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SUPPLEMENTARY INFORMATION

Influence of poly(ethylene glycol) on the micelle formation of alkyl maltosides used in membrane protein crystallization

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ESI Tables

Table 2: Analysis of CMC titration curves of $C_{10}G_2$ in 100 mM PIPES/NaOH (pH 7.0), 5 mM $CaCl_2$ as a function of PEG2000 concentration ([PEG] in % (w/v); detergent concentrations in mM).

[PEG]	C_{ANS} [a]	x_0 [b]	Δx [b]	$x_0 - 2\Delta x$	$x_0/\Delta x$
0	1.30	1.566 ± 0.062	0.179 ± 0.054	1.21 ± 0.17	8.75 ± 2.99
2	–	1.920 ± 0.048	0.206 ± 0.043	1.508 ± 0.134	9.32 ± 2.18
4	1.40	1.99 ± 0.05	0.20 ± 0.04	1.59 ± 0.13	9.95 ± 2.24
6	–	2.295 ± 0.043	0.264 ± 0.038	1.77 ± 0.12	8.69 ± 1.42
8	1.75	–	–	–	–
10	–	2.94 ± 0.11	0.50 ± 0.10	1.94 ± 0.31	5.88 ± 1.40
12	2.00	3.10 ± 0.09	0.53 ± 0.08	2.04 ± 0.25	5.85 ± 1.06
14	–	3.52 ± 0.19	0.67 ± 0.16	2.18 ± 0.51	5.25 ± 1.54
16	2.40	3.58 ± 0.11	0.51 ± 0.10	2.56 ± 0.31	7.02 ± 1.60
17	–	4.20 ± 0.07	0.71 ± 0.06	2.78 ± 0.19	5.92 ± 0.60
18	–	4.14 ± 0.07	0.69 ± 0.07	2.76 ± 0.21	6.00 ± 0.71
20	–	4.37 ± 0.08	0.99 ± 0.08	2.39 ± 0.24	4.41 ± 0.44

[a] Error: ± 5 %, estimated from the graphical analysis of the titration curves.

[b] Error: standard deviation from the sigmoidal fit.

Table 3: Analysis of CMC titration curves of $C_{11}G_2$ in 100 mM PIPES/NaOH (pH 7.0), 5 mM $CaCl_2$ as a function of PEG2000 concentration ([PEG] in % (w/v); detergent concentrations in mM).

[PEG]	C_{ANS} [a]	x_0 [b]	Δx [b]	$x_0 - 2\Delta x$	$x_0/\Delta x$
0	0.38	0.480 ± 0.008	0.048 ± 0.007	0.384 ± 0.022	10.000 ± 1.625
1	–	0.542 ± 0.012	0.070 ± 0.011	0.402 ± 0.034	7.74 ± 1.39
2	0.40	–	–	–	–
3	–	0.673 ± 0.025	0.113 ± 0.024	0.447 ± 0.073	5.96 ± 1.49
4	0.45	–	–	–	–
5	–	0.74 ± 0.04	0.14 ± 0.04	0.46 ± 0.12	5.29 ± 1.80
6	0.49	–	–	–	–
7	–	0.82 ± 0.02	0.15 ± 0.02	0.52 ± 0.06	5.47 ± 0.87
8	0.55	–	–	–	–
10	0.60	1.14 ± 0.06	0.27 ± 0.05	0.60 ± 0.16	4.22 ± 1.01
12	0.65	1.28 ± 0.06	0.31 ± 0.05	0.66 ± 0.16	4.13 ± 0.86
14	0.70	1.36 ± 0.04	0.32 ± 0.04	0.72 ± 0.12	4.25 ± 0.66
16	0.75	1.77 ± 0.09	0.51 ± 0.09	0.75 ± 0.27	3.47 ± 0.79
18	–	1.77 ± 0.07	0.49 ± 0.07	0.79 ± 0.21	3.61 ± 0.66

[a] Error: ± 5 %, estimated from the graphical analysis of the titration curves.

[b] Error: standard deviation from the sigmoidal fit.

Table 4: Analysis of CMC titration curves of $C_{12}G_2$ in 100 mM PIPES/NaOH (pH 7.0), 5 mM $CaCl_2$ as a function of PEG2000 concentration ([PEG] in % (w/v); detergent concentrations in mM).

