Supplementary Materials

For Article:

Croconic Acid Doped Triglycine Sulfate: Crystal Structure, UV-Vis, FTIR, Raman, Photoluminescence Spectroscopy, and Dielectric Properties

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SM.1. *Single crystal XRD*

Table S1.1. Results of refinement of the TGS:CA(80:20) structure (space group $P2_1$ (4)) using single crystal XRD data. Atomic numbers Z, relative coordinates of atoms (x/a, y/b, z/c)[a] and their equivalent isotropic (for non-H atoms) or overall isotropic (for H atoms) temperature factors $U_{eq/iso}$ are shown.

N	Atom	Z	x/a	y/b	z/c	$U_{eq/iso}$(Å^2)
1	S1	16	-0.50029(7)	0.84266(10)	0.22619(12)	0.0324(2)
2	O1	8	-0.6422(2)	0.8411(4)	0.0071(4)	0.0432(5)
3	O2	8	-0.5348(2))	0.8441(3	0.4556(4)	0.0444(5)
4	O5	8	-0.4153(4)	0.9384(2)	0.2083(7)	0.0444(9)
5	O6	8	-0.4125(3)	0.7485(2)	0.2143(7)	0.0442(8)
6	O3	8	0.1065(2)	0.8354(4)	0.0776(4)	0.0511(6)
7	O11	8	-0.0047(3)	0.8267(4)	-0.3328(5)	0.0632(11)
8	C12	6	-0.0106(3)	0.8327(5)	-0.1276(6)	0.0424(8)
9	N17	7	-0.1423(4)	0.8795(3)	0.1624(6)	0.0574(10)
10	H17A	1	-0.232207	0.899519	0.166477	0.069(?)
11	H17B	1	-0.079876	0.934842	0.195904	0.069
12	H17C	1	-0.104135	0.829059	0.275115	0.069
13	C18	6	-0.1601(3)	0.8385(5)	-0.0851(6)	0.0456(7)
14	H18A	1	-0.228699	0.884113	-0.209868	0.055(?)
15	H18B	1	-0.204780	0.768376	-0.103655	0.055
16	O4	8	0.2793(4)	1.0877(3)	0.2237(7)	0.0512(9)
17	N7	7	0.3947(4)	1.0228(3	0.6974(8)	0.0422(10)
18	H7A	1	0.436755	0.986522	0.604936	0.051(?)
19	H7B	1	0.419263	0.992994	0.846837	0.051
20	H7C	1	0.428265	1.089313	0.713656	0.051
21	O13	8	0.0399(4)	1.0610(3)	0.2000(8)	0.0546(9)
22	C16	6	0.1834(5)	1.0604(3)	0.3145(9)	0.0385(10)
23	O8	8	0.2858(4)	0.5909(3)	0.2384(7)	0.0505(9)
24	N9	7	0.4156(4)	0.6665(3)	0.7052(7)	0.0394(9)
25	H9A	1	0.448741	0.713538	0.619965	0.047(?)

26	H9B	1	0.455173	0.603271	0.695924	0.047
27	H9C	1	0.443587	0.686593	0.863506	0.047
28	C10	6	0.2512(5)	0.6603(4)	0.6008(10)	0.0445(11)
29	H10A	1	0.208628	0.730390	0.599292	0.053(?)
30	H10B	1	0.214566	0.615141	0.704914	0.053
31	O14	8	0.0512(4)	0.6125(3)	0.2443(8)	0.0609(10)
32	C15	8	0.1985(6)	0.6165(4)	0.3391(10)	0.0442(12)
33	C1	6	0.2294(6)	1.0224(4)	0.5768(10)	0.0450(11)
34	H1A	1	0.184307	1.067621	0.669245	0.054(?)
35	H1B	1	0.191547	0.951003	0.579060	0.054
36	H3	1	0.190(6)	0.827(6)	0.046(9)	0.089(17)
37	H13	1	0.011(7)	1.082(5)	0.074(9)	0.058(18)

[a] The carbon and nitrogen-bound H atoms shown without estimated standard deviations (e.s.d.s) were placed in calculated positions and were included in the refinement in the 'riding' model approximation.

