Supplementary information

S.1 Crystal structure determination

The crystal structure determination procedure was performed using programs implemented in the Reflex Plus module of Materials Studio software [(1)]. First, lattice constants and space group were determined using X-Cell software [(2)]. Cell parameters together with peak profile parameters (shape -Pseudo-Voigt function-, asymmetry and full width at half maximum), background and zero shift were subsequently refined by Pawley refinement [(3)]. Crystal structure determination was achieved using a rigid body simulated annealing procedure using Powder Solve program [(4)]. The starting geometry of NMU molecule was taken from the known crystal structure of form I [(5)]. Then, the six degrees of freedom (3 translations and 3 rotations) of the latter molecule were allowed to vary in the simulated annealing procedure to achieve the best matching between experimental and calculated X-ray diffraction patterns. The final crystal structure was subsequently obtained after Rietveld refinement[(6)] of the best crystal structure attained from the simulated annealing procedure (low value of the agreement factor Rwp and realistic intermolecular interactions), encompassing refinement of the six degrees of freedom of the rigid body, an isotropic mean temperature factor and parameters describing preferential orientation of crystallites.

S.2 Molecular chains of Form III

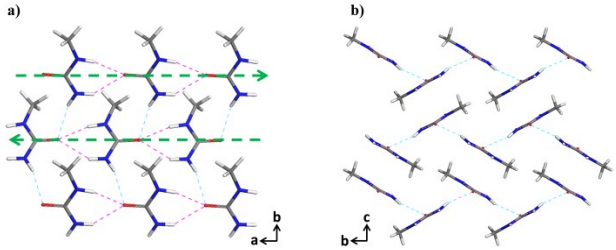

Figure S1. Molecular chains of Form III along a) *c* axis b) *a* axis showing methyl moieties face to face from adjacent layers.

References

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