2962, 2927 and 2885 ν (CH), 1656, 1597 δ (NH), 1455, 1370 and 1334 δ (CH), 1283, 1132 ν (C-N), 1055 and 946 ν (C-O).

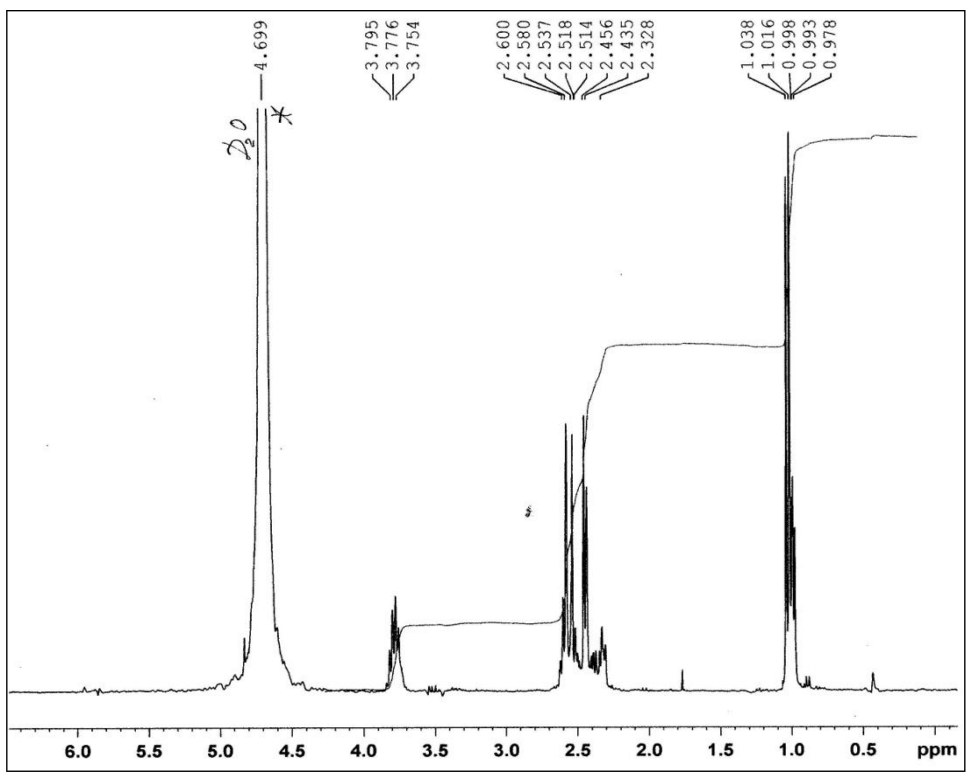

Fig. S2. ^{1}H-NMR spectrum of N,N'-Bis(2-hydroxypropyl)ethylenediamine

^{1}H-NMR, (300.13 MHz, D_2O), δ (ppm): 0.98-1.04 (CH-C$\underline{H_3}$), 2.33-2.60 (C$\underline{H_2}$-N^+H), 3.75-3.80 (C$\underline{H}$-OH).

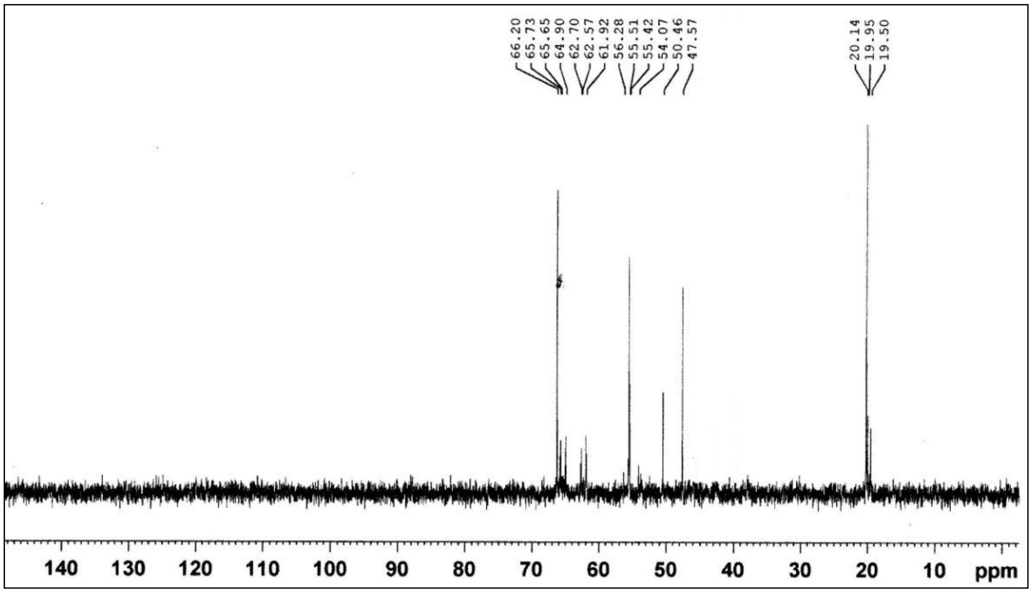

Fig. S3. ^{13}C-NMR spectrum of N,N'-Bis(2-hydroxypropyl)ethylenediamine

^{13}C NMR, (75.47 MHz, D_2O), δ (ppm): 19.5-20.1 ($\underline{C}H_3$-CH), 47.6-56.3 (NH^+-$\underline{C}H_2$-$\underline{C}H_2$-NH^+), 61.9-66.2 (NH^+-$\underline{C}H_2$-$\underline{C}$H-OH).

