Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Molecular aggregation by hydrogen bonding in cold-crystallization behavior of mixed nucleobases analyzed by temperature-controlled infrared spectroscopy

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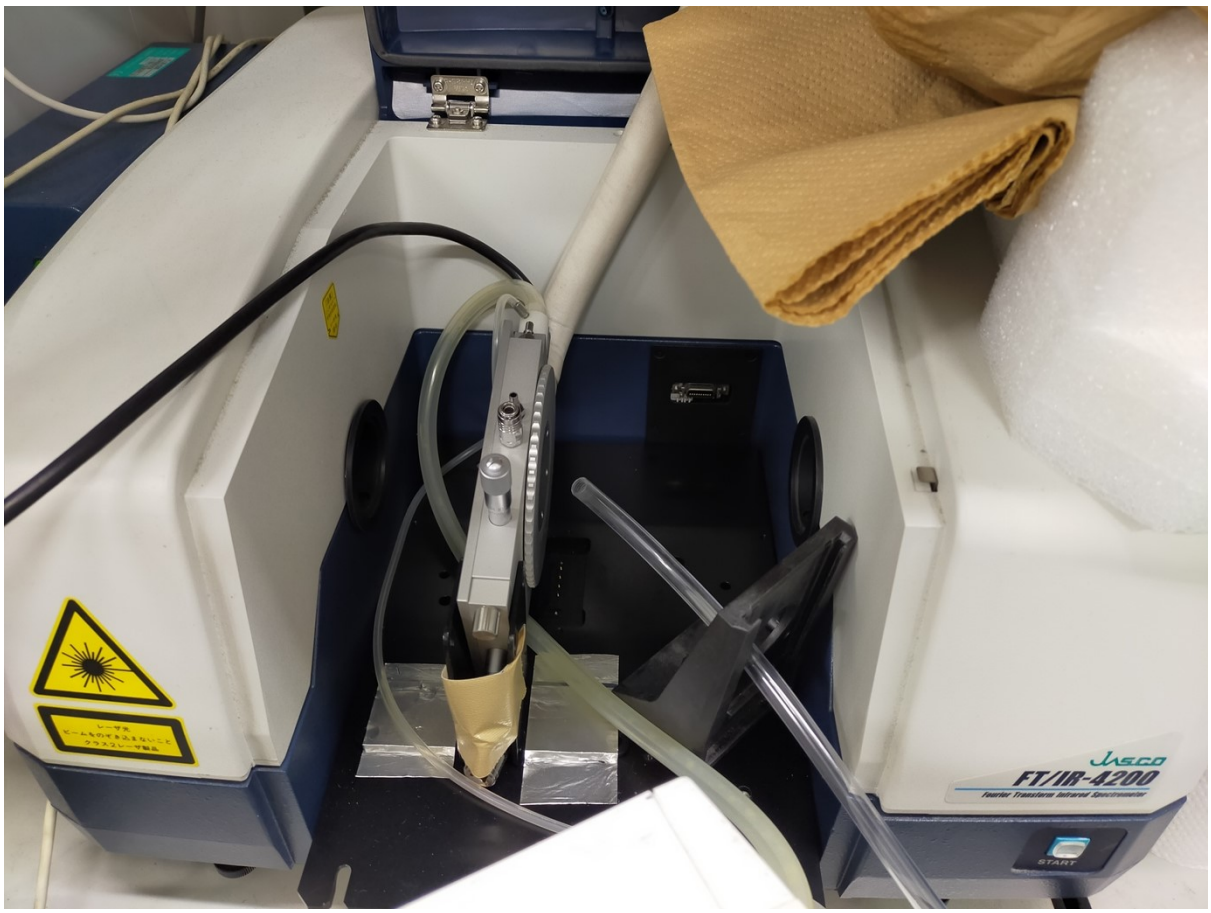


Fig. S1 Photograph of the thermally controlled FTIR spectroscopic system.