[PEG]	C_{ANS} [a]	x_0 [b]	Δx [b]	$x_0 - 2\Delta x$	$x_0/\Delta x$
0	0.09	0.13 ± 0.01	0.02 ± 0.01	0.09 ± 0.03	6.50 ± 3.75
2	0.10	0.211 ± 0.015	0.056 ± 0.014	0.099 ± 0.043	3.77 ± 1.21
3	0.11	0.22 ± 0.01	0.05 ± 0.01	0.12 ± 0.03	4.40 ± 1.08
4	–	0.236 ± 0.008	0.045 ± 0.007	0.146 ± 0.022	5.24 ± 1.00
6	0.12	0.32 ± 0.02	0.08 ± 0.02	0.16 ± 0.06	4.00 ± 1.25
8	0.14	0.34 ± 0.02	0.10 ± 0.02	0.14 ± 0.06	3.40 ± 0.88
10	0.14	0.374 ± 0.013	0.116 ± 0.013	0.142 ± 0.039	3.22 ± 0.48
12	0.18	0.48 ± 0.02	0.16 ± 0.02	0.16 ± 0.06	3.00 ± 0.50
14	–	0.49 ± 0.02	0.15 ± 0.02	0.19 ± 0.06	3.27 ± 0.57
15	–	0.56 ± 0.05	0.19 ± 0.05	0.18 ± 0.15	2.95 ± 1.04
16	0.18	0.60 ± 0.03	0.21 ± 0.03	0.18 ± 0.09	2.86 ± 0.56
18	–	0.70 ± 0.08	0.27 ± 0.07	0.16 ± 0.22	2.59 ± 0.97

[a] Error: ± 5 %, estimated from the graphical analysis of the titration curves.

[b] Error: standard deviation from the sigmoidal fit.

Table 5: Data of the TMT-approach to the CMC (C_0) of C_nG_2.

n	10	11	12
m	85 ± 5 [a]	110 ± 5 [b]	140 ± 5 [a]
a / Å	12.25 ± 0.25 [a]	13.0 ± 0.2 [c]	14.05 ± 0.25 [a]
b / Å	23.50 ± 0.50 [a]	25.5 ± 0.4 [c]	28.75 ± 0.75 [a]
ε	0.85	0.86 [b]	0.87
l_c / Å	14.15	15.42	16.68
V_c / Å^3	296.7	323.6	350.6
V_s / Å^3	28300 ± 1800	35600 ± 1620 [d]	48650 ± 2130
$m\ V_c$ / Å^3	25220 ± 1500	35600 ± 1620	49080 ± 1760
A_c / Å^2	4863 ± 205	5683 ± 179	7094 ± 339
A / Å^2	57 ± 6	52 ± 4	51 ± 5
g_{int}	4.4 ± 0.2	3.8 ± 0.2	3.6 ± 0.2
g_{tr} (TMT)	−16.77 ± 0.25	−18.22 ± 0.27	−19.67 ± 0.29
g_{tr} (SES)	−18.4 ± 0.4	−20.1 ± 0.4	−21.8 ± 0.5
g_{pack}	2.04	2.19	2.48
g_{st}	1.21	1.47	1.53
g_{mic} (TMT)	−9.1 ± 0.5	−10.8 ± 0.5	−12.1 ± 0.5
g_{mic} (SES)	−10.8 ± 0.6	−12.6 ± 0.6	−14.2 ± 0.7
g_{mic} (exp.)	−10.6	−11.9	−13.3
C_0 (TMT) /mM	6.11 ± 3.06	1.12 ± 0.56	0.30 ± 0.15
C_0 (SES) / mM	1.12 ± 0.67	0.18 ± 0.11	0.04 ± 0.03
C_0 (exp.) / mM	1.30 ± 0.07	0.38 ± 0.02	0.090 ± 0.005

[a] Lipfert et al.,[1] [b] Interpolated, [c] Calculated from eqs. (14) to (16), [d] Set equal to $m\ V_c$.

Table 6: Data of the CS-MT-approach to the CMC (C_0) of C_nG_2.

n	10	11	12
g_{dehydr} (CS-MT)	−15.54 ± 0.09	−16.72 ± 0.07	−17.90 ± 0.05 [a]
g_{dehydr} (CS-SES)	−16.8 ± 0.4	−18.2 ± 0.4	−19.6 ± 0.4
g_{hydr}	2.25 ± 0.02 [b]	2.25 ± 0.02 [b]	2.25 ± 0.02 [a]
g_{pack}	2.04 [c]	2.19 [c]	2.48 [c]
g_{st}	1.21 [c]	1.47 [c]	1.53 [c]
g_{mic} (CS-MT)	−10.04 ± 0.11	−10.81 ± 0.09	−11.64 ± 0.07
g_{mic} (CS-SES)	−11.3 ± 0.5	−12.3 ± 0.5	−13.3 ± 0.5
g_{mic} (exp.)	−10.6	−11.9	−13.3
C_0 (CS-MT) /mM	2.39 ± 0.27	1.10 ± 0.10	0.48 ± 0.04
C_0 (CS-SES) / mM	0.68 ± 0.34	0.25 ± 0.13	0.09 ± 0.05
C_0 (exp.) / mM	1.30 ± 0.07	0.38 ± 0.02	0.090 ± 0.005