Table S1.2. Anisotropic atomic displacement parameters U_{ij} for the TGS:CA (80:20).

Atom	U_{11}, (Å²)	U_{22} , (Å²)	U_{33}, (Å²)	U_{23}, (Å²)	U_{13}, (Å²)	U_{12}, (Å²)
S1	0.0319(3)	0.0315(3)	0.0348(4)	0.0005(6)	0.0130(3)	-0.0004(5)
O1	0.0358(10)	0.0557(12)	0.0378(10)	-0.0045(19)	0.0121(8)	-0.0043(19)
O2	0.0523(12)	0.0469(12)	0.0381(11)	0.0010(18)	0.0209(9)	0.001(2)
O5	0.049(2)	0.0342(18)	0.054(2)	-0.0008(15)	0.0222(16)	-0.0074(15)
O6	0.0399(17)	0.0368(18)	0.058(2)	0.0014(15)	0.0192(15)	0.0058(14)
O3	0.0332(10)	0.0727(18)	0.0477(12)	-0.004(2)	0.0143(9)	0.003(2)
O11	0.0517(14)	0.091(3)	0.0470(14)	-0.0030(18)	0.0166(11)	0.0100(19)
C12	0.0401(15)	0.039(2)	0.0480(17)	0.000(2)	0.0147(13)	0.001(2)
N17	0.0381(16)	0.083(3)	0.056(2)	-0.0027(16)	0.0223(14)	-0.0079(15)
C18	0.0367(14)	0.0469(17)	0.0513(17)	0.001(3)	0.0126(12)	-0.002(3)
O4	0.0446(19)	0.060(2)	0.046(2)	0.0139(15)	0.0117(16)	-0.0014(16)
N7	0.049(2)	0.042(2)	0.034(2)	0.0061(15)	0.0124(17)	0.0004(16)
O13	0.0417(18)	0.067(2)	0.050(2)	0.0110(18)	0.0095(16)	0.0069(16)
C16	0.038(2)	0.033(2)	0.042(2)	0.0012(18)	0.0114(19)	-0.0002(17)
O8	0.046(2)	0.059(2)	0.047(2)	-0.0093(15)	0.0176(16)	0.0039(16)
N9	0.0438(19)	0.035(2)	0.036(2)	-0.0002(15)	0.0100(16)	0.0032(16)
C10	0.046(2)	0.047(3)	0.044(2)	-0.005(2)	0.020(2)	-0.001(2)
O14	0.0388(17)	0.084(3)	0.059(2)	-0.0090(18)	0.0163(15)	-0.0104(17)
C15	0.044(2)	0.039(3)	0.049(3)	-0.0002(19)	0.016(2)	-0.0036(18)
C1	0.040(2)	0.049(3)	0.047(3)	0.003(2)	0.016(2)	-0.0030(19)

Table S1.3. Results of refinement of the TGS:CA(90:10) structure (space group $P2_1$ (4)) using single crystal XRD data. Atomic numbers *Z*, relative coordinates of atoms (*x*/*a*, *y*/*b*, *z*/*c*)[a] and their equivalent isotropic (for non-H atoms) or overall isotropic (for H atoms) temperature factors $U_{eq/iso}$ are shown.

