Electronic Supplementary Information (ESI)

Anion-controlled Supramolecular Crystal Structures and Ionic Liquids from Fatty Acid-substituted Ethyl-nicotinate Ionic Compounds

Wei-Jie Chang, Padi Yi-Syong Su and Kwang-Ming Lee*

Department of Chemistry, National Kaohsiung Normal University, 62 Shen-Shung Road, Kaohsiung 82444, Taiwan

Table of contents page

Table S1. Crystal data and structure refinement for salts 1 and 2. 2

Table S2. Hydrogen-bonding details for salts 1 and 2. 3

Figure S1. The single crystal X-ray diffraction pattern of salt **1**. 4

Figure S2. The single crystal X-ray diffraction pattern of salt **2**. 5

Table S1. Crystal data and structure refinement for salts **1** and **2**.

	1	2
Empirical formula	$C_{14}H_{21}BrN_2O_3$	$C_{38}H_{40}BNO_4$
Formula weight	345.24	582.52
Temperature (K)	100(2)	100(2)
wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
space group	P-1	P 21/c
a (Å)	7.6544(2)	13.5715(12)
b (Å)	10.3806(3)	10.6930(9)
c (Å)	10.4938(3)	21.9043(16)
α (°)	105.5910(13)	90
β (°)	102.9580(12)	99.931(2)
γ (°)	95.4460(13)	90
V (Å^3)	771.91(4)	3131.1(3)
Z	2	4
D_c (g·cm^{-3})	1.485	1.242
μ (mm^{-1})	2.672	0.079
F(000)	356	1248
θ (°)	2.07 to 26.40	1.523 to 26.421
reflns collected	12734	26637
unique reflns	3151	6423
Completeness to θ (%)	99.5	100.0
Data / restraints / parameters	3151 / 0 / 186	6423 / 0 / 399
GOF	1.108	0.999
R_1, wR_2 [$I > 2\sigma(I)$]	0.0225, 0.0588	0.0470, 0.0916
R_1, wR_2 (all data)	0.0262, 0.0864	0.0846, 0.1057
CCDC number	1533668	1533667

Table S2. Hydrogen-bonding details for salts **1** and **2**. (D: donor; A: acceptor)

D-H…A	D-H/Å	H⋯A/Å	D⋯A/Å	∠D-H⋯A/deg	Symmetry operation for A
			1		
C13-H13B⋯O1#1	0.990	2.742	3.358	120.71	-*x*, 2-*y*, 2-*z*
C7-H7A⋯O4#1	0.990	2.545	3.397	144.06	-*x*, 2-*y*, 2-*z*
C2-H2⋯O1#2	0.950	2.482	3.096	122.30	1+*x*, *y*, *z*
C1-H1⋯O1#2	0.949	2.760	3.352	105.25	1+*x*, *y*, *z*
C1-H1⋯Br1#3	0.949	2.760	3.695	168.86	1-*x*, 1-*y*, 1-*z*
O4-H41⋯Br1#4	0.641	2.598	3.160	147.87	*x*, *y*, 1+*z*
C5-H5⋯Br1#5	0.949	2.833	3.553	133.49	-*x*, 1-*y*, 1-*z*
C5-H5⋯O3#6	0.949	3.093	2.905	69.74	*x*, 1+*y*, *z*
			2		
C6-H16⋯O4#1	0.990	2.609	3.225	120.35	2-*x*, 1-*y*, 2-*z*
C5-H17··O2#2	0.949	2.922	3.190	97.66	*x*, 1+*y*, *z*
O2-H2⋯O4#3	0.840	1.784	2.618	171.55	2-*x*, -*y*, 2-*z*

