Mononuclear Rearrangement of Heterocycles in Zwitterionic Micelles of Amine Oxide Surfactants

Susanna Guernelli,[a] Antonella Fontana,[b,1] Renato Noto,[c] Domenico Spinelli,[d] and Maria Liria Turco Liveri[e]

[a] *Dipartimento di Chimica Organica "A. Mangini", Università degli Studi di Bologna, Via S. Giacomo 11, 40126 Bologna.*
[b] *Dipartimento di Scienze del Farmaco, Università "G. d'Annunzio", Via dei Vestini 31, 66013 Chieti.*
[c] *Dipartimento di Scienze e Tecnologie Molecolari e Biomolecolari (STEMBIO), Viale delle Scienze, Ed. 16, Parco d'Orleans 2, 90128 Palermo.*
[d] *Dipartimento di Chimica "G. Ciamician", Università degli Studi di Bologna, Via Selmi 2, 40126 Bologna.*
[e] *Dipartimento di Chimica "S. Cannizzaro", Viale delle Scienze, Ed. 17, Parco d'Orleans 2, 90128 Palermo.*

Supporting Material

Figure S1. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1a** → **2a** on the concentration of C_{14} DMAO.

Figure S2. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1b** → **2b** on the concentration of C_{14} DMAO.

Figure S3. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1c** → **2c** on the concentration of C_{14} DMAO.

Figure S4. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1d** → **2d** on the concentration of C_{14} DMAO.

Figure S5. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1e** → **2e** on the concentration of C_{14} DMAO.

Table S1. C.m.c. values for C_{14} DMAO in the presence of the investigated substrates.