N	Atom	*Z*	*x*/*a*	*y*/*b*	*z*/*c*	$U_{eq/iso}$(Å²)
1	S1	16	-0.00057(8)	0.61108(9)	0.22657(13)	0.0167(2)
2	O8	8	-0.2135(4)	0.3587(4)	0.2398(7)	0.0353(9)
3	O5	8	0.0846(4)	0.7069(2)	0.2096(7)	0.0267(8)
4	O1	8	-0.1424(3)	0.6102(4)	0.0092(5)	0.0268(6)
5	O2	8	-0.0340(3)	0.6126(3)	0.4585(5)	0.0281(6)
6	O13	8	-0.5388(4)	0.3291(3)	-0.1951(7)	0.0346(9)

7	O6	8	0.0870(4)	0.5166(2)	0.2123(7)	0.0280(8)
8	O3	8	-0.3935(3)	0.6021(4)	0.0798(5)	0.0342(7)
9	C15	6	-0.2998(6)	0.3840(4)	0.3414(9)	0.0263(10)
10	O11	8	-0.5050(4)	0.5916(4)	-0.3309(6)	0.0457(12)
11	N9	7	-0.0816(5)	0.4351(3)	0.7070(7)	0.0248(8)
12	H9A	1	-0.050132	0.487501	0.633478	0.030(?)
13	H9B	1	-0.042050	0.374336	0.680412	0.030
14	H9C	1	-0.052336	0.447348	0.869527	0.030
15	O4	8	-0.7793(4)	0.3544(3)	-0.2224(7)	0.0339(9)
16	O14	8	-0.4479(5)	0.3791(4)	0.2510(8)	0.0452(11)
17	H14	1	-0.474951	0.356914	0.107993	0.068(?)
18	N7	7	-0.8942(5)	0.2915(3)	-0.6984(8)	0.0254(9)
19	H7A	1	-0.918776	0.260485	-0.846365	0.031(?)
20	H7B	1	-0.927481	0.357890	-0.717562	0.031
21	H7C	1	-0.936272	0.256370	-0.604622	0.031
22	N17	7	-0.6424(5)	0.6485(4)	0.1649(8)	0.0383(10)
23	H17A	1	-0.732567	0.665870	0.170380	0.046(?)
24	H17B	1	-0.583875	0.705650	0.193543	0.046
25	H17C	1	-0.600141	0.599884	0.280151	0.046
26	C1	6	-0.7286(6)	0.2910(4)	-0.5770(10)	0.0291(10)
27	H1A	1	-0.683855	0.336908	-0.668025	0.035(?)
28	H1B	1	-0.690847	0.219961	-0.581299	0.035
29	C18	6	-0.6601(4)	0.6055(5)	-0.0829(7)	0.0286(8)
30	H18A	1	-0.729056	0.649920	-0.209444	0.034(?)
31	H18B	1	-0.703580	0.535191	-0.098639	0.034
32	C12	6	-0.5103(4)	0.5998(5)	-0.1251(7)	0.0267(9)
33	C10	6	-0.2477(6)	0.4286(4)	0.6036(10)	0.0285(10)
34	H10A	1	-0.290385	0.498480	0.601430	0.034(?)
35	H10B	1	-0.283552	0.383588	0.708507	0.034
36	C16	6	-0.6820(5)	0.3278(4)	-0.3116(9)	0.0252(9)
37	H3	1	-0.301(8)	0.595(7)	0.072(11)	0.07(2)

[a] The carbon and nitrogen-bound H atoms shown without estimated standard deviations (e.s.d.s) were placed in calculated positions and were included in the refinement in the 'riding' model approximation.

Table S1.4. Anisotropic atomic displacement parameters U_{ij} for tTGS:CA (90:10).

Atom	U_{11}, (Å²)	U_{22} , (Å²)	U_{33}, (Å²)	U_{23}, (Å²)	U_{13}, (Å²)	U_{12}, (Å²)
S1	0.0160(4)	0.0160(4)	0.0194(4)	0.0005(4)	0.0076(3)	-0.0001(4)
O8	0.0286(19)	0.046(2)	0.0314(19)	-0.0077(15)	0.0103(15)	0.0044(16)
O5	0.0288(19)	0.0187(17)	0.0365(19)	-0.0001(14)	0.0164(15)	-0.0074(14)
O1	0.0179(11)	0.0390(15)	0.0212(11)	-0.0032(17)	0.0041(9)	-0.0032(18)
O2	0.0364(15)	0.0308(14)	0.0218(12)	0.0022(16)	0.0160(11)	0.0009(18)
O13	0.0216(16)	0.043(2)	0.0346(18)	-0.0044(16)	0.0039(13)	-0.0010(15)
O6	0.0249(17)	0.0206(18)	0.0388(19)	-0.0005(15)	0.0112(15)	0.0060(14)
O3	0.0174(12)	0.053(2)	0.0317(14)	-0.0015(18)	0.0084(11)	0.0048(18)
C15	0.028(2)	0.021(2)	0.030(2)	-0.0012(17)	0.0110(18)	-0.0023(17)

