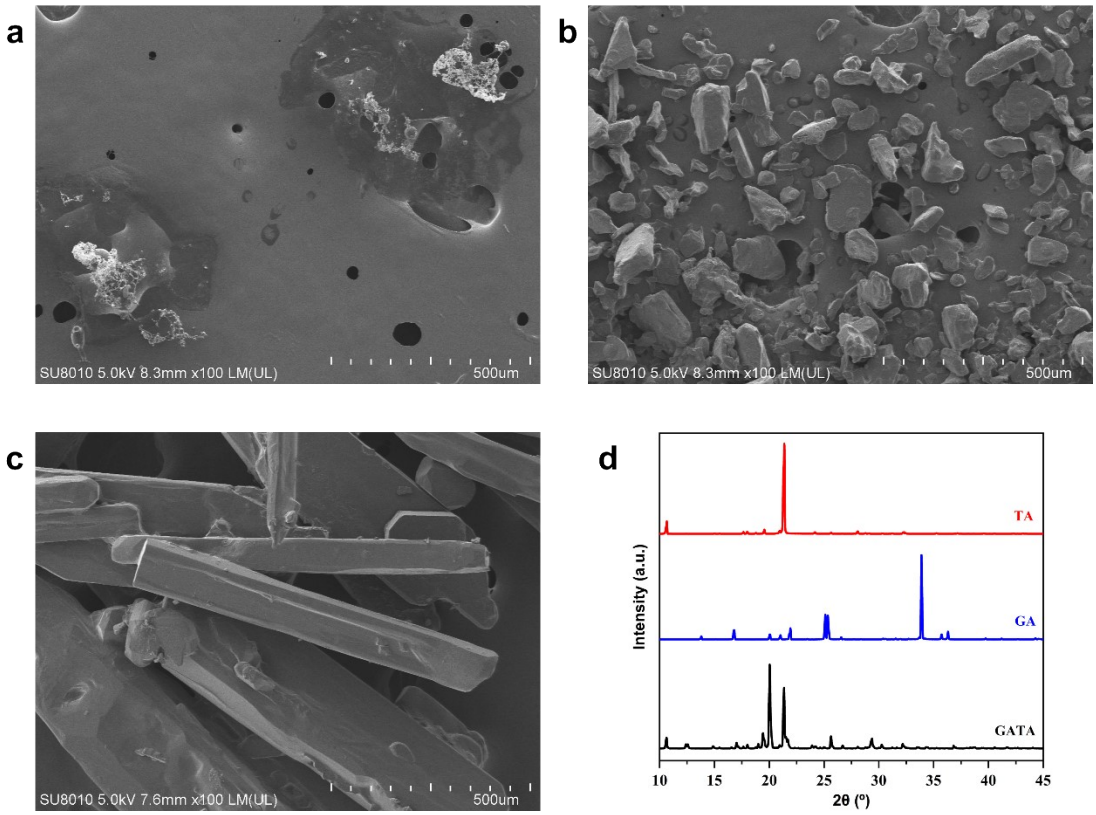

Figure S1. Microstructure of GA, TA, and GATA. (a) Scanning electron microscopy (SEM) image of GA; (b) SEM image of TA; (c) SEM image of GATA; (d) XRD patterns of GA, TA, and GATA.