1 Corresponding author Fax +39 0871 *3554790. E-mail address*: fontana@unich.it

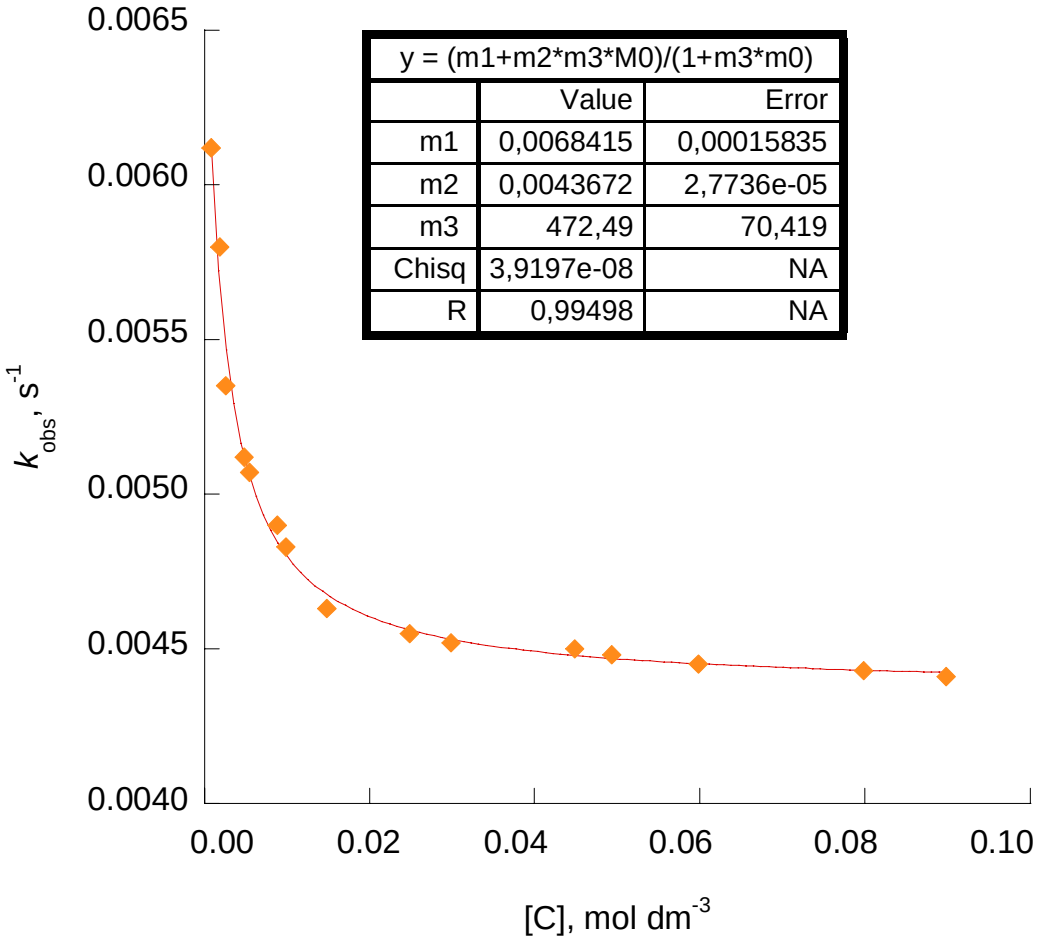
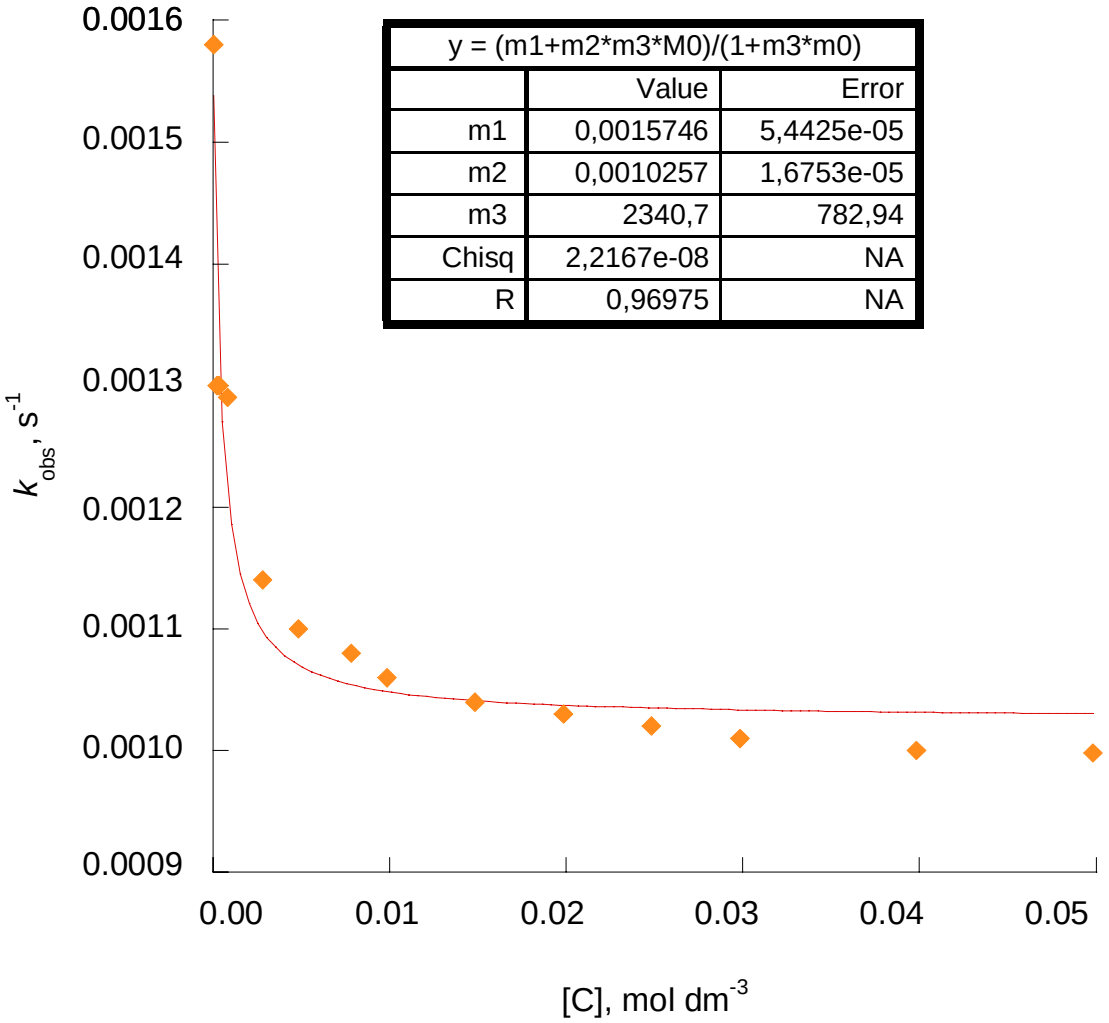


Figure S1. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1a** → **2a** on the concentration of C_{14} DMAO (concentration corrected for the corresponding c.m.c. of the surfactant, 1.5×10^{-4} mol dm^{-3}) in the presence of borate buffer (p*H* 9.6), ionic strength 2.0×10^{-2} mol dm^{-3}, at 313.1 ± 0.1 K.