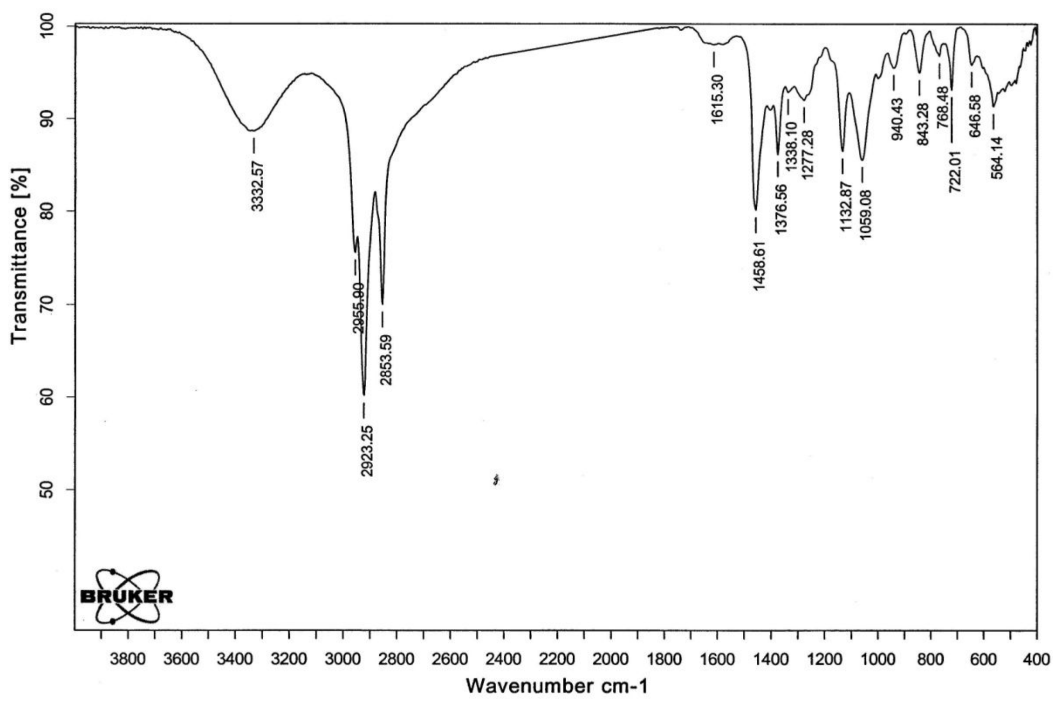

Fig. S4. IR spectrum of $C_9C_2C_9$[iso-Pr(OH)]

IR-spectrum ν, cm^{-1}: 3332 ν (OH) and (NH), 2923 and 2853 ν (CH), 1458 and 1376 δ

(CH), 1132 ν (C-N), 1059 and 940 ν (C-O), 722 δ -$(CH_2)_x$.

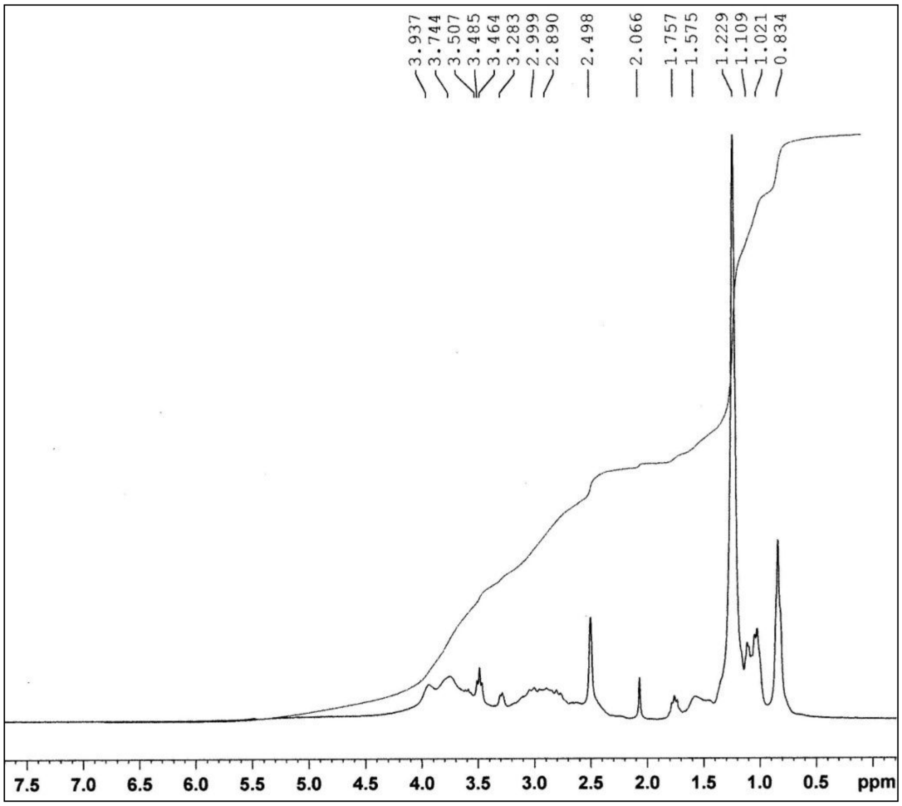

Fig. S5. ^{1}H-NMR spectrum of $C_9C_2C_9$[iso-Pr(OH)]

^{1}H-NMR, (300.13 MHz, DMSO-d_6), δ (ppm): 0.83 (C*H*$_3$), 1.02-1.11 (CH-C*H*$_3$), 1.23 (C*H*$_2$ chain), 1.58-1.76 (C*H*$_2$-CH_2-N^+H), 2.89-3.74 (C*H*$_2$-N^+H), 3.94 (C*H*-OH).

