



Cite this: *Soft Matter*, 2023,
19, 6851

Correction: Cross-linkable, phosphobetaine-based, zwitterionic amphiphiles that form lyotropic bicontinuous cubic phases†

Lauren N. Bodkin,^a Zachary A. Krajnak,^a Ruiqi Dong,^b Chinedum O. Osuji^b and Douglas L. Gin^{*a}

DOI: 10.1039/d3sm90094k

rsc.li/soft-matter-journal

Correction for 'Cross-linkable, phosphobetaine-based, zwitterionic amphiphiles that form lyotropic bicontinuous cubic phases' by Lauren N. Bodkin *et al.*, *Soft Matter*, 2023, **19**, 3768–3772, <https://doi.org/10.1039/D3SM00269A>.

The authors regret the following mistake in the chemical structure of monomer **1f** shown in the original article and its Electronic Supporting Information (ESI). Please note the original ESI was replaced with a corrected version on 24/08/2023, and is also available with this Correction article.†

After publication, it was brought to the authors' attention that a 4-dimethylaminopyridine (DMAP) moiety is typically more nucleophilic and undergoes alkylation at the pyridine ring nitrogen rather than at the dimethylamino group nitrogen position (*J. Chem. Educ.* 2011, **88**, 328–330). Consequently, the structure of **1f** may actually be the structural isomer shown in updated Fig. 1 below, in which the DMAP unit is tethered to the phosphonate unit *via* an ethyl spacer to the pyridine ring nitrogen, instead of the original published structure where the DMAP unit is tethered *via* an ethyl linkage to the dimethylamine nitrogen. It was determined *via* nuclear Overhauser effect spectroscopy (NOESY) experiments that the corrected structure for monomer **1f** shown in updated Fig. 1 below is more likely than the original published one.

NOESY reveals through-space correlations of hydrogen atom interactions within a molecule. This spectroscopic method is necessary when dealing with nitrogen in the structure since heteroatoms typically inhibit through-bond correlations seen with other methods. For the original published structure of **1f** (where the dimethylamino group nitrogen atom is attached to the phosphonate moiety *via* an ethyl spacer and the pyridine ring nitrogen is at the end of the molecule), it would be expected to see the correlations originating from the hydrogens next to the pyridine-ring nitrogen (A) to grow progressively weaker with increasing distance from hydrogens B to C to D to E. However, this was not the case observed.

The 1D NOESY spectrum for monomer **1f** (see Fig. C1 here) shows that the hydrogens next to the pyridine ring nitrogen (A) are near the other pyridine ring hydrogens (B) as well as the hydrogens on the methylene unit connected to the pyridine nitrogen (D), with slightly weaker correlations to the hydrogens on the dimethylamino group (C) and the methylene unit nearest the phosphonate group (E). These results suggest that ring hydrogens (A) are more centrally located in the formed zwitterionic headgroup, and more consistent with the updated structure of **1f**.

^a Department of Chemistry, University of Colorado, Boulder, CO 80309, USA. E-mail: douglas.gin@colorado.edu

^b Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA

† Electronic supplementary information (ESI) available. See DOI: <https://doi.org/10.1039/d3sm90094k>