O11	0.0349(17)	0.071(4)	0.0316(16)	-0.0042(18)	0.0117(13)	0.008(2)
N9	0.0302(19)	0.023(2)	0.0205(17)	-0.0007(14)	0.0077(15)	0.0042(16)
O4	0.031(2)	0.042(2)	0.0276(18)	-0.0099(15)	0.0078(15)	0.0021(16)
O14	0.0283(19)	0.071(3)	0.035(2)	-0.0107(19)	0.0100(16)	-0.016(2)
N7	0.028(2)	0.023(2)	0.0210(18)	-0.0056(14)	0.0028(15)	0.0002(15)
N17	0.0227(18)	0.058(3)	0.039(2)	-0.0007(18)	0.0163(16)	-0.0057(17)
C1	0.025(2)	0.035(3)	0.028(2)	-0.0035(18)	0.0093(18)	0.0012(19)
C18	0.0184(15)	0.031(2)	0.0347(19)	-0.004(2)	0.0066(13)	-0.001(2)
C12	0.0196(16)	0.027(3)	0.0326(19)	0.0005(18)	0.0084(14)	0.0016(19)
C10	0.030(2)	0.030(3)	0.028(2)	-0.0068(19)	0.0132(18)	0.000(2)
C16	0.023(2)	0.019(2)	0.031(2)	-0.0027(17)	0.0048(17)	0.0003(16)

Table S1.5. Bond lengths (Å) in TGS:CA (80:20) and TGS:CA (90:10) structure according to results of structure refinement using single crystal XRD data (Table S1.1., S1.3.).

Bond	TGS:CA (80:20)	TGS:CA (90:10)
S1− O1	1.484(2)	1.481(3)
S1 − O2	1.459(2)	1.470(3)
S1 − O5	1.472(3)	1.476(3)
S1− O6	1.462(3)	1.471(4)
O3 − C12	1.306(4)	1.305(5)
O3 − H3	0.87(5)	0.90(7)
O1 − C12	1.198(4)	1.203(5)
C12 − C18	1.509(4)	1.516(5)
N17 − H17A	0.8900	0.8900
N17 − H17B	0.8900	0.8900
N17 − H17C	0.8900	0.8900
N17 − C18	1.464(5)	1.478(6)
C18 − H18A	0.9700	0.9700
C18 − H18B	0.9700	0.9700
O4 − C16	1.235(6)	1.242(6)
N7 − H7A	0.8900	0.8900
N7 − H7B	0.8900	0.8900
N7 − H7C	0.8900	0.8900
N7 − C1	1.468(7)	1.476(7)
O13 − C16	1.282(6)	1.285(6)
O13 − H13	0.73(5)	−
C16 − C1	1.493(7)	1.505(7)
O8 − C15	1.199(6)	1.198(6)
N9 − H9A	0.8900	0.8900
N9 − H9B	0.8900	0.8900
N9 − H9C	0.8900	0.8900
N9 − C10	1.455(6)	1.475(7)
C10 − H10A	0.9700	0.9700
C10 − H10B	0.9700	0.9700
C10 − C15	1.512(7)	1.520(7)
O14 − C15	1.303(6)	1.314(7)
C1 − H1A	0.9700	0.9700
C1 − H1B	0.9700	0.9700

