Alkylated distyrylbenzene as a model to clarify substitution pattern effect on liquid properties

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Alkyl-π functional molecular liquids (FMLs) constructed by attaching bulky yet flexible alkyl chains to the functional π-conjugated core unit are a new kind of soft matter.[1] Richer optoelectronic properties from larger π-conjugated moiety is in trade-off relationship with lower viscosity of alky-π FMLs. For instance, liquid porphyrins possessing electret properties exhibit relatively high viscosity in the range of 15.7-75.1 Pa·s, which might cause limitations when fabricating into devices.[2] Therefore, establishment of rational molecular design strategy for predictable creation of alkyl-π FMLs with richer optoelectronic property as well as lower viscosity is particularly essential.

In order to clarify the relationship between the molecular structure of alkyl-π FMLs and its thermal, optical and liquid-physical properties, we have investigated substitution pattern effect on distyrylbenzene (DSB) model system. That is attaching 2-octyldodecyl (C_8C_{12}) chains at 3,5-, 2,4-, 2,5- and 2,6-substituted position of the both terminal phenyl units, and another is various length of alkyl chains including 2-hexyldecyl (C_6C_{10}), 2-decyltetradecyl ($C_{10}C_{14}$), 2-dodecylhexadecyl ($C_{12}C_{16}$) at 2,5-substituted positions. A 2,5-substituted derivative with $C_{10}C_{14}$ chains exhibits the lowest viscosity as kinetically-stable liquid. Moreover, we have confirmed the applicability of 2,5-$C_{10}C_{14}$ substitution pattern on dicyanostyrylbenzene (DCS). Although a bare DCS moiety aggregates easily, 2,5-$C_{10}C_{14}$-DCS shows comparable low viscosity as 2,5-$C_{10}C_{14}$-DSB and retaining its intrinsic optical property. In this presentation, the liquid properties of alkylated DSB and DCS derivatives will be discussed further.

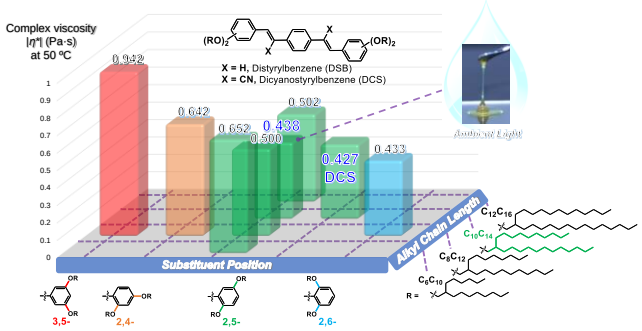

Figure 1. Complex viscosity $|\eta^*|$ of alkylated DSB and DCS derivatives at 50 ºC.

1) T. Nakanishi, ed., Functional Organic Liquids. **2019**, Wiley-VCH Verlag GmbH & Co. KGaA. 2) A. Ghosh, et al, *Nat. Commun*., **2019**, *10*, 1042.