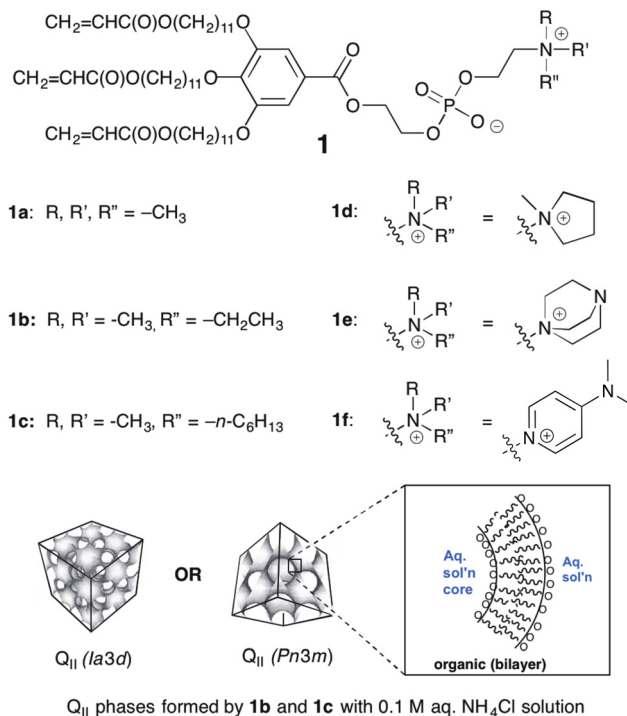


Fig. 1 Structures of cross-linkable, zwitterionic phosphobetaine monomers **1a–f** and schematic representations of the Q_{II} phase formed by **1b** and **1c** with 0.1 M aq. NH₄Cl solution. (Q_{II} unit cell images partially reproduced from ref. 17 with permission. Copyright American Chemical Society, 1997.)

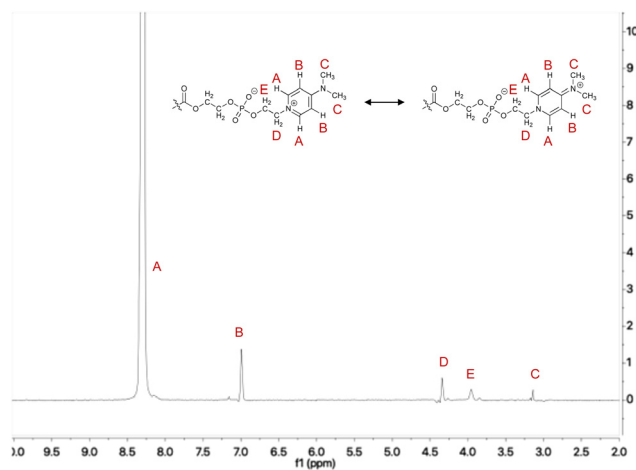
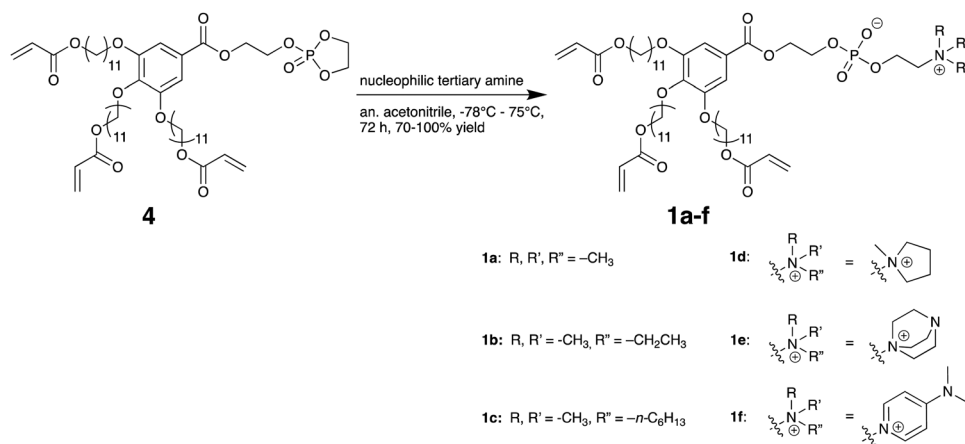


Fig. C1 1D NOESY spectrum for monomer **1f**.

Monomer **1f** is not one of the new phosphobetaine-based, zwitterionic compounds in the original article that exhibits the desired bicontinuous cubic phase formation behaviour, which are the focus of the article. Consequently, the updated structure of **1f** is a technical correction and does not change the overall conclusions of the original paper.