Table S1.6. Bond angles (°) in in TGS:CA (80:20) and TGS:CA (90:10) structure according to results of structure refinement using single crystal XRD data (Table S1.2)

	TGS:CA (80:20) Bond angles (°)	TGS:CA (90:10) Bond angles (°)
O2 – S1 – O1	110.38(12)	110.37(17)
O2 – S1 – O5	110.3(2)	109.9(2
O2 – S1 – O6	110.9(2)	111.2(2)
O5 – S1 – O1	107.7(2)	107.8(2)
O6 – S1 – O1	107.9(2)	108.0(2)
O6 – S1 – O5	109.64(12)	109.52(17)
C12 – O3 – H3	111(3)	119(4)
O3 – C12 – C18	113.4(3)	113.5(3)
O11 – C12 – O3	125.1(3)	125.3(4)
O11 – C12 – C18	121.5(3)	121.1(4)
H17A – N17 – H17B	109.5	109.5
H17A – N17 – H17C	109.5	109.5
H17B – N17 – H17C	109.5	109.5
C18 – N17 – H17A	109.5	109.5
C18 – N17 – H17B	109.5	109.5
C18 – N17 – H17C	109.5	109.5
C12 – C18 – H18A	109.2	109.3
C12 – C18 – H18B	109.2	109.3
N17 – C18 – C12	111.8(3)	111.7(3)
N17 – C18 – H18A	109.2	109.3
N17 – C18 – H18B	109.2	109.3
H18A – C18 – H18B	107.9	107.9
H7A – N7 – H7B	109.5	109.5
H7A – N7 – H7C	109.5	109.5
H7B – N7 – H7C	109.5	109.5
C1 – N7 – H7A	109.5	109.5
C1 – N7 – H7B	109.5	109.5
C1 – N7 – H7C	109.5	109.5
C16 – O13 – H13	119(5)	
O4 – C16 – O13	125.1(5)	125.2(5)
O4 – C16 – C1	120.9(4)	120.1(4)
O13 – C16 – C1	113.9(5)	114.7(5)
H9A – N9 – H9B	109.5	109.5
H9A – N9 – H9C	109.5	109.5
H9B – N9 – H9C	109.5	109.5
C10 – N9 – H9A	109.5	109.5
C10 – N9 – H9B	109.5	109.5
C10 – N9 – H9C	109.5	109.5
N9 – C10 – H10A	109.3	109.5
N9 – C10 – H10B	109.3	109.5
N9 – C10 – C15	111.5(4)	110.8(4)
H10A – C10 – H10B	108.0	108.1
C15 – C10 – H10A	109.3	109.5
C15 – C10 – H10B	109.3	109.5
O8 – C15 – C10	122.1(4)	122.6(4)
O8 – C15 – O14	126.4(5)	127.2(5)
O14 – C15 – C10	111.5(5)	110.2(5)

N7 – C1 – C16	111.4(4)	111.6(4)
N7 – C1 – H1A	109.3	109.3
N7 – C1 – H1B	109.3	109.3
C16 – C1 – H1A	109.3	109.3
C16 – C1 – H1B	109.3	109.3
H1A – C1 – H1B	108.0	108.0