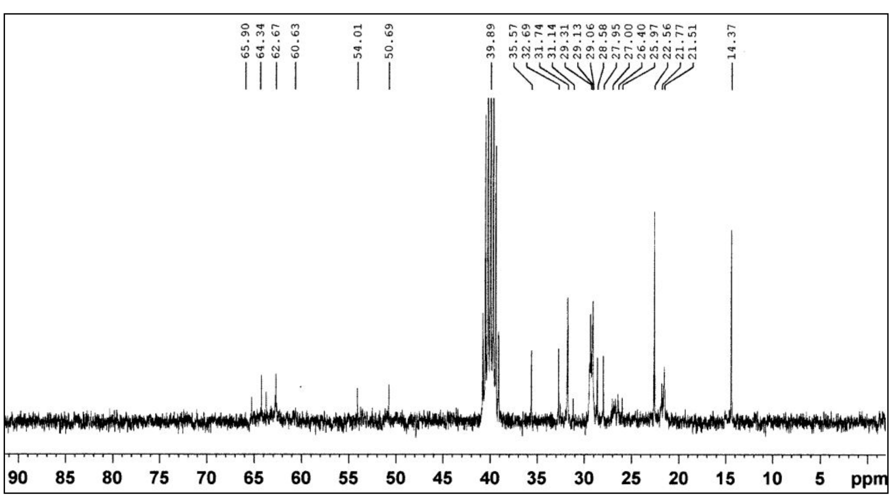

Fig. S6. ^{13}C-NMR spectrum of $C_9C_2C_9$[iso-Pr(OH)]

^{13}C NMR, (75.47 MHz, DMSO-d_6), δ (ppm): 14.4 ($\underline{C}H_3$), 21.5 ($\underline{C}H_3$-CH), 22.6–32.7 (alkyl group $\underline{C}H_2$), 54.2-54.6 (NH^+-$\underline{C}H_2$-CH_2), 59.8-65.9 (NH^+-CH_2-$\underline{C}$H-OH).

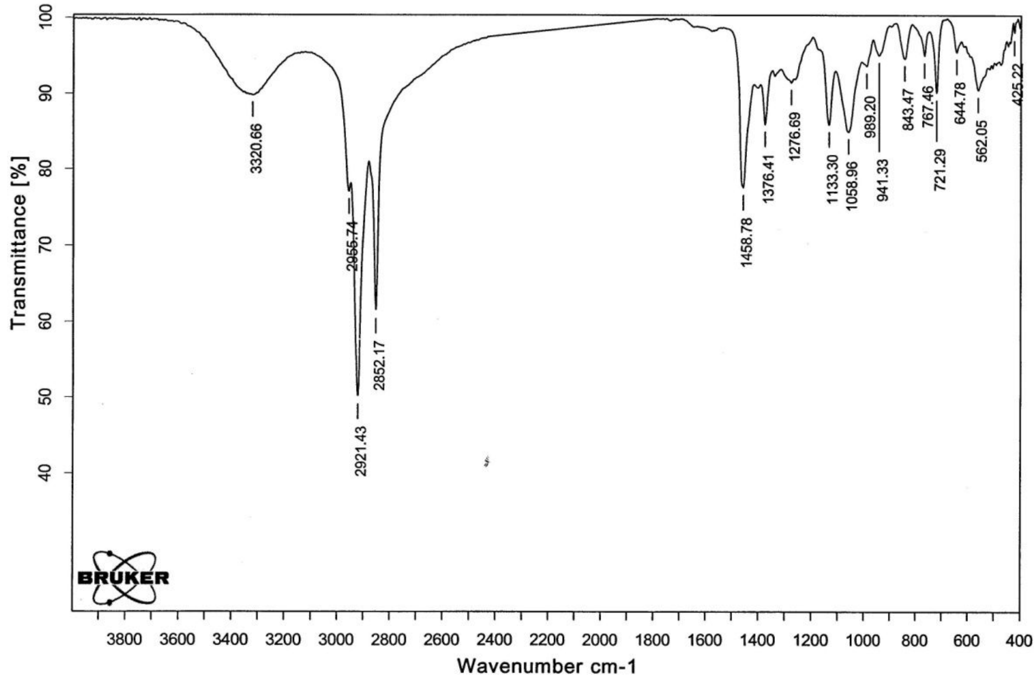

Fig. S7. IR spectrum of $C_{12}C_2C_{12}$[iso-Pr(OH)]

IR-spectrum ν, cm^{-1}: 3220 ν (OH) and (NH), 2955, 2921 and 2852 ν (CH), 1458, 1376 and 1276 δ (CH), 1133 ν (C-N), 1058 and 941 ν (C-O), 721 δ -$(CH_2)_x$-.

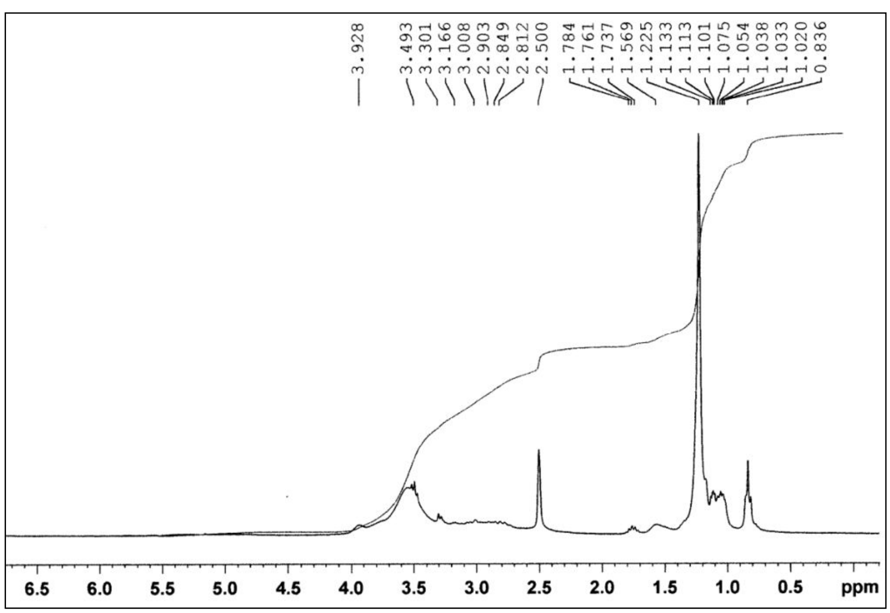

Fig. S8. ^{1}H-NMR spectrum of $C_{12}C_2C_{12}$[iso-Pr(OH)]

^{1}H-NMR, (300.13 MHz, DMSO-d_6), δ (ppm): 0.84 (C$\underline{H_3}$), 1.02-1.11 (CH-C$\underline{H_3}$), 1.22 (C$\underline{H_2}$ chain), 1.57-1.78 (C$\underline{H_2}$-CH_2-N^+H), 2.81-3.49 (C$\underline{H_2}$-N^+H), 3.93 (C$\underline{H}$-OH).