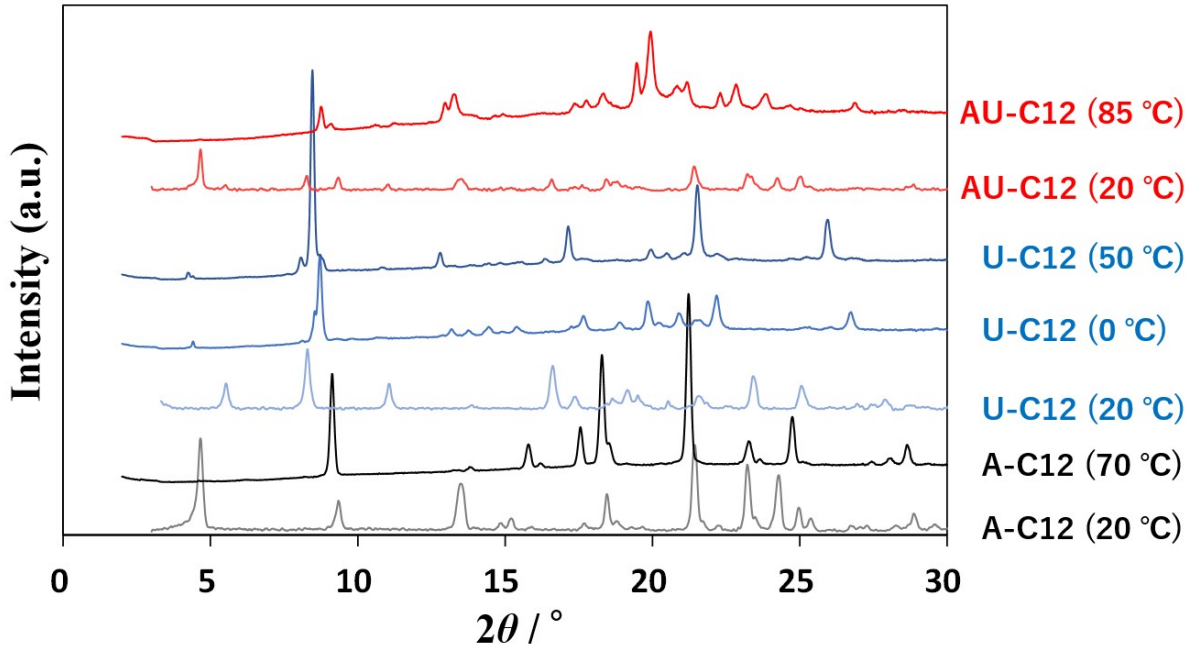


Fig. S2 Comparison of PXRD patterns between A-C12, U-C12, and AU-C12. A-C12, U-C12, and AU-C12 (20 °C, room temperature) were the samples crystallized from solution and measured before thermal treatment. A-C12 (70 °C) was the sample crystallized in the cooling process. U-C12 (0 °C) and U-C12 (50 °C) were the samples formed by solid-solid transition in the heating and cooling processes. AU-C12 (85 °C) was the sample formed by cold crystallization in the heating process. The PXRD patterns at 20 °C were measured using a diffractometer (Ultima IV, Rigaku, Japan).