y = (m1+m2*m3*M0)/(1+m3*m0)		
	Value	Error
m1	0,0015746	5,4425e-05
m2	0,0010257	1,6753e-05
m3	2340,7	782,94
Chisq	2,2167e-08	NA
R	0,96975	NA

Figure S2. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1b** → **2b** on the concentration of C_{14} DMAO (concentration corrected for the corresponding c.m.c. of the surfactant, 1.7×10^{-4} mol dm^{-3}) in the presence of borate buffer (p*H* 9.6), ionic strength 2.0×10^{-2} mol dm^{-3}, at 313.1 ± 0.1 K.

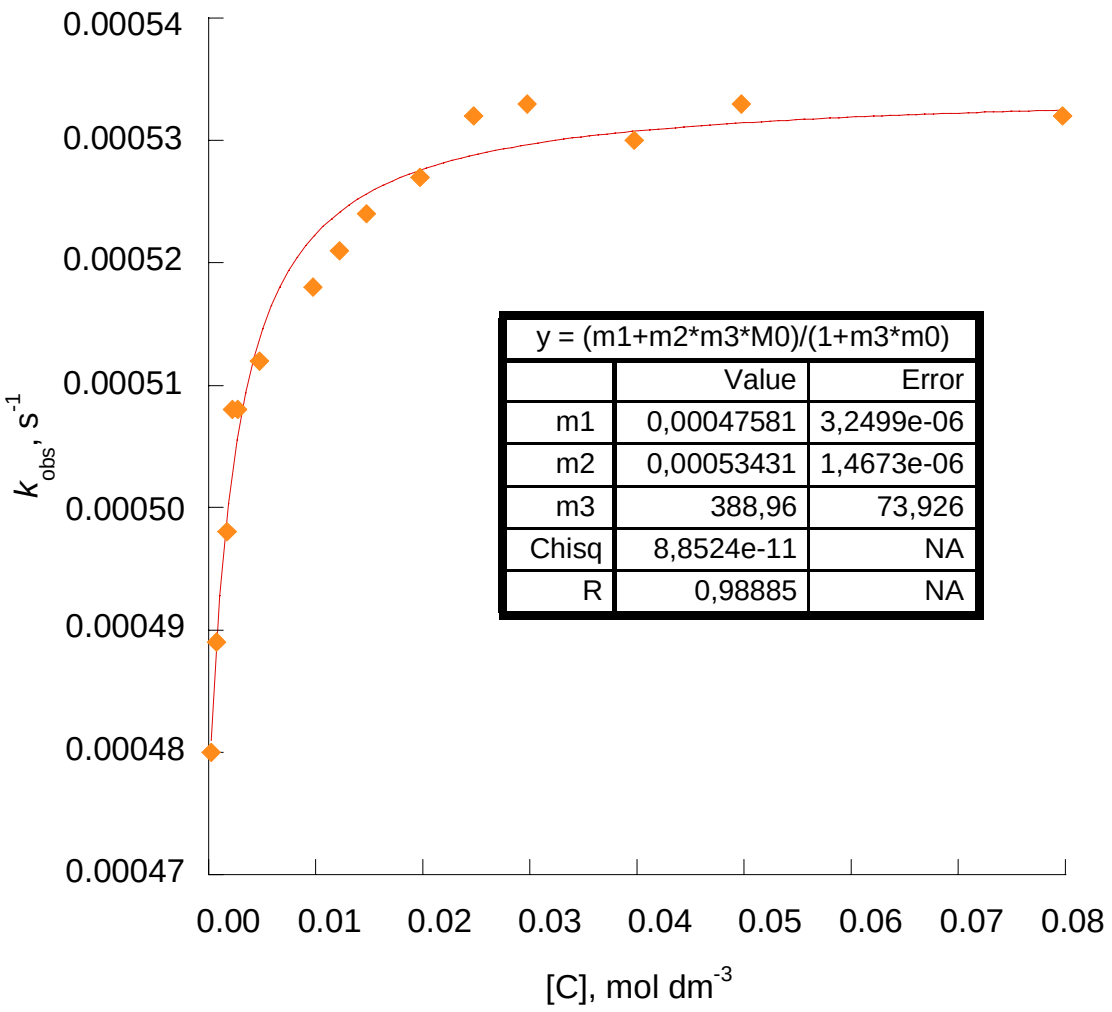


Figure S3. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1c** → **2c** on the concentration of C_{14} DMAO (concentration corrected for the corresponding c.m.c. of the surfactant, 2.5×10^{-4} mol dm^{-3}) in the presence of borate buffer (p*H* 9.6), ionic strength 2.0×10^{-2} mol dm^{-3}, at 313.1 ± 0.1 K.