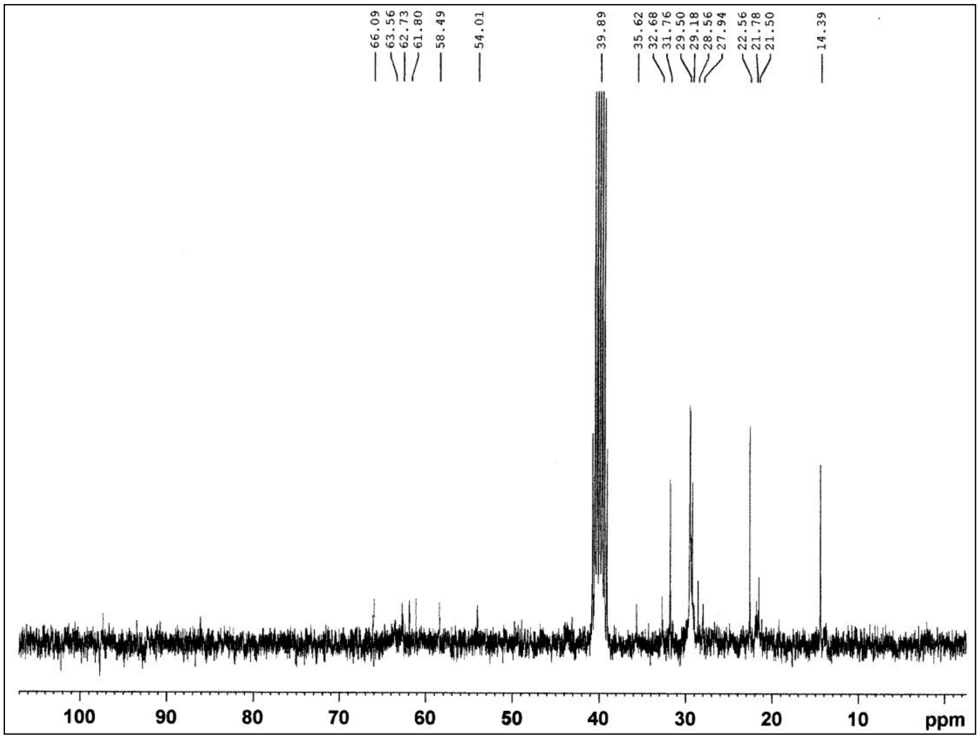

Fig. S9. ^{13}C-NMR spectrum of $C_{12}C_2C_{12}$[iso-Pr(OH)]

^{13}C NMR, (75.47 MHz, DMSO-d_6), δ (ppm): 14.4 ($\underline{C}H_3$), 21.5 ($\underline{C}H_3$-CH), 22.6–32.6 (alkyl group $\underline{C}H_2$), 54.0-58.5 (NH^+-$\underline{C}H_2$-CH_2), 61.8-66.1 (NH^+-$\underline{C}H_2$-$\underline{C}$H-OH).

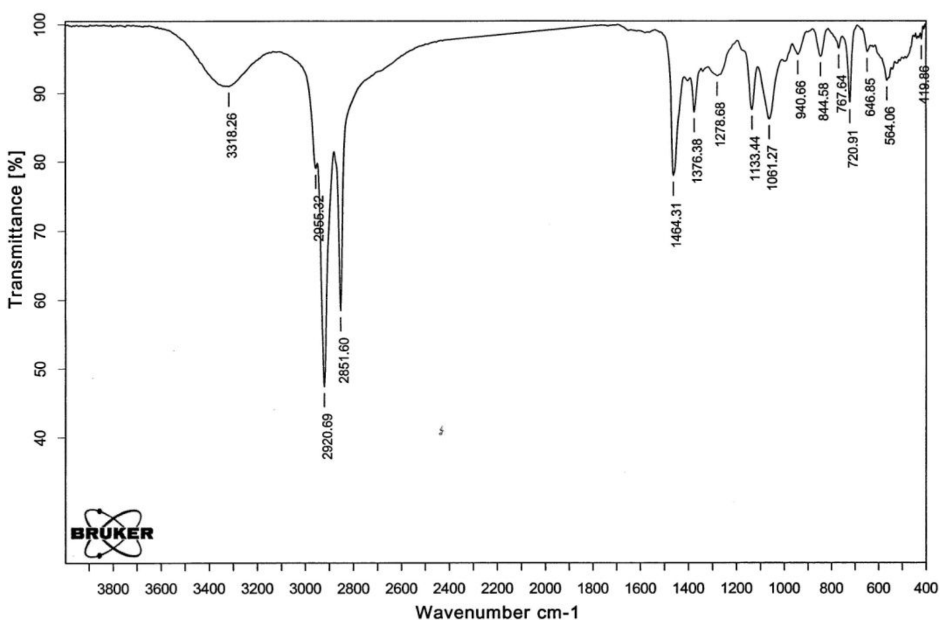

Fig. S10. IR spectrum of $C_{14}C_2C_{14}$[iso-Pr(OH)]

IR-spectrum ν, cm^{-1}: 3318 ν (OH) and (NH), 2955, 2920 and 2851 ν (CH), 1464, 1376 and 1278 δ (CH), 1133 ν (C-N), 1061 and 940 ν (C-O), 721 δ -$(CH_2)_x$.