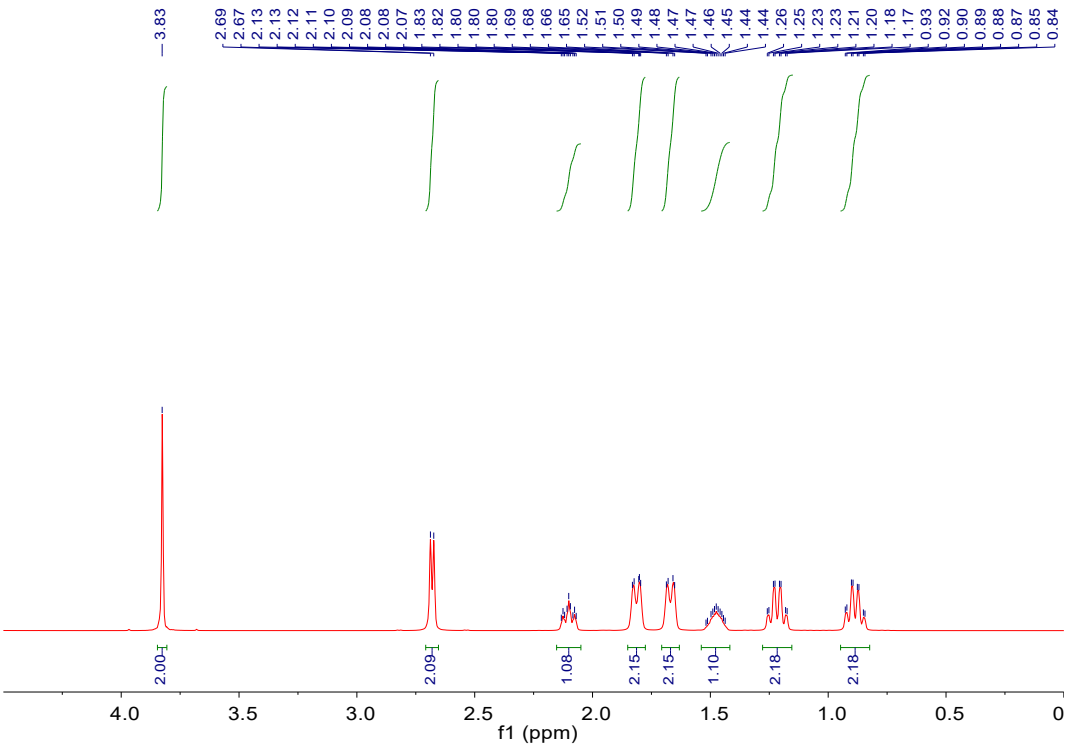

Figure S2. [1]H NMR of GATA. **[1]H NMR** (500 MHz, D_2O) δ 3.83(s, 2H), 2.68 (dd, J = 10Hz, 2H), 2.10 (t, 15Hz, 1H), 1.83–1.80 (m, 1H), 1.69–1.65 (m, 1H), 1.47 (s, 1H), 1.23–1.20 (dd, J = 5, 5Hz, 2H), 0.90–0.87 (dd, J = 5, 5 Hz, 1H).