[a] Stephenson et al.,[2] [b] Set equal to g_{hydr} of $C_{12}G_2$. [c] Same as in TMT (Table 5).

ESI Figures

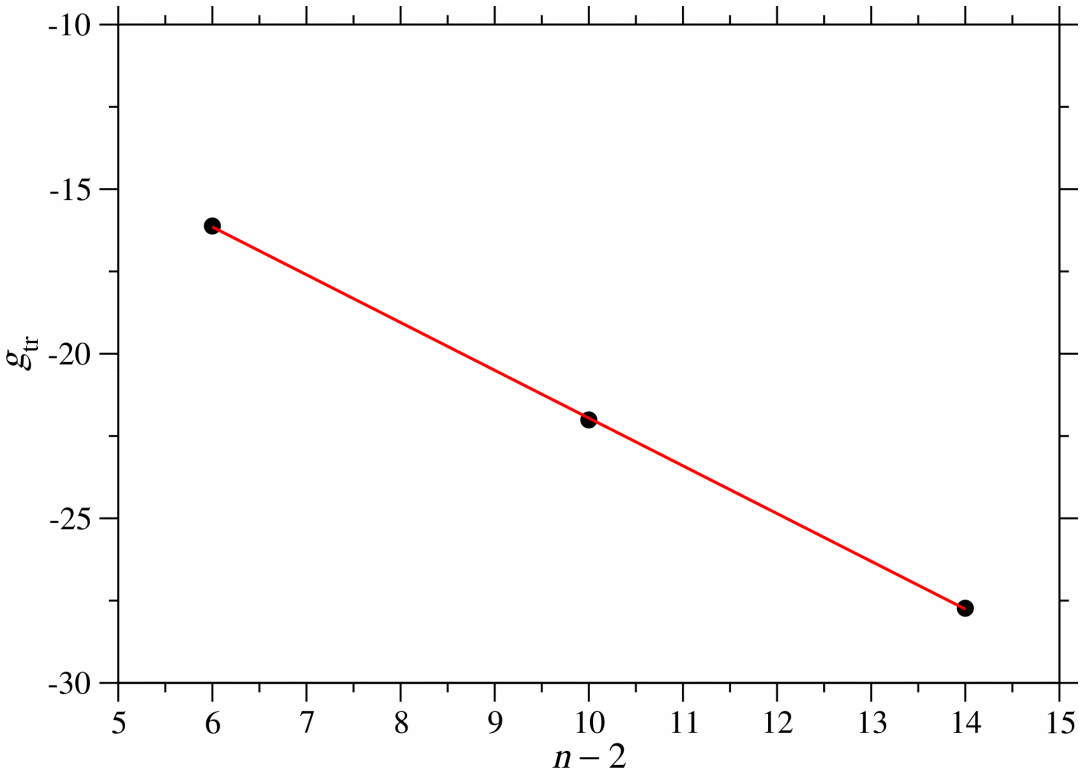

Figure 9.

Plot of g_{tr} for oil droplets of alkanes with umber n of carbon atoms as determined by Stephenson al.[3] based on MD simulations (black circles; "mean" in Table A1 of ref. 3) over $n-2$. The red line is a linear regression, where the slope of –1.45 is the group contribution $g_{tr}(CH_2)$, while the intercept of –7.44 is twice the group contribution $g_{tr}(CH_3)$.

