Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supplementary Information

For

Lidocaine barbiturate: a promising material for second harmonic generation

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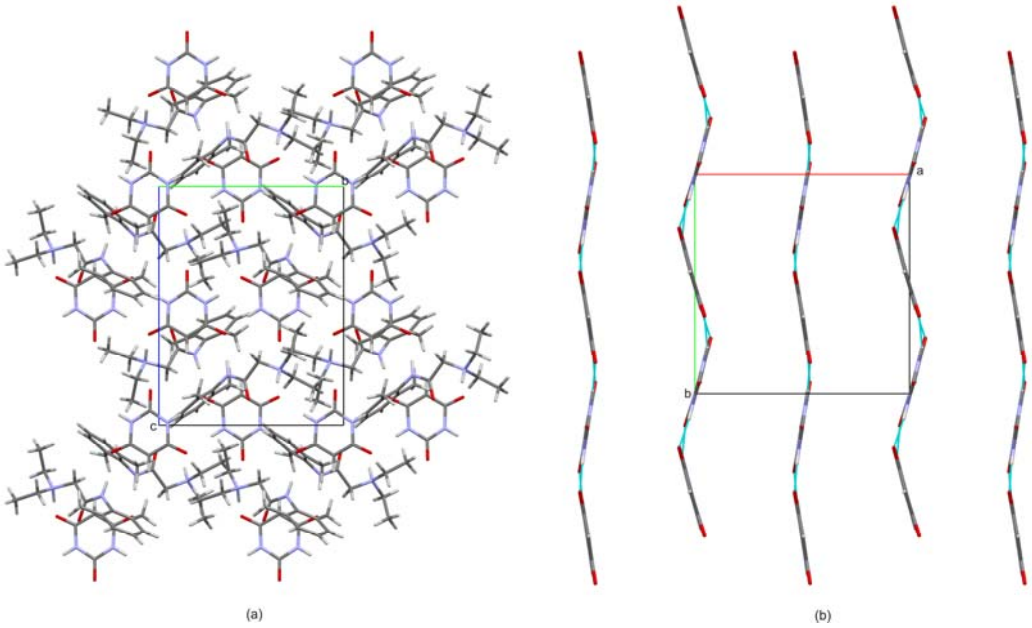

Fig. S1 (a) Packing of the structure components viewed along **a**. (b) Side-shape of the tapes viewed along **c**. Both drawings were prepared in Mercury.

Table S1 Hydrogen bond geometry for (I) (Å / °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1A–H1A...O4A$^{\#1}$	0.89(1)	1.86(1)	2.745(2)	172(2)
N3A–H3A...O6A$^{\#2}$	0.89(1)	1.86(1)	2.745(2)	174(2)
N1B–H1B...O4B$^{\#3}$	0.89(1)	1.95(1)	2.833(2)	174(2)
N3B–H3B...O6B$^{\#4}$	0.89(1)	1.93(1)	2.813(2)	177(2)
N1–H1...O6A	0.89(1)	1.89(2)	2.697(2)	151(2)
N3–H3...O6B$^{\#4}$	0.90(1)	1.90(1)	2.792(2)	177(2)
N2–H2...O4B	0.90(1)	1.90(1)	2.728(2)	152(2)
N4–H4...O4A$^{\#5}$	0.89(1)	1.91(1)	2.797(2)	177(3)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1, *y*-1/2, -*z*+1; #2 -*x*+1, *y*+1/2, -*z*+1; #3 -*x*+2, *y*-1/2, -*z*+2; #4 -*x*+2, *y*+1/2, -*z*+2; #5 -*x*+1, *y*-1/2, -*z*+2

Table S2 Static first hyperpolarizability tensor components calculated for barbiturate (barb_a, barb_b) and lidocaine (lid_a, lid_b) non-optimised ions using B3LYP/6-31G(2d,2p) and B3LYP/6-311G(2d,2p). βtot in 10^{-30} esu units.

	β_{xxx}	β_{xxy}	β_{xyy}	β_{yyy}	β_{xxz}	β_{xyz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}	β_{tot}[a]
B3LYP/6-31G(2d,2p)											
barb_a	-97.74	-143.28	79.55	31.50	6.34	-3.35	-2.39	1.65	0.41	-0.09	0.97
barb_b	-91.29	-148.00	78.32	33.62	-0.32	-2.44	0.33	2.85	-0.63	-0.18	1.00
lid_a	379.40	-28.51	-28.42	-24.40	41.17	-22.67	-12.63	59.74	12.07	-37.88	3.57
lid_b	-454.07	-5.00	-46.44	-61.22	57.68	0.73	6.62	26.92	-1.21	-18.35	4.15
B3LYP/6-311G(2d,2p)											
barb_a	-120.67	-176.40	97.82	40.68	7.47	-4.39	-1.86	3.90	10.06	-2.32	1.10
barb_b	-117.41	-178.89	93.83	46.71	1.53	-2.39	0.06	3.11	10.21	0.70	1.07
lid_a	415.43	-34.41	-20.96	-26.77	32.83	-19.98	-13.74	69.45	8.21	-53.99	4.05
lid_b	-487.69	-8.55	-61.36	-39.34	62.64	-6.12	-1.37	18.15	2.27	-20.81	4.62

[a] $\beta_{tot} = \{(\beta_{xxx}+B_{xyy}+\beta_{xzz})^2+(\beta_{yyy}+\beta_{yzz}+\beta_{yxx})^2+(\beta_{zzz}+\beta_{zxx}+\beta_{zyy})^2\}^{1/2}$.