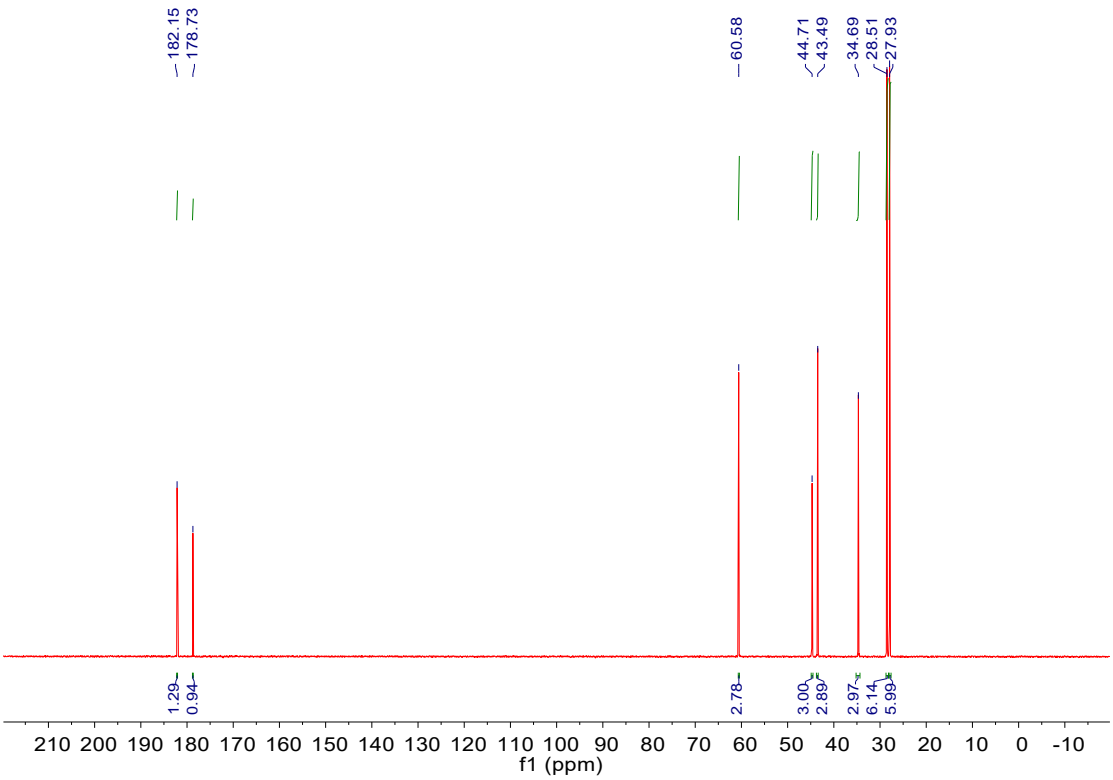

Figure S3. ^{13}C NMR of GATA. **^{13}C NMR** (500 MHz, D_2O) δ 182.15 (s), 178.73 (s), 60.58 (s), 44.71 (s), 43.49 (s), 34.69 (s), 28.51 (s).