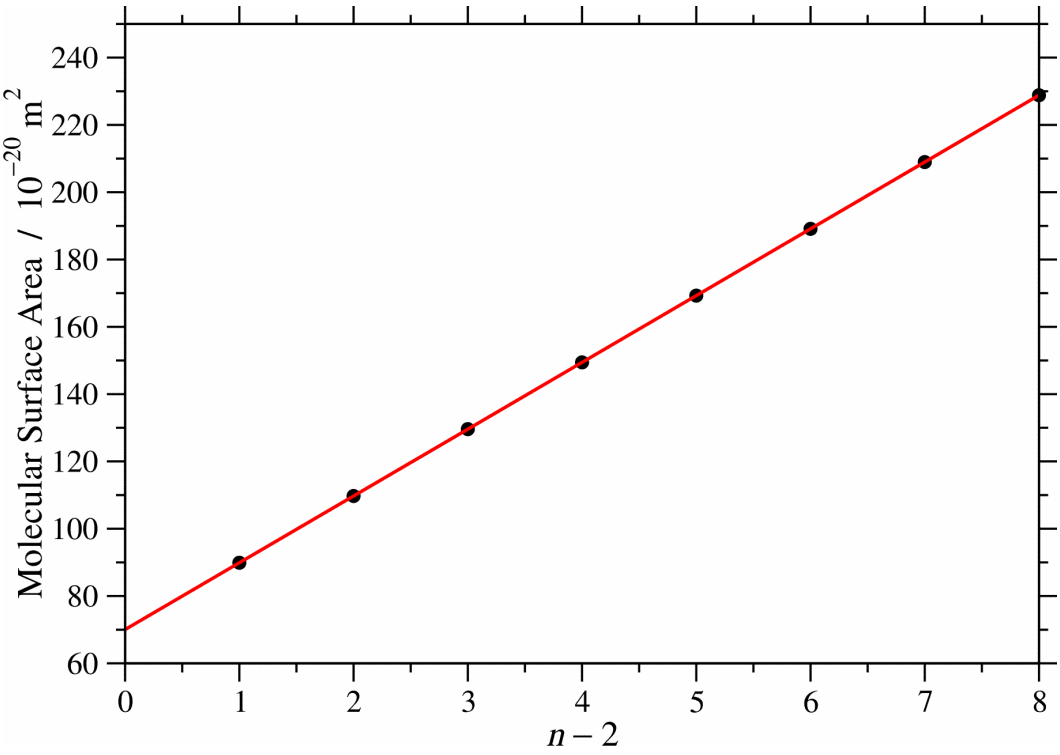

Figure 10.

Plot of the surface area of alkanes with number n of carbon atoms as calculated by Tuñón et al.[4] (black circles) over $n - 2$. The red line is a linear regression, where the slope of 19.85 Å^2 is the group contribution S(CH_2), while the intercept of 70.04 Å^2 is twice the group contribution S(CH_3) and corresponds to the molecular surface area of ethane.

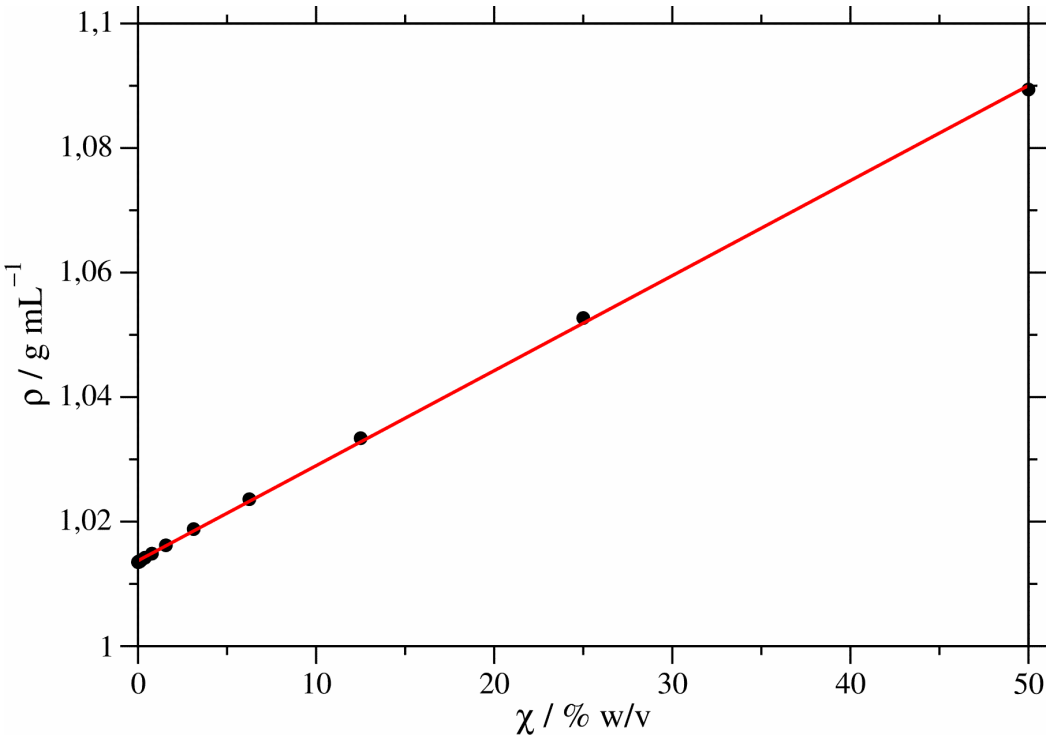

Figure 11.