The updated versions of the ESI **Scheme S3**, **Fig. S12**, **Fig. S13**, and **Table S1** that show the corrected structure and data for **1f** are also provided here.





Scheme S3 Synthesis of monomers **1a-f** from compound **4**.

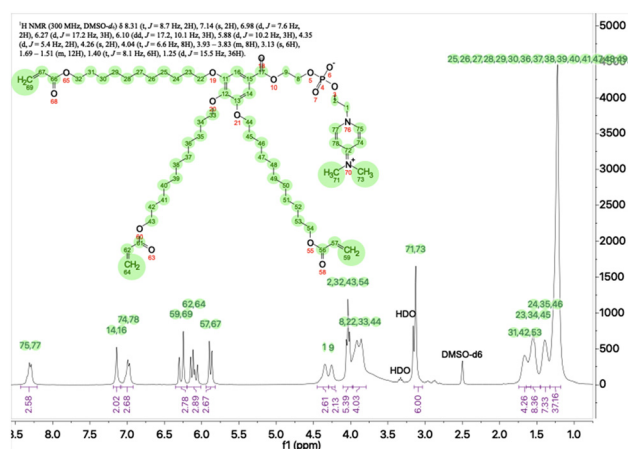


Fig. S12 ¹H NMR spectrum of monomer **1f** revealing only deuterated solvent peaks and no other impurities. Deuterated solvent residual peaks are labeled in black (above peaks), hydrogen assignments are labeled in green (above peaks), and integration ranges are labeled in purple (below peaks).

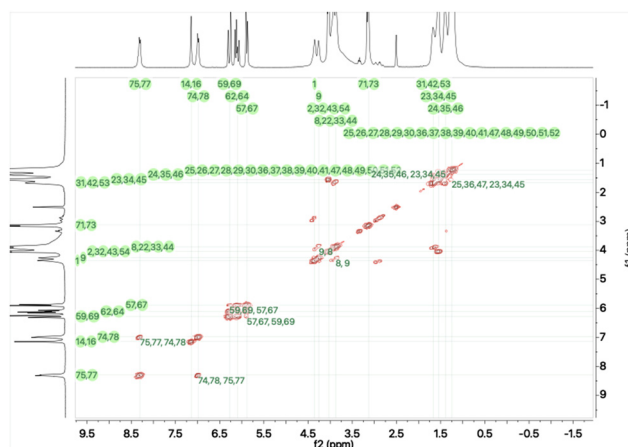
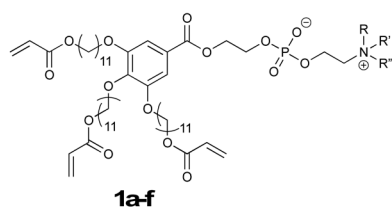


Fig. S13 ¹H-¹H COSY 2D-NMR spectrum of monomer **1f** revealing correlations within the zwitterionic headgroup. Hydrogen assignments are labeled in green.



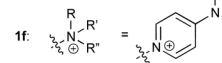
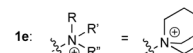
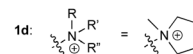
Table S1 Summary of the preliminary qualitative Q-phase formation behaviour of monomers **1a–f** studied in this work when mixed with 0.1 M aq. NH_4Cl and observed from 25–100 °C, as determined *via* PLM-based solvent-penetration scan screening studies



1a: R, R', R'' = -CH₃

1b: R, R' = -CH₃, R'' = -CH₂CH₃

1c: R, R' = -CH₃, R'' = -*n*-C₆H₁₃



Monomer:	1a	1b	1c	1d	1e	1f
Potential Q phase <i>via</i> penetration scan studies:	Yes	Yes	Yes	Yes	Yes	Yes
Potential Q-phase temp. range (°C):	59.5–79.5	55.8–75.8	36.5–91.5	64.9–84.9	52.1–72.1	36.3–76.3

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