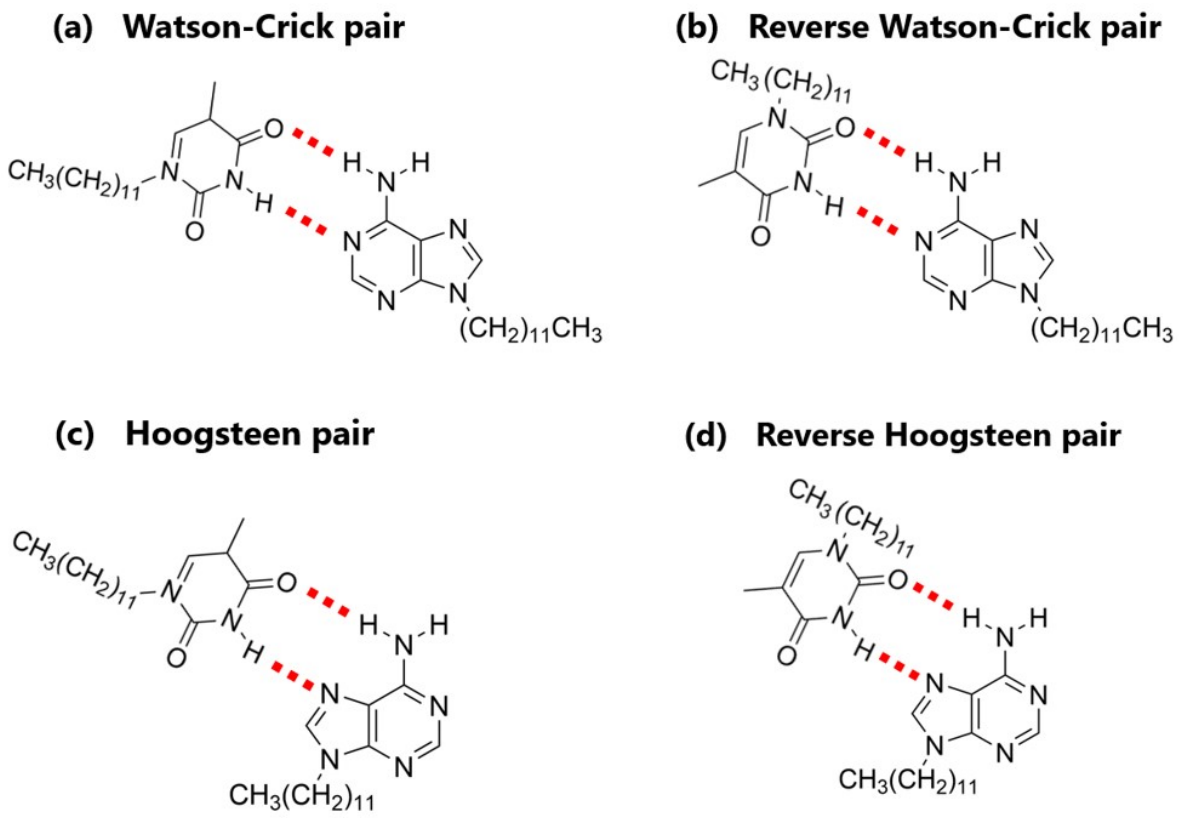
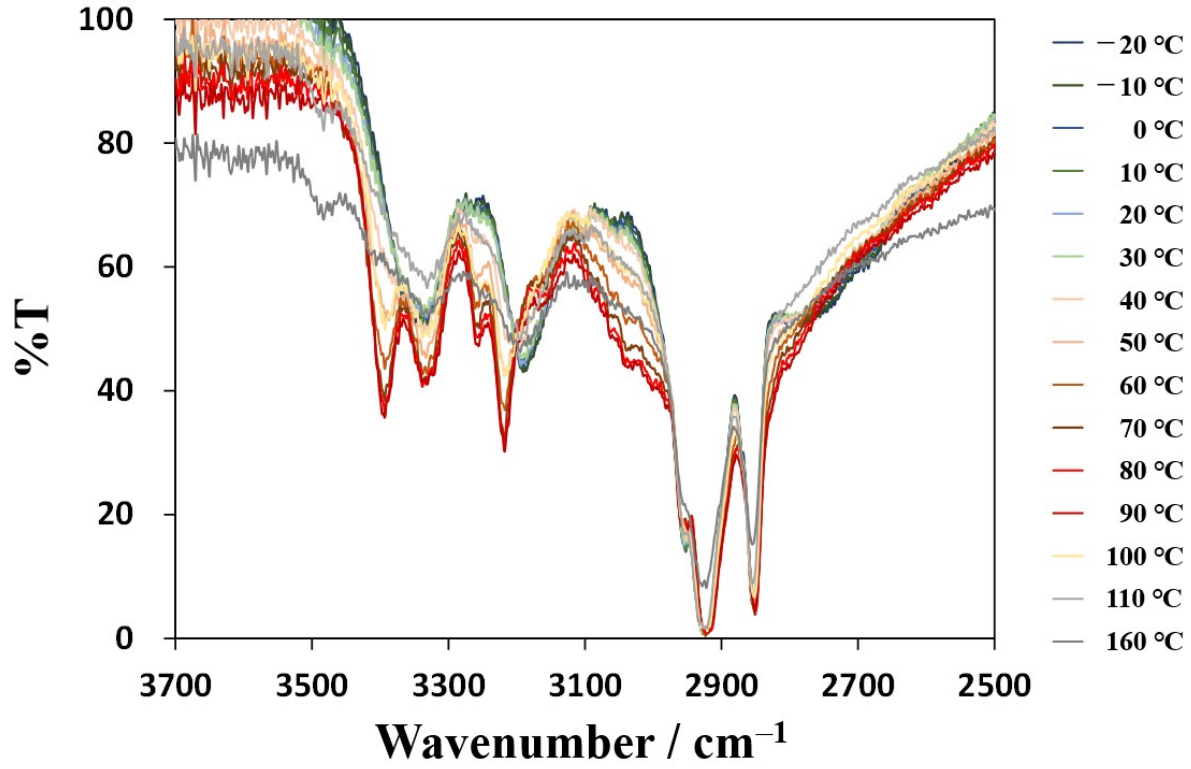


