Corrigendum

The authors of this Communication wish to alter the proposed structure of annulene 1, a system that had previously been reported by Yamaguchi et al.[1] After one of the authors (F.M.M.) had originally inspected the then available analytical data (¹H and ¹³C NMR spectra, elemental analysis, and ESI-MS data), he affirmed that they were (and still are) consistent with the annulene system. In particular, parent mass spectral signals at m/z 531.44353, 587.50648, and 643.56867 for the R= $C_{12}H_{25}$, $C_{14}H_{29}$, and $C_{16}H_{33}$ derivatives, respectively, all correspond to the mass of $[1-Cl^-]^+$. Recently, however, Prof. M. Cristl suggested^[2] that the pyridinium salt 2 would be an alternative and more likely possibility. There exists an intriguing ambiguity in this case because 1 and 2 have indistinguishable NMR spectra and elemental analyses and because our [1-2 Cl-]2+ base peak and the [2-Cl-]+ parent peak happen to have identical masses. We are now able to differentiate the two structures through weak ¹³C-containing MS signals. These signals have a shift one mass unit higher than the all-12C signal (consistent with $[2-Cl^-]^+$) as opposed to 0.5 units higher (consistent with $[1-2Cl^-]^{2+}$). In view of these new data, our peaks at m/z > 500 must, we surmise, arise from dimers of 2 in the gas phase. Fortunately, the altered identity of the compound in no way affects our high-level calculations on the annulene structure. Moreover, our conclusion based on the NMR data, namely, that the terminal methyl groups of the chains loop within a micelle so as to contact the micelle surface, remains valid, although the micelles are now more classical in nature than we had previously envisioned.

$$CI_{+}/N$$
 $R=N$
 $N=R$
 $R=C_{12}H_{25}, C_{14}H_{29}, and C_{16}H_{33}$

[1] I. Yamaguchi, Y. Gobara, M. Sato, Org. Lett. 2006, 8, 4279.

[2] M. Christl, private communication.

[12]Annulene Gemini Surfactants: Structure and Self-Assembly

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