



**Fig.S1:** Inversion centers of nylon 54 monomer salt.

**Table S1.** Experimental solubility of nylon 54 monomer salt in different proportions of methanol-water mixtures at different temperatures.

$x_2$	$x_1$							
	283.2 K	$10^3$ sd	293.2 K	$10^3$ sd	303.2 K	$10^3$ sd	313.2 K	$10^3$ sd
0.70	0.0452	0.6673	0.0496	0.7145	0.0536	0.3408	0.0548	0.4134
0.75	0.0426	0.8342	0.0468	0.4120	0.0510	0.6129	0.0533	0.5708
0.80	0.0389	0.7125	0.0438	0.8134	0.0464	0.4301	0.0514	0.6372
0.85	0.0342	0.7459	0.0392	0.4748	0.0403	0.5212	0.0467	0.5899
0.90	0.0267	0.5498	0.0319	0.5901	0.0338	0.4378	0.0412	0.4589
0.95	0.0154	0.6412	0.0216	0.6145	0.0220	0.8609	0.0289	0.5543

**Table S2.** Parameters of the (CNIBS)/Redlich–Kister model for nylon 54 monomer salt at different temperatures.

	283.2 K	293.2 K	303.2 K	313.2 K
$B_0$	9.185	7.583	-0.137	5.518
$B_1$	-34.836	-30.778	-9.300	-23.940
$B_2$	5.712	6.383	0.445	3.862
$B_3$	54.653	47.251	22.640	37.883
$B_4$	-39.542	-35.054	-17.983	-27.350
$10^3$ rmsd	1.50	1.92	2.18	2.64

**Table S3.** Parameters of the modified Apelblat model for nylon 54 monomer salt in pure water.

solvent	A	B	C	$10^3$ rmsd
pure water	17.426	-3569.732	-1.311	0.0224

**Table S4.** The hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) of nylon 54 monomer salt.

D-H $\cdots$ A	D-H	H $\cdots$ A	D $\cdots$ A	D-H $\cdots$ A
N1-H1A $\cdots$ O3 <sup>i</sup>	0.89	1.91	2.795(2)	179
N1-H1B $\cdots$ O2 <sup>ii</sup>	0.89	1.93	2.769(3)	156
N1-H1C $\cdots$ O3 <sup>iii</sup>	0.89	1.91	2.798(2)	173
N2-H2A $\cdots$ O1	0.89	1.92	2.795(3)	166
N2-H2B $\cdots$ O4	0.89	1.84	2.726(3)	170
N2-H2C $\cdots$ O1 <sup>iv</sup>	0.89	1.93	2.752(2)	153

Symmetry codes: ( i )  $1+x, 3/2-y, 1/2+z$ ; ( ii )  $1+x, y, z$ ; ( iii )  $1+x, y, 1+z$ ; ( iv )  $x, 3/2-y, -1/2+z$ .