

SUPPORTING INFORMATION

NEW PHARMACEUTICAL SALTS OF TRAZODONE

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Table S1. ^{13}C CP/MAS NMR chemical shifts (ppm) of T:HCl and T:OHN.

Group	Assignment	T:HCl δ [ppm]		T:OHN δ [ppm]		T:HCl δ_{exp} - T:OHN δ_{exp} [ppm]
		EXP	CAL*	EXP	CAL*	
C	1	148,37	146,19	149,02	147,56	-0,65
CH	2	121,62	118,35	118,18	117,39	3,44
CH	3	132,32	132,57	129,83	130,09	2,49
CH	4	108,63	111,25	107,76	109,85	0,87
CH	5	126,08	125,74	125,85	125,66	0,23
C	6	142,64	142,05	141,89	142,06	0,75
CH ₂	7	48,26	44,6	46,35	42,25	1,91
CH ₂	8	26,4	19,8	25,79	22,76	0,61
CH ₂	9	56,54	50,87	53,75	50,35	2,79
CH ₂	10	50,3	49,79	46,35	41,83	3,95
CH ₂	11	48,26	41,62	44,16	40,02	4,1
CH ₂	12	48,26	44,34	46,35	42	1,91
CH ₂	13	50,3	46,14	52,66	49,09	-2,36
C	14	148,37	150,1	150,94	149,54	-2,57
CH	15	108,63	111,71	115,44	112,48	-6,81
CH	16	131,3	131,05	129,83	129,57	1,47
CH	17	121,24	116,77	118,18	117,38	3,06
C	18	142,64	142,01	141,89	139,97	0,75
CH	19	110,93	112,89	115,44	115,15	-4,51
C	20			112,15	110,25	
C	21			161,63	165,95	
C	22			161,63	165,95	
CH	23			127,91	126,62	
CH	24			124,07	125,53	
CH	25			127,91	128,98	
CH	26			129,83	130,38	
C	27			135,86	134,87	
CH	28			141,89	141,58	
CH	29			129,83	129,13	
C	30			173,97	175,35	

* CASTEP computed δ values have been obtained from all atoms positions optimization (the lattice parameters were fixt to their experimental values);

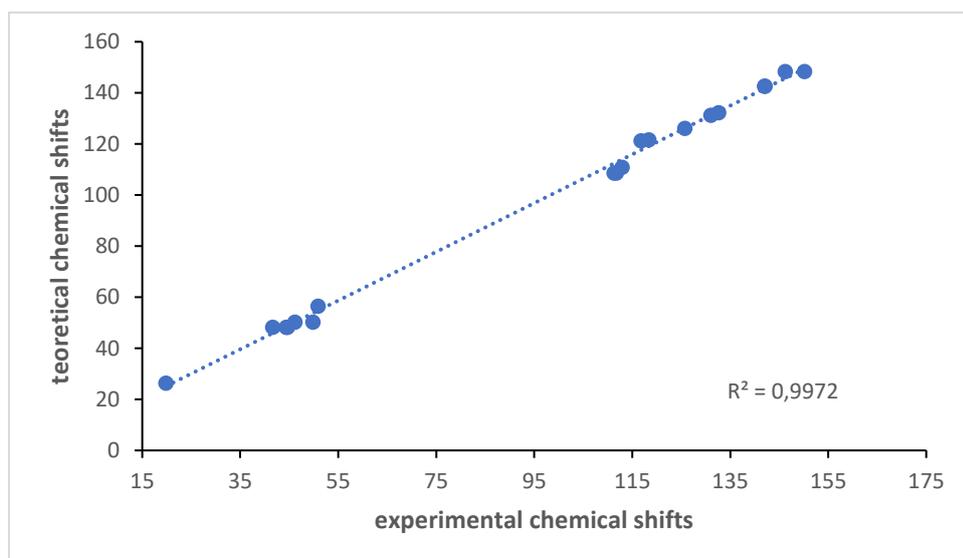


Fig 1S. Comparison of experimental and teoretical chemical shifts of carbon-13 of **T:HCl**.