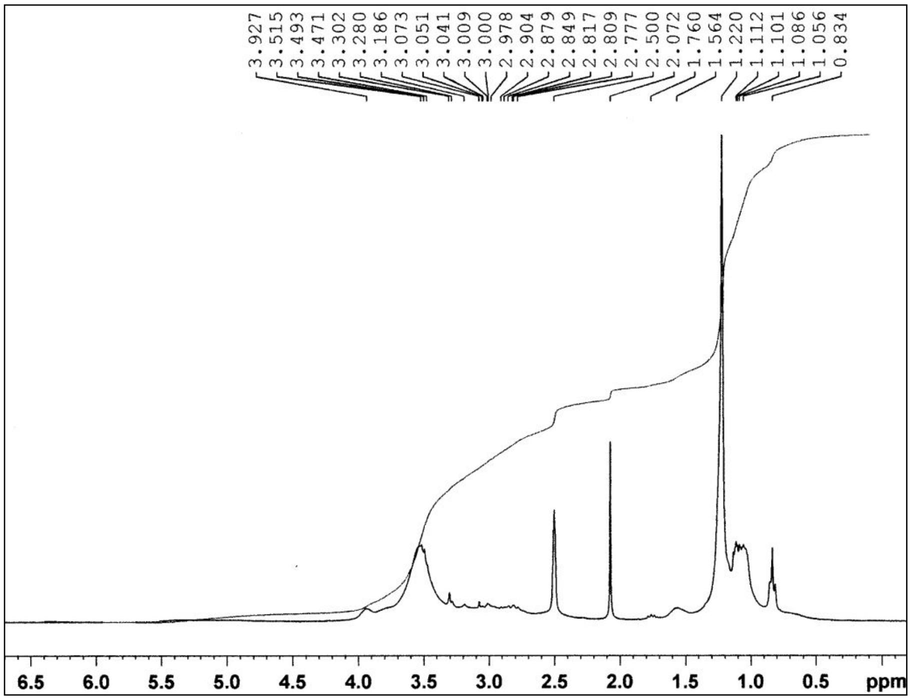

Fig. S11. ^{1}H-NMR spectrum of $C_{14}C_2C_{14}$[iso-Pr(OH)]

^{1}H-NMR, (300.13 MHz, DMSO-d_6), δ (ppm): 0.83 (C$\underline{\mathit{H}}_3$), 1.06-1.11 (CH-C$\underline{\mathit{H}}_3$), 1.22 (C$\underline{\mathit{H}}_2$ chain), 1.56-1.76 (C$\underline{\mathit{H}}_2$-CH_2-N^+H), 2.78-3.52 (C$\underline{\mathit{H}}_2$-N^+H), 3.93 (C$\underline{\mathit{H}}$-OH).

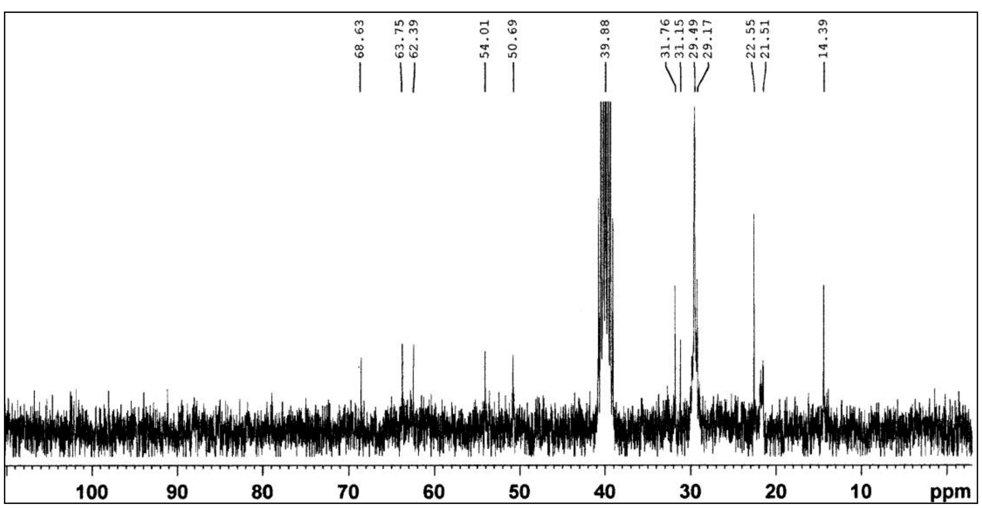

Fig. S12. ^{13}C-NMR spectrum of $C_{14}C_2C_{14}$[iso-Pr(OH)]

^{13}C NMR, (75.47 MHz, DMSO-d_6), δ (ppm): 14.4 ($\underline{C}H_3$), 21.5 ($\underline{C}H_3$-CH), 22.6–31.8 (alkyl group $\underline{C}H_2$), 50.7-54.0 (NH^+-$\underline{C}H_2$-CH_2), 62.4-68.6 (NH^+-$\underline{C}H_2$-$\underline{C}$H-OH).

