Tetrabenzoporphyrin (BP) is a p-type molecular semiconductor having strong photoabsorption around 450 nm at which the solar-light intensity is highest. Accordingly BP has been among the prototypical active-layer components in organic solar cells (OSCs). At the same time, BP is extremely low in solubility and thus its processing by cost-effective wet processes is essentially impossible. This issue has been evaded via a stepwise pathway so-called “thermal precursor approach”, in which a soluble precursor 1,4:8,11:15,18:22,25-tetraethano-29H,31H-tetrabenzo[b,g,l,q]porphyrin (CP) is solution-deposited then quantitatively converted to BP in situ by a thermally induced retro-Diels–Alder reaction (Scheme 1a). Through this approach, power conversion efficiencies (PCEs) of over 5% have been achieved with solution-processed active layers containing BP or its derivatives. However, the open-circuit voltage ($V_{OC}$) in these devices is considerably lower as compared to the state-of-the-art systems, primarily because of the high energy level of the highest-occupied-molecular orbital (HOMO).

In this work, we examine the performance of CF$_3$BP, a new derivative of BP, as an active-layer material in OSCs. CF$_3$BP is not soluble enough to process as solution, and thus deposited by the thermal precursor approach using CF$_3$CP as a precursor compound (Scheme 1b). Owing to the two strongly electron-withdrawing trifluoromethyl groups, the HOMO and lowest unoccupied molecular orbital (LUMO) levels of CF$_3$BP are considerably lower than those of BP. This leads to a significant improvement in $V_{OC}$ when CF$_3$BP is used as a p-type material (up to 0.96 V from 0.58 V with BP). In addition, the low-lying LUMO allows CF$_3$BP to serve as an n-type material in OSCs. The thin-film characteristics and device performance will be discussed in detail in the presentation.

Scheme 1. Synthesis of BP (a) and CF$_3$BP (b) from the corresponding thermal precursors.