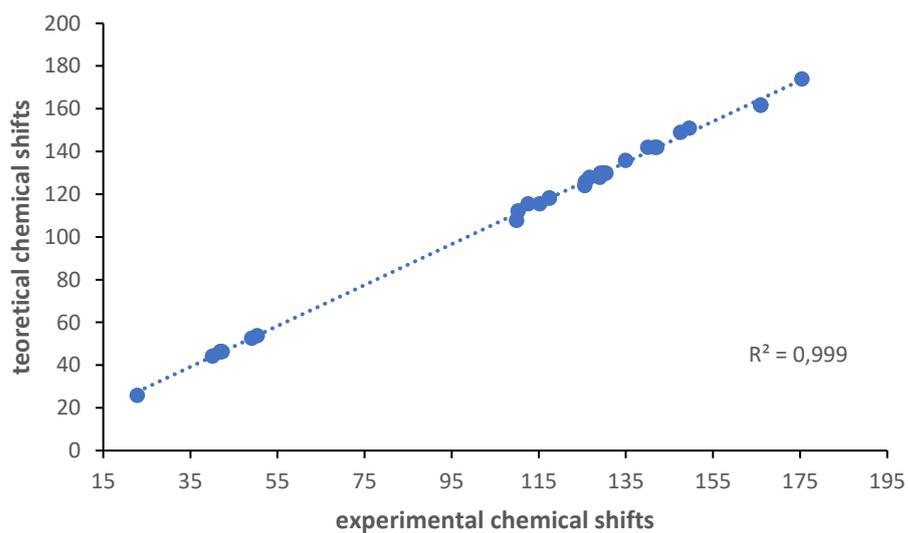


Fig 2S. Comparison of experimental and teoretical chemical shifts of carbon-13 of **T:OHN**.

Table. S2. Geometry of main weak intermolecular interactions in **T:OHN** crystal.

	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N4–H4...O5	1.72(2)	2.651(2)	169.4(18)
O4–H4B...O3	1.50(3)	2.457(2)	159(3)
O5–H5A...O2 ⁱ	1.86	2.710(2)	177.1
O5–H5B...O3 ⁱⁱ	1.85	2.695(2)	176.8
C9–H9B...O2 ⁱⁱ	2.49	3.351(2)	147
C10–H10A...O1 ⁱⁱⁱ	2.44	3.166(3)	132
C10–H10A...Cg1a ^{iv}	2.91	3.327(2)	107
C11–H11B...Cg2a ^{iv}	2.73	3.645(2)	158
C12–H12A...O4 ^v	2.48	3.405(2)	160
C13–H13A...O2 ⁱⁱ	2.55	3.390(2)	146
C15–H15...O4 ^v	2.54	3.454(2)	169
C30–H30...O5 ⁱ	2.59	3.486(3)	161
Cg(t6)...Cg(1a) ⁱⁱ		4.184(2)	
Cg(PhCl)...Cg(PhCl) ^{iv}		4.766(2)	

Footnote:

Symmetry operations: [i] -x,1-y,1-z; [ii] 1/2-x,-1/2+y,3/2-z; [iii] -1/2+x,1/2-y,-1/2+z; [iv] 1-x,1-y,1-z; [v] 1-x,1-y,2-z.

Ring codes: Cg1a, Cg2a – rings of the anion; Cg(t6) – six membered ring of the fused 9-membered ring (head); Cg(PhCl) – chlorophenyl ring.

Table. S3 Geometry of main weak intermolecular interactions in **T:HCl** crystal.

	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N4–H49...Cl2	1.97	3.0418	173
C8–H31...Cl2 ⁱ	2.68	3.5870	140
C9–H50...Cl2 ⁱⁱ	2.54	3.5833	157
C10–H40...Cl2 ⁱⁱⁱ	2.69	3.7176	155
C11–H34...O1 ⁱⁱⁱ	2.37	3.2058	132
C12–H35...O1 ⁱ	2.50	3.2541	125
C13–H36...Cl2 ⁱⁱ	2.63	3.6541	154
C19–H47...O1 ⁱⁱⁱ	2.31	3.3964	173
Cg(t5)...Cg(t6) ⁱⁱ		4.6241	
Cg(PhCl)...Cg(PhCl) ^{iv}		4.8828	

Footnote:

Symmetry operations: [i] [-x, 2-y, 1-z]; [ii] x, 3/2-y, -1/2+z; [iii] -x, -1/2+y, 3/2-z; [iv] -1-x, 1-y, 1-z

Ring codes: Cg(t5), Cg(t6) – five- and six membered ring of the fused 9-membered ring (head); Cg(PhCl) – chlorophenyl ring.