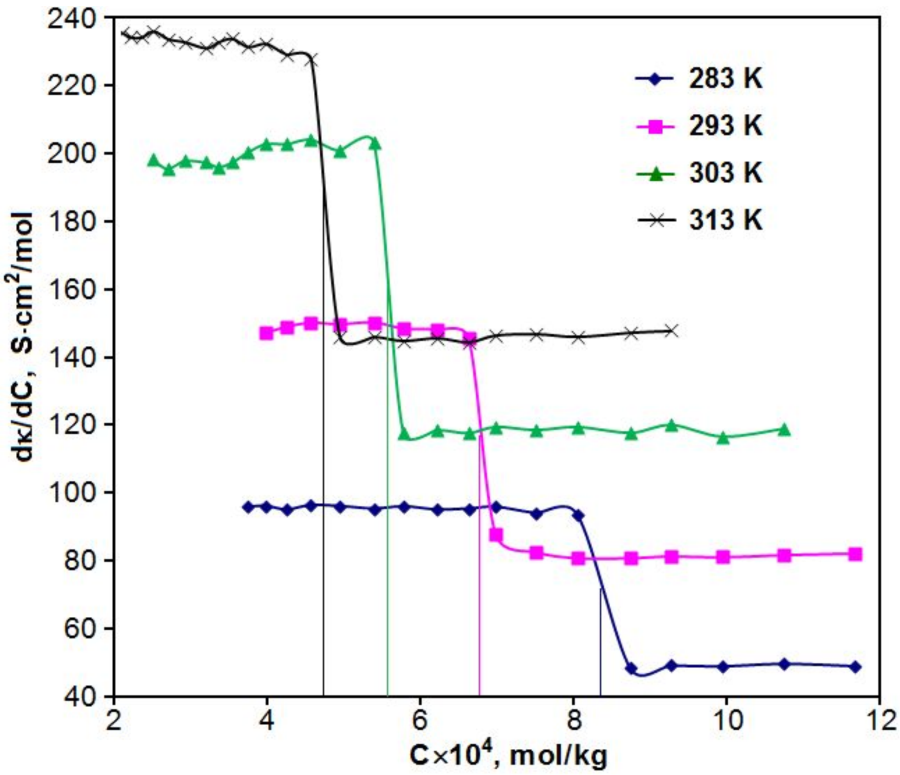

Fig. S13. The dependence of differential electrical conductivity (dκ/dC) on concentration of $C_{14}C_2C_{14}$[iso-Pr(OH)] at different temperatures. Temperature, K: 1. 283; 2. 293; 3. 303; 4. 313.

Table S1. Dependence of surface tension γ from natural logarithm of molality b for $C_9C_2C_9$[iso-Pr(OH)] at different temperatures (p=0.1 MPa)[a]

ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m
T=283 K		T=293 K		T=303 K		T=313 K	
-12.3727	69.95	-12.3727	65.38	-12.3727	61.65	-12.3727	58.01
-11.6796	65.54	-11.6796	61.06	-11.6796	57.84	-11.6796	54.35
-11.2741	62.90	-11.2741	58.70	-11.2741	55.53	-11.2741	52.17
-10.9864	60.90	-10.9864	56.91	-10.9864	53.85	-10.9864	50.62
-10.0702	54.65	-10.0702	51.63	-10.0702	48.84	-10.0702	46.04
-9.37701	50.31	-9.37701	47.52	-9.37701	45.19	-9.37701	42.47
-8.97154	47.67	-8.97154	45.00	-8.97154	42.86	-8.97154	40.37
-8.68386	45.57	-8.68386	43.17	-8.68386	41.15	-8.68386	38.82
-7.76757	39.75	-7.76757	37.50	-7.76757	36.10	-7.76757	34.08
-7.07442	35.10	-7.07442	33.46	-7.07442	32.30	-7.07442	30.82
-6.66896	32.30	-6.66896	31.00	-6.66896	30.28	-6.66896	29.58
-6.54379	31.50	-6.54379	30.60	-6.54379	30.20	-6.54379	29.50
-6.38127	30.90	-6.38127	30.10	-6.38127	30.00	-6.38127	29.40
-5.97581	30.90	-5.97581	30.08	-5.97581	30.01	-5.97581	29.35
-5.68813	30.88	-5.68813	30.05	-5.68813	29.94	-5.68813	29.32
-5.46498	30.85	-5.46498	30.03	-5.46498	29.92	-5.46498	29.28

[a]The standard uncertainties u(γ) = 0.1 mN/m; u(T) = 0.01 K; u(p) = 10 kPa.

Table S2. Dependence of surface tension γ from natural logarithm of molality b for $C_{12}C_2C_{12}$[iso-Pr(OH)] at different temperatures (p=0.1 MPa)[a]

ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m
T=283 K		T=293 K		T=303 K		T=313 K	
-12.5059	72.28	-12.5059	69.40	-12.5059	66.25	-12.5059	62.10
-11.8128	66.60	-11.8128	63.72	-11.8128	60.89	-11.8128	57.20
-11.4073	63.40	-11.4073	60.51	-11.4073	57.39	-11.4073	54.20
-11.1196	61.28	-11.1196	58.30	-11.1196	55.40	-11.1196	52.24
-10.2034	53.50	-10.2034	51.30	-10.2034	48.20	-10.2034	45.10
-9.51021	48.00	-9.51021	45.60	-9.51021	43.10	-9.51021	40.30
-9.10474	44.70	-9.10474	42.40	-9.10474	39.90	-9.10474	37.30
-8.81706	42.30	-8.81706	40.10	-8.81706	37.60	-8.81706	35.30
-7.90077	34.60	-7.90077	33.00	-7.90077	30.60	-7.90077	28.70
-7.20762	29.20	-7.20762	27.34	-7.20762	26.40	-7.20762	25.96
-6.94526	28.00	-6.94526	27.00	-6.94526	26.20	-6.94526	25.76
-6.80216	27.50	-6.80216	27.00	-6.80216	26.10	-6.80216	25.66
-6.67699	27.50	-6.67699	27.00	-6.67699	26.10	-6.67699	25.40
-6.51448	27.40	-6.51448	26.90	-6.51448	26.10	-6.51448	25.30

[a]The standard uncertainties u(γ) = 0.1 mN/m; u(T) = 0.01 K; u(p) = 10 kPa.

Table S3. Dependence of surface tension γ from natural logarithm of molality b for $C_{14}C_2C_{14}$[iso-Pr(OH)] at different temperatures (p=0.1 MPa)[a]

ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m	ln*b* (mol/kg)	γ, mN/m
T=283 K		T=293 K		T=303 K		T=313 K	
-12.5858	70.50	-12.5858	66.26	-12.5858	62.73	-12.5858	59.00
-11.8926	65.55	-11.8926	61.58	-11.8926	58.39	-11.8926	54.90
-11.4872	62.44	-11.4872	59.00	-11.4872	55.75	-11.4872	52.26
-11.1995	60.49	-11.1995	57.00	-11.1995	53.88	-11.1995	50.38
-10.2832	54.00	-10.2832	50.81	-10.2832	47.93	-10.2832	45.00
-9.59006	49.18	-9.59006	46.21	-9.59006	43.56	-9.59006	40.76
-9.18460	46.29	-9.18460	43.48	-9.18460	40.91	-9.18460	38.00
-8.89692	44.27	-8.89692	41.52	-8.89692	39.00	-8.89692	36.31
-7.98063	37.71	-7.98063	35.31	-7.98063	33.11	-7.98063	30.69
-7.28748	32.90	-7.28748	30.71	-7.28748	29.68	-7.28748	28.67
-6.88201	31.00	-6.88201	30.20	-6.88201	29.06	-6.88201	28.00
-6.59433	30.50	-6.59433	29.80	-6.59433	28.50	-6.59433	27.42
-6.18887	30.00	-6.18887		-6.18887		-6.18887	

[a]The standard uncertainties u(γ) = 0.1 mN/m; u(T) = 0.01 K; u(p) = 10 kPa.