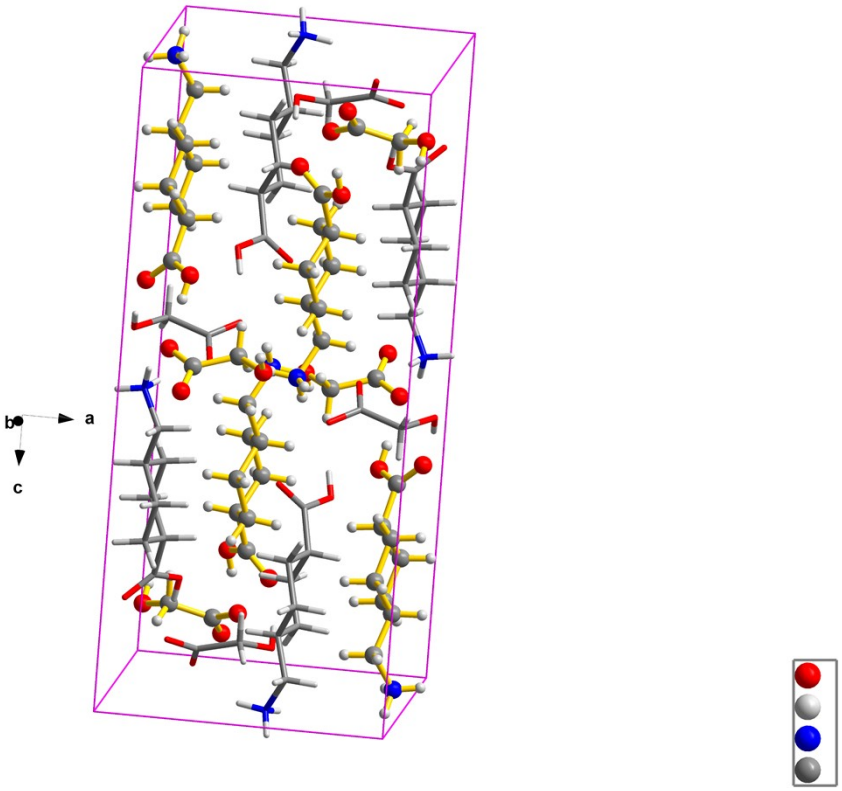

Figure S4. Crystal cell of GATA

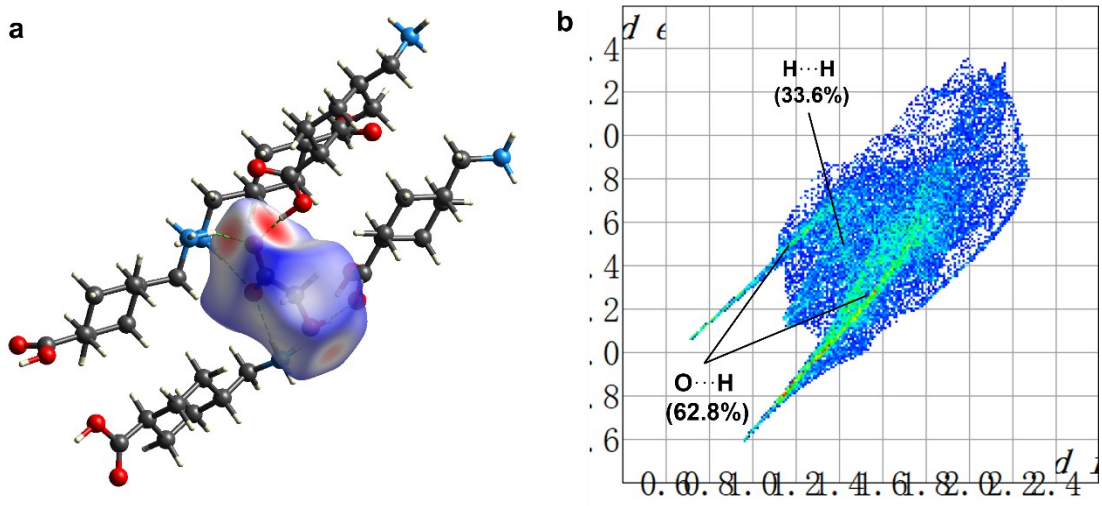

Figure S5. (a) 3D Hirshfeld d_{norm} surface of GA anion. (b) 2D fingerprint plot of GA anion with atom–atom contact contributions.

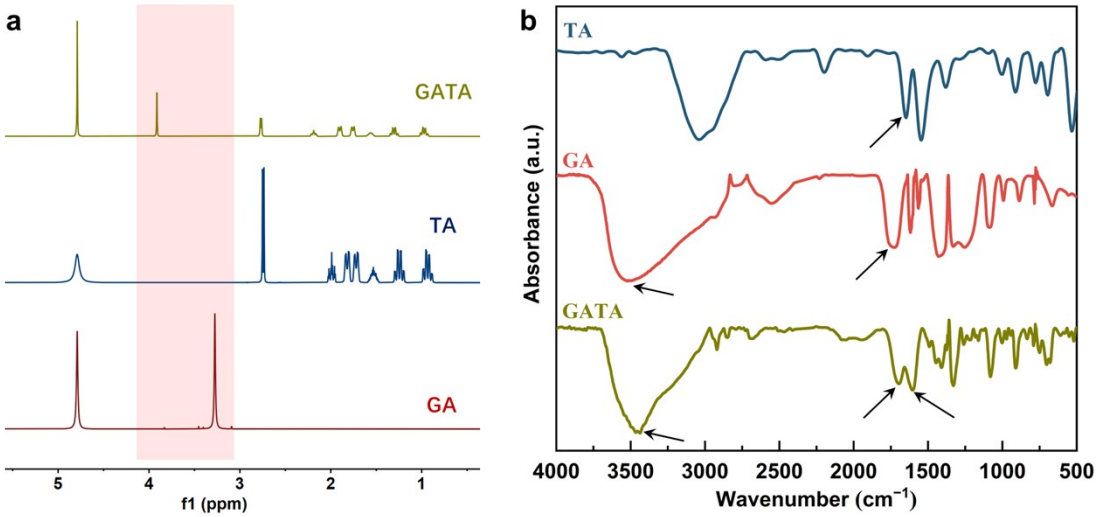

Figure S6. (a) ^{1}H NMR and (b) FTIR spectra of GA, TA, and GATA.