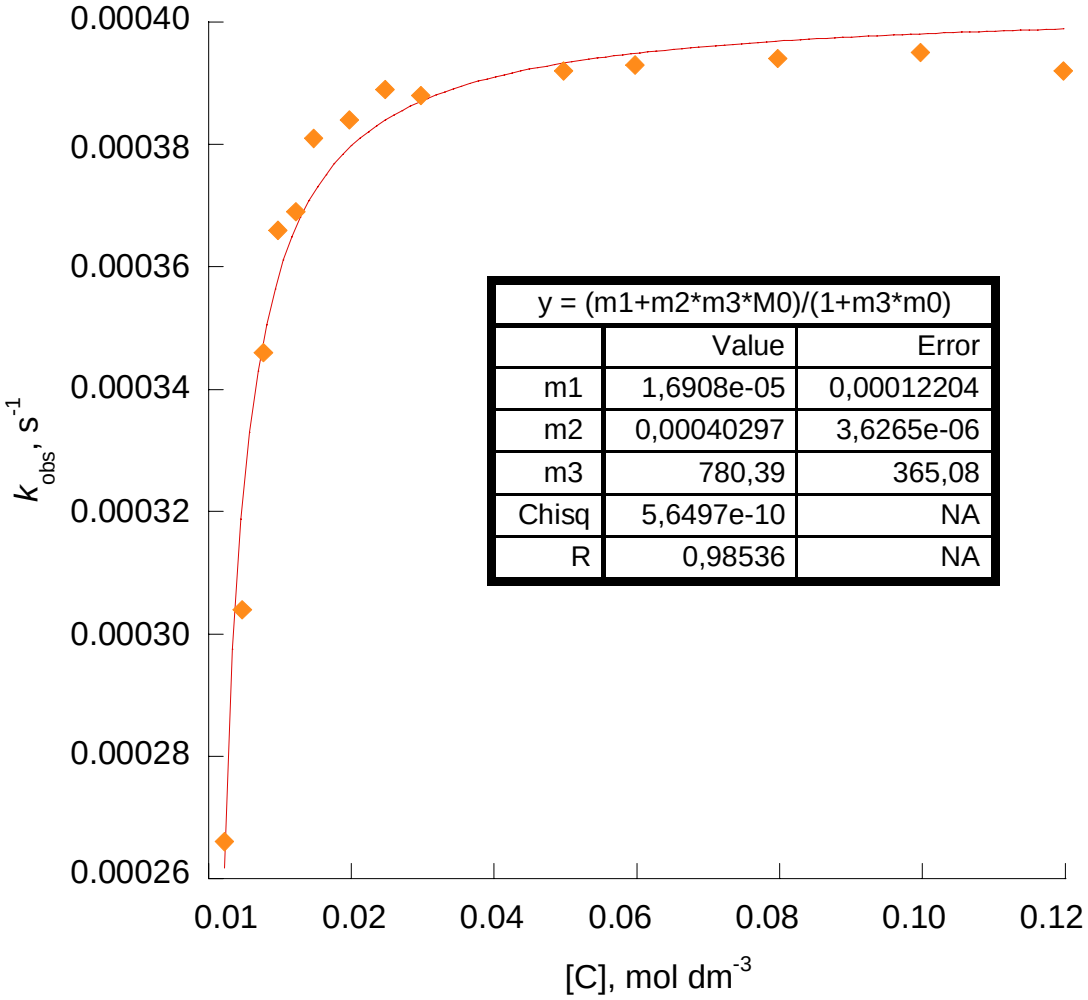
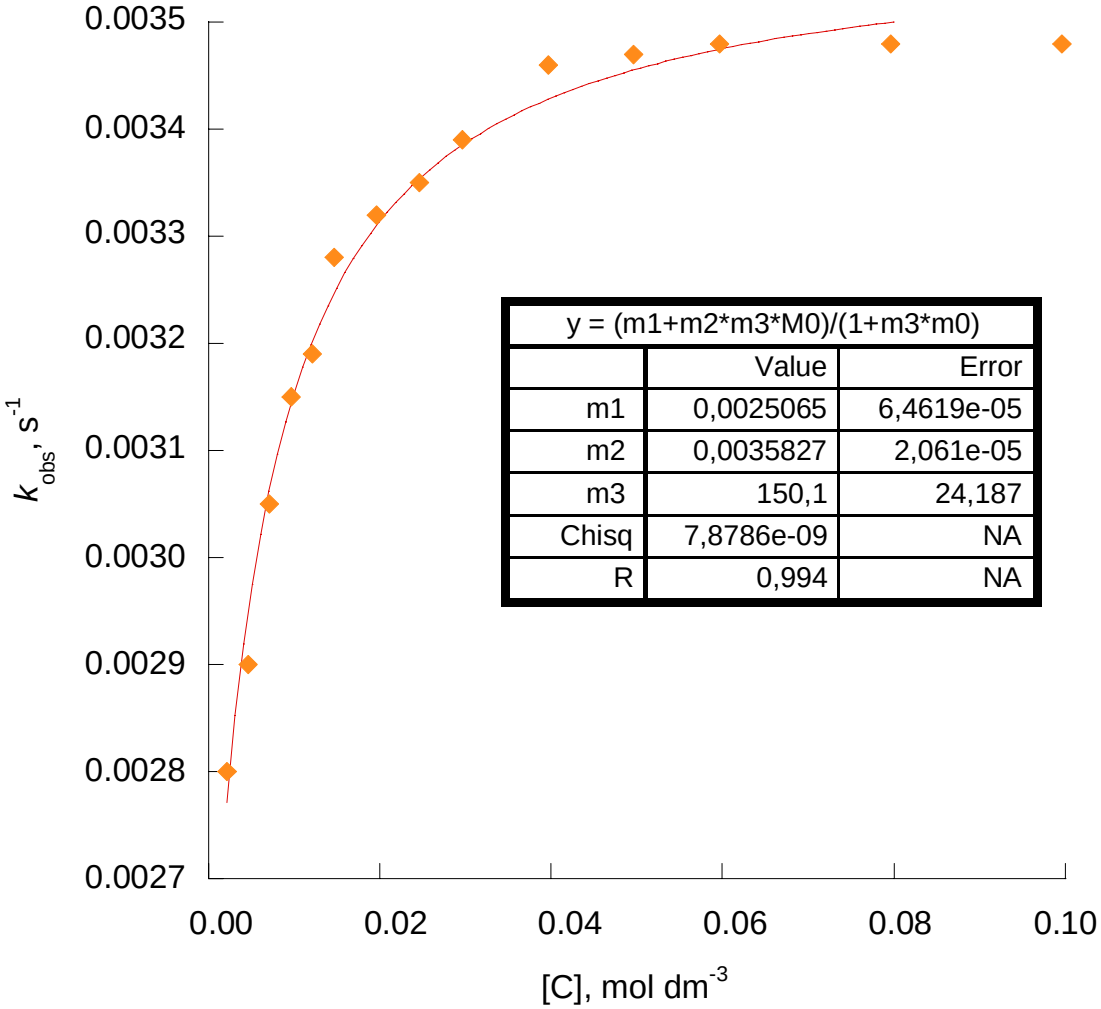


Figure S4. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1d** → **2d** on the concentration of C_{14} DMAO (concentration corrected for the corresponding c.m.c. of the surfactant, 2.8×10^{-4} mol dm^{-3}) in the presence of borate buffer (p*H* 9.6), ionic strength 2.0×10^{-2} mol dm^{-3}, at 313.1 ± 0.1 K.



y = (m1+m2*m3*M0)/(1+m3*m0)		
	Value	Error
m1	0,0025065	6,4619e-05
m2	0,0035827	2,061e-05
m3	150,1	24,187
Chisq	7,8786e-09	NA
R	0,994	NA

Figure S5. Dependence of the observed rate constant (k_{obs}, s^{-1}) for the MRH **1e** → **2e** on the concentration of C_{14} DMAO (concentration corrected for the corresponding c.m.c. of the surfactant, 3.3×10^{-4} mol dm^{-3}) in the presence of borate buffer (p*H* 9.6), ionic strength 2.0×10^{-2} mol dm^{-3}, at 313.1 ± 0.1 K.

Table S1. C.m.c. values for C_{14} DMAO in the presence of the investigated substrates.

	C.m.c. ($/10^4$, mol dm^{-3})
1a	1.5
1b	1.7
1c	2.5
1d	2.8
1e	3.3