Table S4. The dependence of specific electrical conductivity κ from concentration b of $C_9C_2C_9$[iso-Pr(OH)] at different temperatures (p=0.1 MPa)[a]

$b\cdot10^4$, mol/kg	κ, μS/cm	$b\cdot10^4$, mol/kg	κ, μS/cm	$b\cdot10^4$, mol/kg	κ, μS/cm	$b\cdot10^4$, mol/kg	κ, μS/cm
T=283 K		T=293 K		T=303 K		T=313 K	
2.3441	67.2	2.3441	81.2	2.3441	90.6	2.3441	103.5
2.5394	70.5	2.5394	85.6	2.5394	95.0	2.5394	112.3
2.7703	74.2	2.7703	90.0	2.7703	101.2	2.7703	122.1
3.0473	79.0	3.0473	96.0	3.0473	109.2	3.0473	133.1
3.3859	84.0	3.3859	104.2	3.3859	118.0	3.3859	147.2
3.5851	88.0	3.5851	108.0	3.5851	124.0	3.5851	155.2
3.8092	91.3	3.8092	112.1	3.8092	130.0	3.8092	165.0
4.0631	95.6	4.0631	117.1	4.0631	137.1	4.0631	175.4
4.3533	100.4	4.3533	124.4	4.3533	145.4	4.3533	186.8
4.6882	106.9	4.6882	132.1	4.6882	155.0	4.6882	200.0
5.0789	113.4	5.0789	140.8	5.0789	165.3	5.0789	216.1
5.5406	121.2	5.5406	150.0	5.5406	178.7	5.5406	234.4
6.0947	131.2	6.0947	161.9	6.0947	193.8	6.0947	257.6
6.7719	142.0	6.7719	176.7	6.7719	213.0	6.7719	285.1
7.6183	157.2	7.6183	195.3	7.6183	235.9	7.6183	320.0
8.7067	176.0	8.7067	218.9	8.7067	266.2	8.7067	364.5
9.8301	194.9	9.8301	243.0	9.8301	298.0	9.8301	409.6
10.9000	213.3	10.9000	265.8	10.9000	327.0	10.9000	454.2
11.2864	220.3	11.2864	274.1	11.2864	338.0	11.2864	461.3
11.7205	228.2	11.7205	284.8	11.7205	350.8	11.7205	471.8
12.6972	244.5	12.6972	304.5	12.6972	377.6	12.6972	491.2
13.8515	264.6	13.8515	330.5	13.8515	393.3	13.8515	516.0
14.4000	274.4	14.4000	341.7	14.4000	400.7	14.4000	528.2
15.2367	288.8	15.2367	350.0	15.2367	412.5	15.2367	545.9
16.0832	303.0	16.0832	358.7	16.0832	424.3	16.0832	563.5
16.9296	317.7	16.9296	367.1	16.9296	435.6	16.9296	582.3
17.7761	324.2	17.7761	375.8	17.7761	447.2	17.7761	598.9
18.6226	330.7	18.6226	384.3	18.6226	458.8	18.6226	617.1
19.4691	337.3	19.4691	393.3	19.4691	470.6	19.4691	635.9
20.3156	343.7	20.3156	402.0	20.3156	482.4	20.3156	654.1
21.1621	350.2						
22.0085	356.6						

[a]The standard uncertainties $u_r(\kappa) = 0.02$, $u(T) = 0.1$ K, and $u(P) = 10$ kPa; $u(b) = 0.0005$ mmol/kg.

Table S5. The dependence of specific electrical conductivity κ from concentration b of $C_{12}C_2C_{12}$[iso-Pr(OH)] at different temperatures (p=0.1 MPa)[a]

$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm
T=283 K		T=293 K		T=303 K		T=313 K	
5.3346	12.5	5.3346	13.4	5.3346	16.9	5.3346	17.9
5.9273	13.5	5.9273	14.6	5.9273	17.8	5.9273	19.2
6.2760	14.3	6.2760	15.3	6.2760	19.0	6.2760	20.1
6.6682	15.2	6.6682	15.8	6.6682	19.5	6.6682	21.2
7.1128	15.9	7.1128	16.7	7.1128	20.4	7.1128	22.3
7.6209	17.1	7.6209	17.7	7.6209	20.8	7.6209	23.5
8.2071	18.2	8.2071	18.5	8.2071	22.0	8.2071	24.9
8.8910	19.6	8.8910	19.9	8.8910	23.5	8.8910	26.6
9.6993	20.0	9.6993	21.6	9.6993	24.7	9.6993	28.7
10.6692	21.9	10.6692	23.3	10.6692	26.6	10.6692	31.0
11.8547	23.7	11.8547	24.9	11.8547	28.7	11.8547	33.9
13.3365	25.7	13.3365	27.2	13.3365	31.4	13.3365	37.2
15.2417	28.9	15.2417	30.6	15.2417	35.2	15.2417	42.2
17.7820	32.1	17.7820	35.3	17.7820	40.0	17.7820	48.0
19.0521	34.4	19.0521	37.4	19.0521	42.3	19.0521	50.9
20.5177	36.9	20.5177	40.0	20.5177	45.0	20.5177	54.7
22.2275	38.6	22.2275	42.7	22.2275	48.0	22.2275	58.6
24.2482	42.4	24.2482	46.3	24.2482	52.0	24.2482	63.6
26.6730	45.9	26.6730	50.2	26.6730	56.2	26.6730	69.2
29.6367	49.8	29.6367	54.9	29.6367	62.1	29.6367	76.2
31.3800	53.1	31.3800	58.3	31.3800	65.2	31.3800	80.5
33.3412	56.0	33.3412	61.2	33.3412	69.0	33.3412	85.1
35.5640	59.1	35.5640	64.6	35.5640	72.8	35.5640	90.4
38.1043	62.8	38.1043	69.5	38.1043	77.5	38.1043	96.3
41.0354	67.3	41.0354	74.7	41.0354	82.9	41.0354	103.5
44.4550	72.3	44.4550	80.0	44.4550	89.5	44.4550	111.9
48.4963	78.3	48.4963	87.3	48.4963	97.0	48.4963	121.0
53.3460	85.5	53.3460	95.7	53.3460	106.0	53.3460	133.2
54.9760	88.0	54.9760	98.5	54.9760	109.0	54.9760	137.0
59.2733	94.7	59.2733	105.6	59.2733	117.8	59.2733	142.7
62.2370	99.0	62.2370	110.0	62.2370	124.1	62.2370	147.0
66.6825	105.9	66.6825	117.7	66.6825	129.0	66.6825	152.9
74.0916	117.0	74.0916	130.0	74.0916	136.5	74.0916	163.2
80.8272	126.8	80.8272	136.2	80.8272	142.7	80.8272	172.6
86.0419	134.3	86.0419	140.6	86.0419	147.6	86.0419	179.4
91.1327	142.0	91.1327	145.0	91.1327	152.3	91.1327	186.5
95.2607	145.0	95.2607	148.7	95.2607	156.1	95.2607	192.0
102.5884	150.4	102.5884	154.8	102.5884	163.9	102.5884	202.1
111.1375	156.4	111.1375	162.1	111.1375	172.9	111.1375	
121.2409	163.6	121.2409	170.8	121.2409	183.2	121.2409	
133.3649	172.3	133.3649	181.1	133.3649	195.8	133.3649	
148.1833	183.0	148.1833	193.6	148.1833	211.6	148.1833	