Fig. S3 Multiple types of complementary hydrogen bonds: (a) Watson-Crick structure, (b) reverse Watson-Crick structure, (c) Hoogsteen structure, and (d) reverse Hoogsteen structure.

(a)



(b)

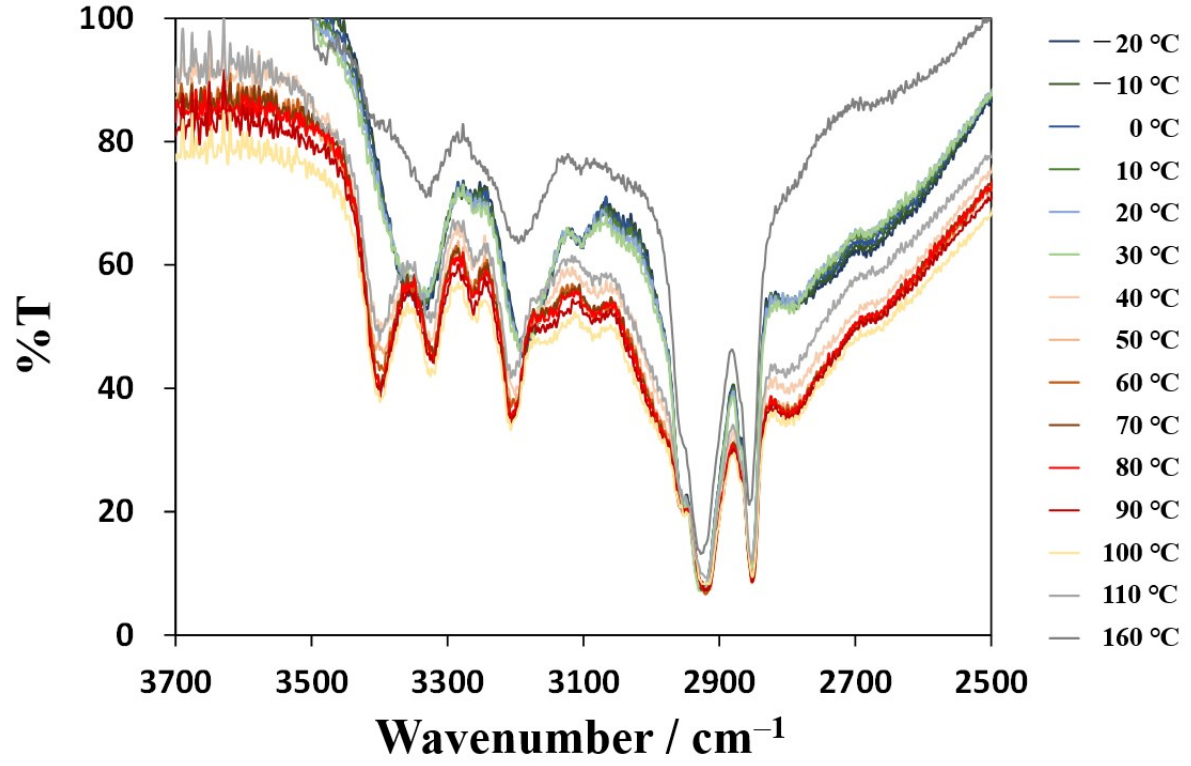


Fig. S4 Temperature-controlled IR spectra of second heating process of (a) AT-C12 and (b) AU-C12. The spectra were measured at a step of 10 °C.