

Correction to "A New Tetracyclic Lactam Building Block for Thick, Broad-Bandgap Photovoltaics"

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Supporting Information

Page 11579. Further analysis of the spectroscopic data of the NT monomer suggested that the majority product is the *O*-alkylated instead of *N*-alkylated product. The amide functionality displays ambident reactivity, and the ratio of *N*- or *O*-alkylation is governed by factors such as the employed halide on the alkyl reactant and the thermodynamic stability of the final product. For amide-containing structures employed in conjugated polymers, the *N*-alkylated product is usually the majority product. However, recently He et al. reported a new conjugated building block that favored *O*-alkylation over *N*-alkylation under reaction conditions similar to those we employed.²

To unambiguously determine which isomer was formed, we synthesized a crystalline C8-NT unit under conditions similar to those used for the initial 2-hexyldecyl-substituted NT unit. Analysis by single-crystal X-ray diffraction and comparison of the other spectroscopic data confirmed that the majority product after alkylation is *O*-alkylated. The correct structures of the NT unit and PTNT are depicted in Figure 1.

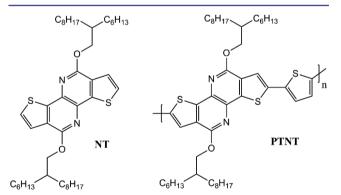


Figure 1. Chemical structures of the NT building block and PTNT.

Even though this diverges from our initially proposed structure, it does not influence the discussion and conclusion regarding the favorable physicochemical properties and photovoltaic performance of PTNT.

ASSOCIATED CONTENT

S Supporting Information

Experimental details, NMR characterization, and single-crystallography data confirming the new structure of NT and PTNT. This material is available free of charge via the Internet at http://pubs.acs.org.

REFERENCES

- (1) Mayr, H.; Breugst, M.; Ofial, A. R. Angew. Chem., Int. Ed. 2011, 50, 6470.
- (2) He, B.; Pun, A. B.; Klivansky, L. M.; McGough, A. M.; Ye, Y.; Zhu, J.; Guo, J.; Teat, S. J.; Liu, Y. Chem. Mater. 2014, 26, 3920.

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