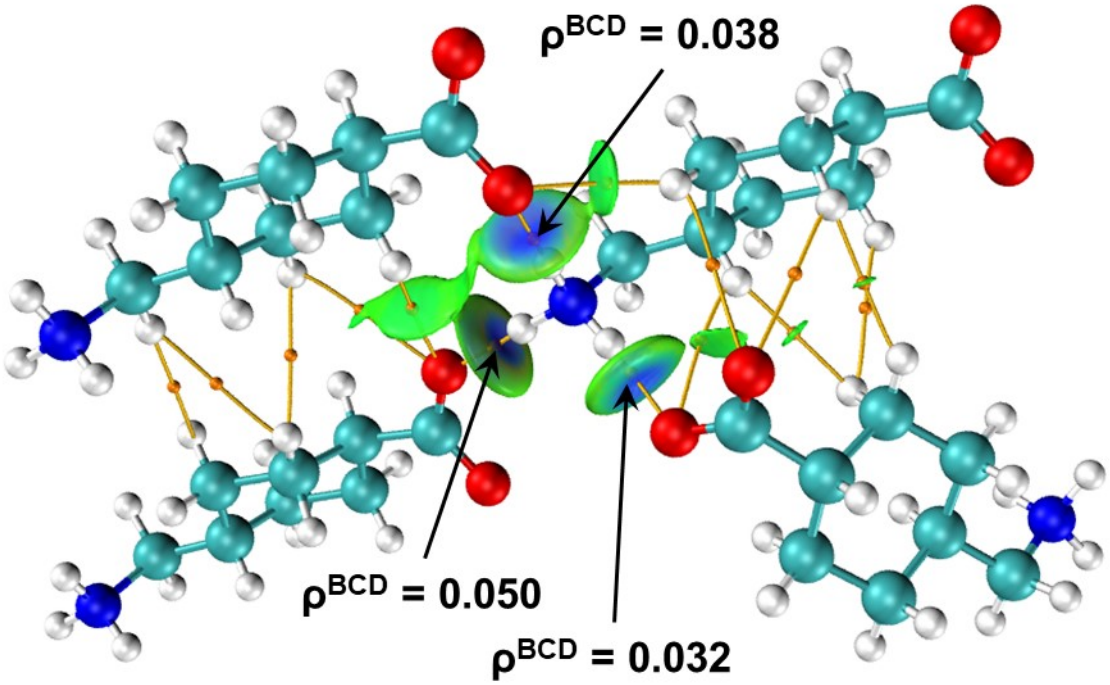

Figure S7. IGMH and AIM analysis of TA.

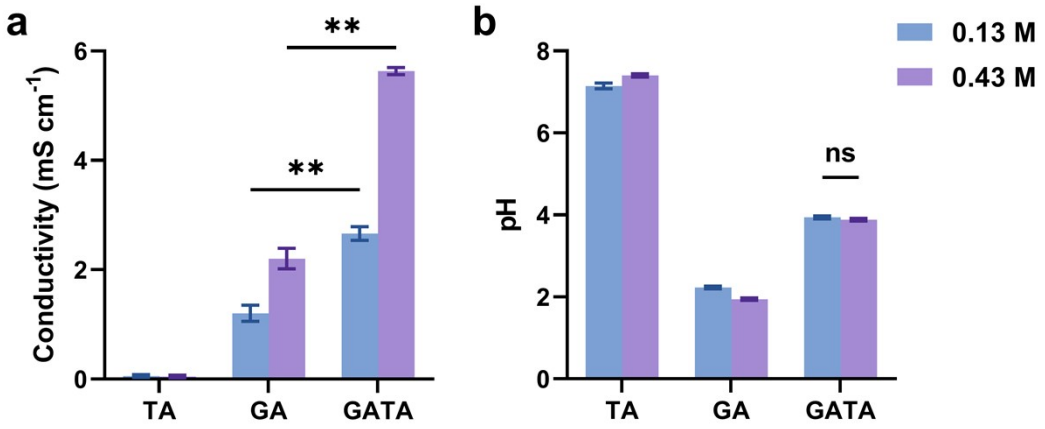

Figure S8. (a) Conductivity and (b) pH of GA, TA, or GATA solutions at different concentrations. Results are the mean ± SD for $n = 3$; ns = no significant, $^{**}p < 0.01$.