[a]The standard uncertainties $u_r(\kappa) = 0.02$, $u(T) = 0.1$ K, and $u(P) = 10$ kPa; $u(b) = 0.0005$ mmol/kg.

Table S6. The dependence of specific electrical conductivity κ from concentration b of $C_{14}C_2C_{14}$[iso-Pr(OH)] salt at different temperatures (p=0.1 MPa)[a]

$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm	$b\cdot10^5$, mol/kg	κ, μS/cm
T=283 K		T=293 K		T=303 K		T=313 K	
4.9252	8.2	4.9252	12.1	4.9252	15.0	4.9252	16.5
5.4724	8.7	5.4724	13.0	5.4724	16.3	5.4724	17.7
5.7943	9.0	5.7943	13.8	5.7943	17.3	5.7943	18.2
6.1565	9.5	6.1565	14.4	6.1565	17.8	6.1565	19.5
6.5669	9.9	6.5669	15.4	6.5669	18.5	6.5669	20.3
7.0359	10.2	7.0359	16.0	7.0359	19.7	7.0359	21.5
7.5772	11.0	7.5772	16.8	7.5772	20.4	7.5772	22.8
8.2086	11.9	8.2086	17.4	8.2086	22.0	8.2086	24.4
8.9548	12.5	8.9548	18.5	8.9548	23.6	8.9548	25.7
9.8503	13.3	9.8503	20.0	9.8503	25.0	9.8503	28.0
10.9448	14.5	10.9448	21.0	10.9448	27.4	10.9448	30.6
12.3129	15.6	12.3129	23.2	12.3129	30.1	12.3129	33.7
14.0719	17.5	14.0719	26.1	14.0719	33.7	14.0719	38.0
16.4172	19.7	16.4172	29.5	16.4172	38.1	16.4172	43.1
17.5899	20.6	17.5899	31.1	17.5899	40.7	17.5899	46.2
18.9429	22.1	18.9429	33.1	18.9429	43.3	18.9429	49.2
20.5215	23.6	20.5215	35.5	20.5215	46.8	20.5215	52.8
22.3871	25.2	22.3871	38.2	22.3871	50.5	22.3871	57.4
24.6258	27.6	24.6258	41.8	24.6258	54.8	24.6258	62.5
27.3620	30.0	27.3620	45.6	27.3620	60.4	27.3620	68.7
28.9716	31.5	28.9716	48.0	28.9716	63.7	28.9716	72.3
30.7823	33.5	30.7823	50.7	30.7823	67.2	30.7823	76.6
32.8344	35.1	32.8344	53.2	32.8344	71.2	32.8344	81.4
35.1797	37.5	35.1797	57.2	35.1797	75.9	35.1797	86.7
37.8859	40.1	37.8859	61.0	37.8859	81.5	37.8859	93.2
41.0430	43.1	41.0430	65.7	41.0430	87.3	41.0430	100.3
44.7742	46.9	44.7742	71.3	44.7742	95.1	44.7742	108.8
49.2516	51.2	49.2516	78.0	49.2516	103.9	49.2516	114.9
53.0823	54.8	53.0823	84.0	53.0823	112.0	53.0823	120.6
57.4603	59.0	57.4603	90.0	57.4603	117.0	57.4603	126.9
61.5646	62.9	61.5646	95.5	61.5646	122.0	61.5646	133.2
65.1216	66.7	65.1216	101.0	65.1216	126.0	65.1216	138.2
70.3595	71.8	70.3595	105.6	70.3595	132.5	70.3595	146.0
75.7718	76.6	75.7718	110.0	75.7718	138.8	75.7718	154.3
82.0861	82.3	82.0861	115.4	82.0861	146.6	82.0861	163.4
87.9494	85.1	87.9494	120.0	87.9494	153.5	87.9494	172.2
94.7147	88.5	94.7147	125.5	94.7147	161.7	94.7147	182.2
102.6076	92.3	102.6076	131.9	102.6076	170.9		
111.9356	96.9	111.9356	139.6	111.9356	182.4		
123.1291	102.4	123.1291	148.8				

[a]The standard uncertainties $u_r(\kappa)$ = 0.02, u(T) = 0.1 K, and u(P) = 10 kPa; u(b) = 0.0005 mmol/kg.