Mass density ρ of the used buffer (100 mM PIPES, pH 7.0, 5 mM $CaCl_2$) as a function of the mass concentration of PEG2000 χ (black circles). The red line has slope 0.0015 and intercept 1.0137.

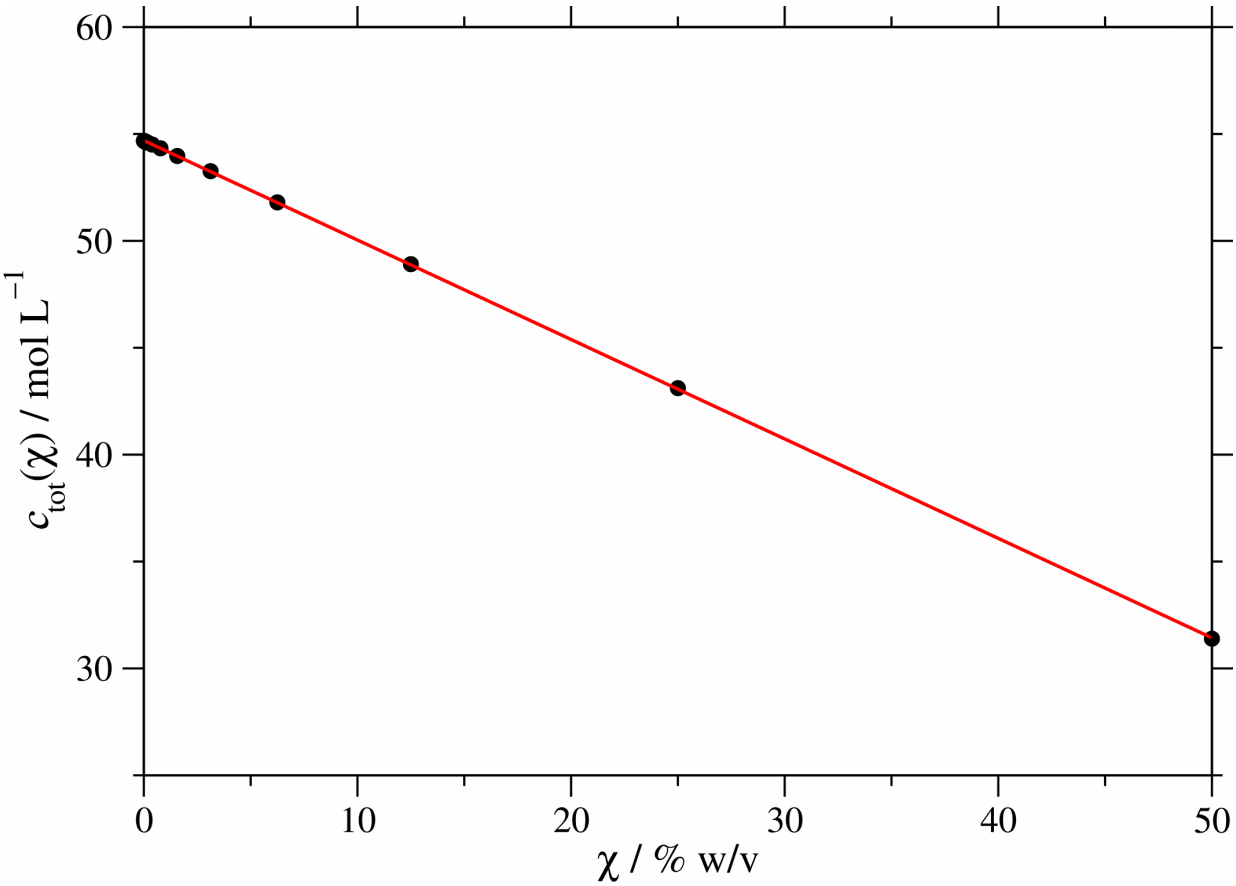

Figure 12.

Total molarity $c_{tot}(\chi)$ of the used buffer (100 mM PIPES, pH 7.0, 5 mM $CaCl_2$) as a function of the mass concentration of PEG2000 χ (black circles). The red line has slope 0.465 and intercept 54.691.