Table S1. Crystal data and structure refinement

Compound	GATA
CCDC	2410510
Empirical formula	$C_{10}H_{19}NO_5$
Formula weight	233.26
Temperature/K	169.99(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	9.4867(3)
b/Å	11.8536(3)
c/Å	21.3590(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2401.85(13)
Z	8
ρ_{calc}g/cm^3	1.290
μ/mm^{-1}	0.867
F(000)	1008.0
Crystal size/mm^3	0.12 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.28 to 146.754
Index ranges	$-11 \leq h \leq 10$, $-12 \leq k \leq 14$, $-19 \leq l \leq 26$
Reflections collected	5723
Independent reflections	2365 [Rint = 0.0219, Rsigma = 0.0247]
Data/restraints/parameters	2365/0/148
Goodness-of-fit on F2	1.048
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0429, wR_2 = 0.1126
Final R indexes [all data]	R_1 = 0.0482, wR_2 = 0.1167
Largest diff. peak/hole/e Å-3	0.20/-0.24

Table S2. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å2 $\times 10^3$) for GATA.

Atom	x	y	z	U(eq)
O1	2048.5(16)	5892.9(13)	8230.4(6)	54.8(4)
O2	382.6(14)	7117.0(11)	8484.2(6)	47.3(3)
N1	669.2(13)	8351.7(11)	5103.6(6)	28.5(3)
C1	1276.1(17)	6787.1(14)	8121.4(8)	33.1(4)
C2	1601.5(16)	7315.8(13)	7495.7(8)	32.2(4)
C3	1100(2)	8534.9(14)	7448.3(8)	41.9(4)
C4	1482(2)	9025.3(14)	6810.5(8)	40.4(4)
C5	900.6(15)	8327.0(12)	6271.2(7)	28.1(3)
C6	1381.9(17)	7099.8(13)	6327.7(7)	30.7(3)
C7	976.4(17)	6604.9(12)	6964.5(7)	30.8(3)
C8	1348.5(15)	8875.7(13)	5659.7(7)	30.7(3)
O3	1658.6(10)	4955.7(8)	9289.2(5)	28.0(3)
O4	2381.9(11)	3402.8(9)	9775.9(5)	31.7(3)
O5	5115.9(11)	3728.1(11)	9396.2(6)	39.9(3)
C9	2609.0(14)	4261.6(12)	9462.5(6)	23.1(3)
C10	4104.3(15)	4570.0(14)	9272.2(7)	32.1(4)

U(eq) is defined as 1/3 of the trace of the orthogonalized UIJ tensor

Table S3. Anisotropic displacement parameters (Å2 × 10^3) for GATA

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	60.2(9)	66.1(9)	38.1(6)	20.0(6)	15.2(6)	31.9(7)
O2	46.4(7)	42.1(7)	53.4(7)	-0.5(6)	14.4(6)	6.1(6)
N1	24.1(6)	26.2(6)	35.2(6)	5.7(5)	5.6(5)	3.4(5)
C1	30.6(8)	33.1(8)	35.5(8)	-1.9(7)	-3.1(7)	0.4(6)
C2	28.3(8)	32.6(8)	35.7(8)	3.4(7)	-3.8(6)	0.3(6)
C3	58.2(11)	27.4(9)	40.1(9)	-6.9(7)	-7.2(8)	-2.4(8)
C4	50.7(10)	24.2(8)	46.5(10)	0.1(7)	-7.7(8)	-6.6(7)
C5	22.4(7)	25.8(7)	36.2(8)	3.0(6)	-1.9(6)	-0.4(6)
C6	32.9(8)	23.9(8)	35.4(8)	1.1(6)	1.4(6)	1.4(6)
C7	35.1(8)	20.2(7)	37.0(8)	1.0(6)	2.0(7)	1.3(6)
C8	21.0(7)	27.3(8)	43.9(9)	7.3(7)	-1.4(6)	-2.2(6)
O3	27.2(5)	27.9(6)	28.8(5)	1.5(4)	0.4(4)	3.3(4)
O4	23.5(5)	30.4(6)	41.4(6)	9.2(5)	3.4(4)	1.9(4)
O5	20.8(5)	50.4(7)	48.5(7)	-6.3(6)	-1.8(5)	2.0(5)
C9	22.6(7)	25.2(7)	21.4(6)	-4.3(5)	-0.1(5)	-0.4(5)
C10	23.3(7)	37.8(9)	35.2(8)	2.2(7)	-0.7(6)	-5.5(6)

The anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…]

Table S4. Bond lengths in GATA

Bond	Length/Å	Bond	Length/Å
O1–C1	1.309(2)	C5–C6	1.529(2)
O2–C1	1.213(2)	C5–C8	1.520(2)
N1–C8	1.487(2)	C6–C7	1.530(2)
C1– C2	1.508(2)	O3–C9	1.2755(17)
C2–C3	1.525(2)	O4–C9	1.2372(17)
C2–C7	1.533(2)	O5–C10	1.4097(19)
C3–C4	1.525(2)	C9–C10	1.5203(19)
C4–C5	1.522(2)		

Table S5. Bond angles in GATA

Bond	**Angle/°**	**Bond**	**Angle/°**
O1–C1–C2	112.30(14)	C4–C5–C8	108.45(13)
O2–C1– O1	122.57(16)	C8–C5–C6	113.04(13)
O2–C1–C2	125.11(15)	C5–C6–C7	111.08(13)
C1–C2–C3	112.88(14)	C2–C7–C6	110.48(13)
C1–C2–C7	110.39(13)	N1–C8–C5	112.74(12)
C3–C2–C7	110.57(13)	O3–C9–C10	115.26(12)
C2–C3–C4	110.29(15)	O4–C9–O3	124.39(13)
C5–C4–C3	112.52(14)	O4–C9–C10	120.33(13)
C4–C5–C6	110.46(13)	O5–C10–C9	114.50(13)

Table S6. Torsion angles in GATA

Bond	Angle/°	Bond	Angle/°
O1–C1–C2–C3	-161.01(15)	C3–C4–C5–C8	-179.41(14)
O1–C1–C2–C3	74.68(18)	C4–C5–C6–C7	55.21(17)
O2–C1–C2–C3	20.8(2)	C4–C5–C8–N1	-171.97(13)
O2–C1–C2–C7	-103.53(19)	C5–C6–C7–C2	-57.09(17)
C1–C2 –C3–C4	179.06(14)	C6–C5–C8–N1	65.19(16)
C1–C2–C7–C6	-176.53(13)	C7–C2–C3–C4	-56.73(19)
C2–C3–C4–C5	56.0(2)	C8–C5–C6–C7	176.92(13)
C3–C2–C7–C6	57.84(18)	O3–C9–C10–O5	-172.27(12)
C3–C4–C5–C6	-55.02(19)	O4–C9–C10–O5	9.3(2)

Table S7. Hydrogen atom coordinates (Å × 10^4) and isotropic displacement parameters (Å2 × 10^3) of GATA

Atom	x	y	z	U(eq)
H1	1876.92	5652.42	5652.42	82
H1A	834.71	8774.31	8774.31	34
H1B	-256.11	8302.72	8302.72	34
H1C	1022.34	7664.42	7664.42	34
H2	2628.12	7315.99	7315.99	39
H3A	1537.2	8980.89	8980.89	50
H3B	86.94	8565.01	8565.01	50
H4A	1113.72	9787.01	9787.01	49
H4B	2499.56	9066.43	9066.43	49
H5	-130.92	8343.62	8343.62	34
H6A	2396.56	7060.93	7060.93	37
H6B	951.14	6656.23	6656.23	37
H7A	-42.07	6586.46	6586.46	37
H7B	1322.98	5836.98	5836.98	37
H8A	1108.53	9670.83	9670.83	37
H8B	2363.97	8816.6	8816.6	37
H5A	5045.28	3223.32	3223.32	60
H10A	4114.46	4734.46	4734.46	39
H10B	4375.77	5253.12	5253.12	39