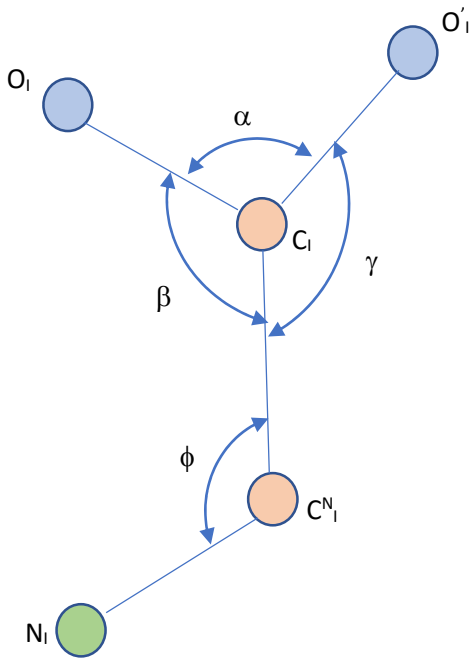
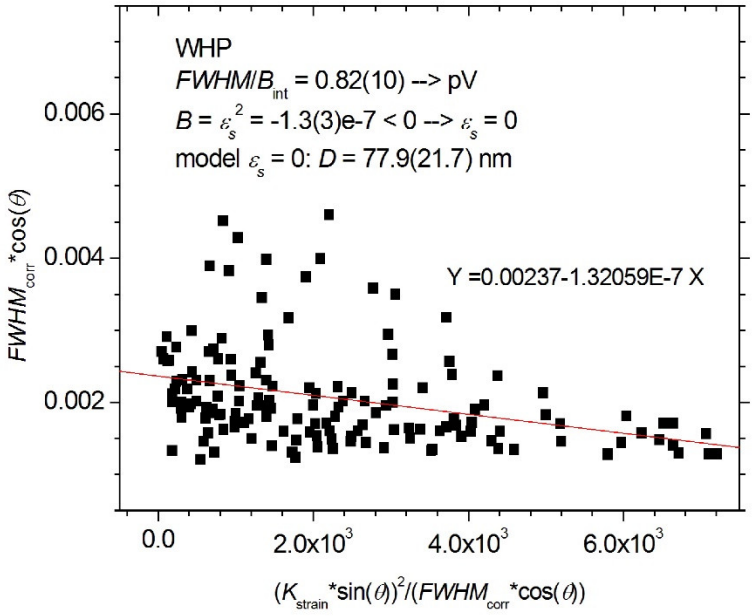
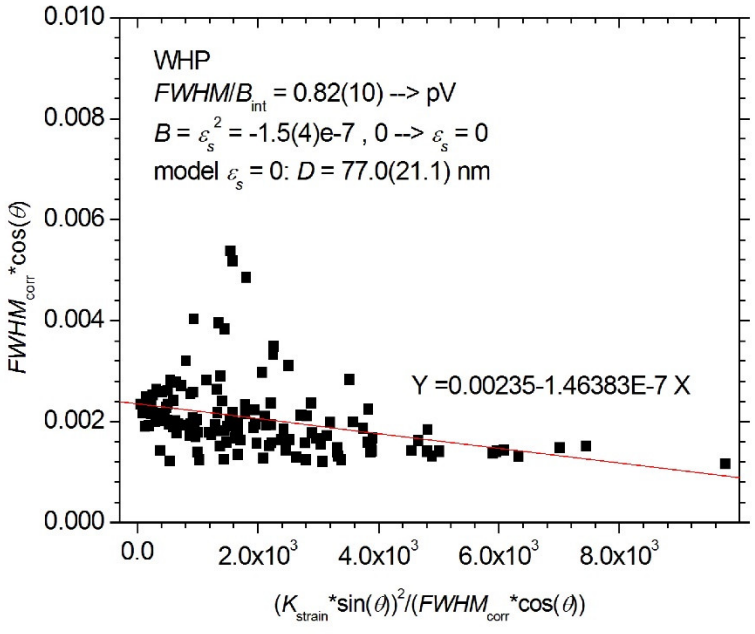


Figure S1.1. Schematic representation of a glycine molecule. α, β, γ, ϕ - angles between bonds.

SM.2. *Powder XRD. WHP graphs for TGS and TGS:CA (90:10).*



(a)



(b)

Figure S2.1. WHP graphs for. (a) TGS, (b) TGS:CA (90:10). $FWHM_{corr}$ is full width at half maximum of the XRD reflection corrected to instrumental broadening, $K_{strain} = 4$, θ is half of Bragg angle of the reflection after angular corrections applied. Equation of linear WHP graph is $Y = A + B \cdot X$, where X and Y are quantities shown in horizontal and vertical axes, respectively. Other designations are given in the text of the paper.