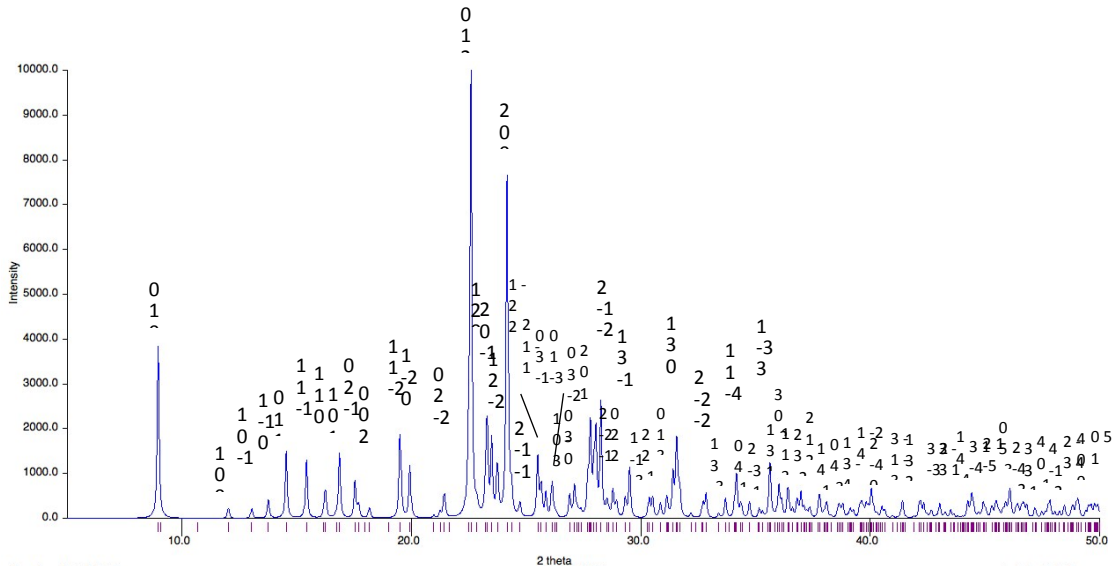

Figure S1. The single crystal X-ray diffraction pattern of salt **1**.

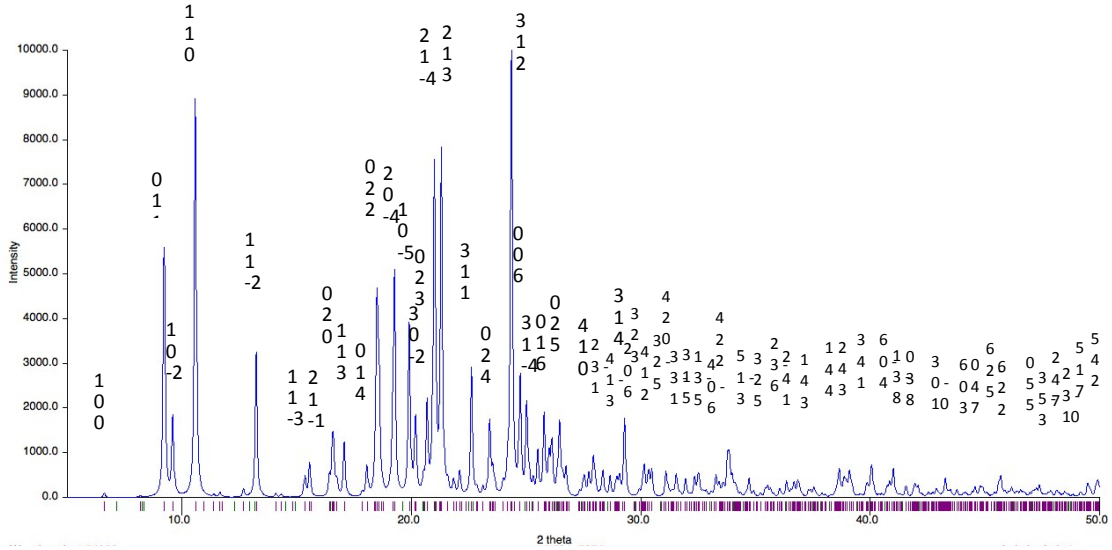

Figure S2. The single crystal X-ray diffraction pattern of salt **2**.