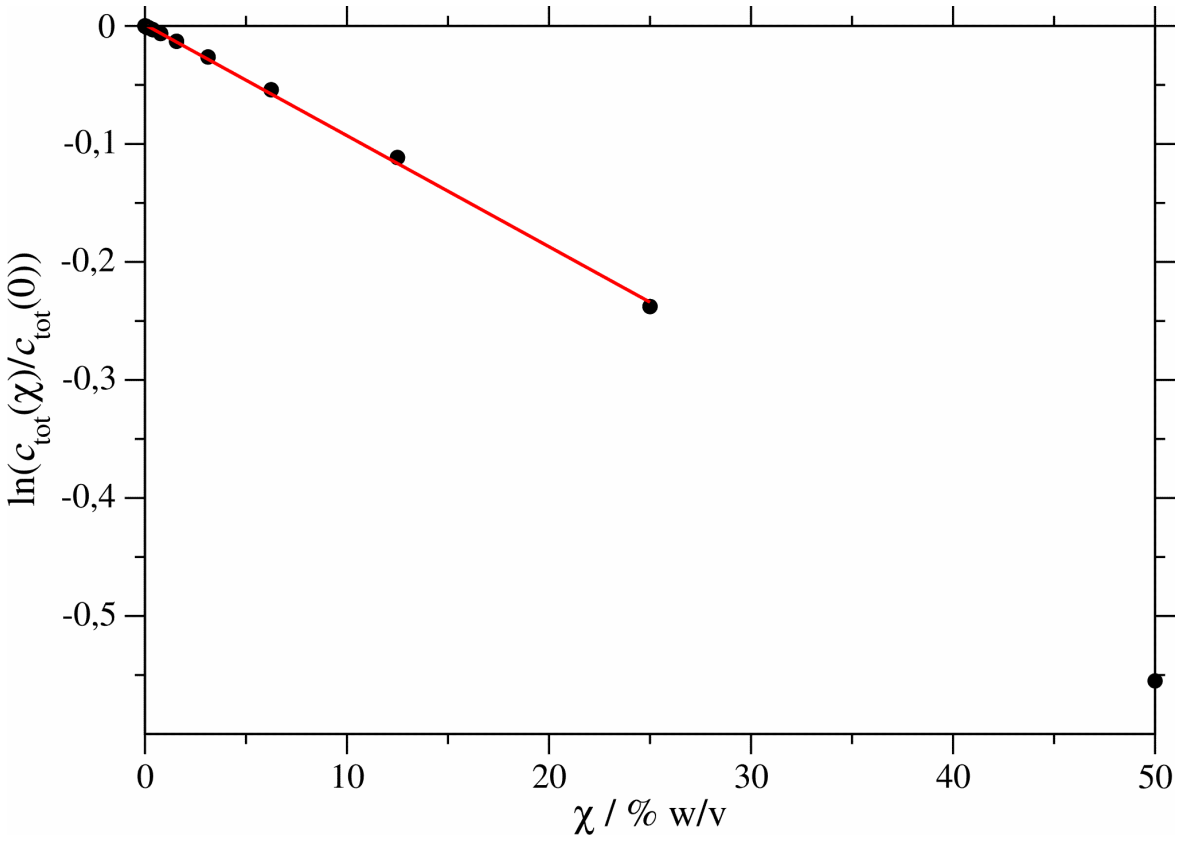

Figure 13.

Molarity correction term $\ln(c_{tot}(\chi)/c_{tot}(0))$ of the used buffer (100 mM PIPES, pH 7.0, 5 mM $CaCl_2$) as a function of the mass concentration of PEG2000 χ (black circles). The red line is a linear regression for $\chi \leq 25$ % w/v with slope – 0.01.

ESI References

1. J. Lipfert, L. Columbus, V. B. Chu, S. A. Lesley and S. Doniach, *J. Phys. Chem. B*, 2007, **111**, 12427-12438.
2. B. C. Stephenson, A. Goldsipe, K. J. Beers and D. Blankschtein, *J. Phys. Chem. B*, 2007, **111**, 1045-1062.
3. B. C. Stephenson, A. Goldsipe, K. J. Beers and D. Blankschtein, *J. Phys. Chem. B*, 2007, **111**, 1025-1044.
4. I. Tunón, E. Silla and J. L. Pascual-Ahuir, *Prot. Eng.*, 1992, **5**, 715-716.