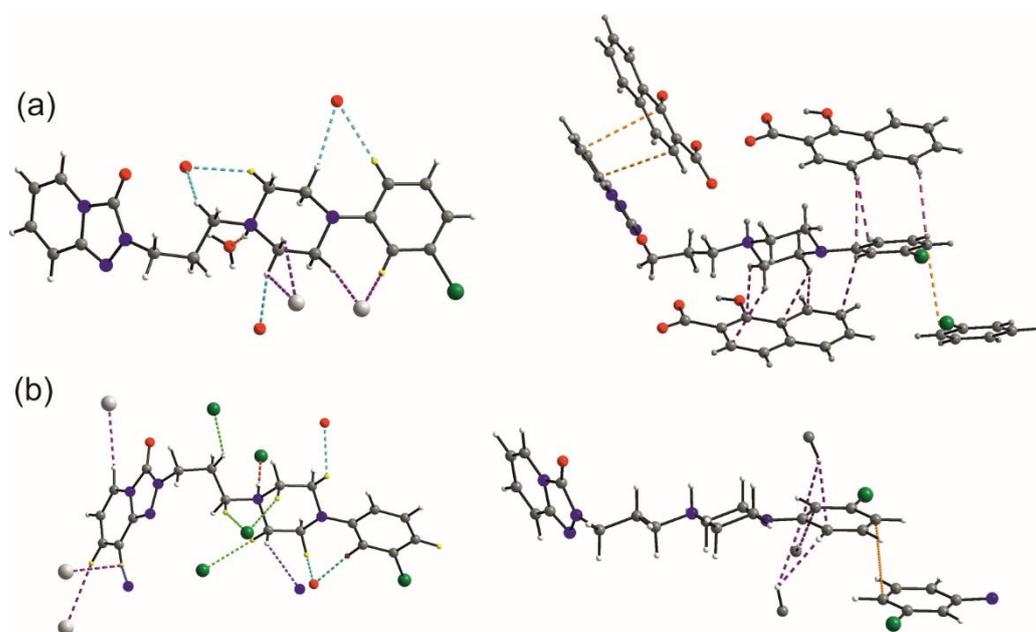


Fig 3S. Weak interactions motives found in **T:OHN** (a) and **T:HCl** (b) crystals.

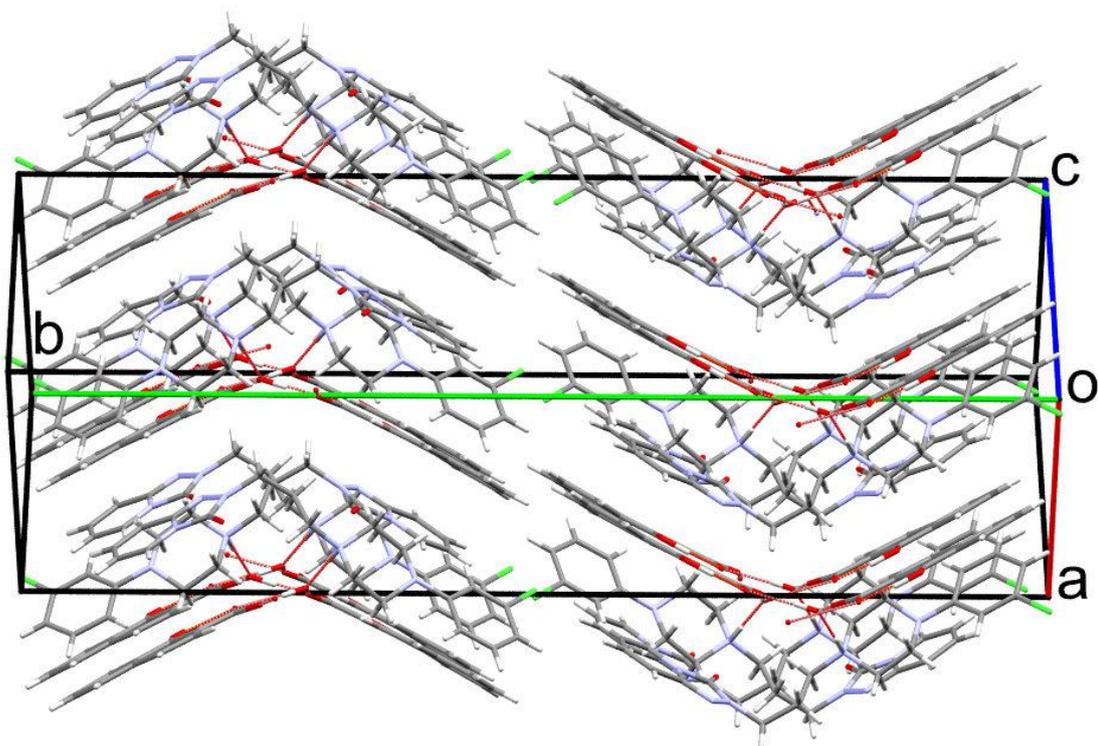


Fig 4S. Packing diagram for **T:OHN** crystal. View along [101] direction.

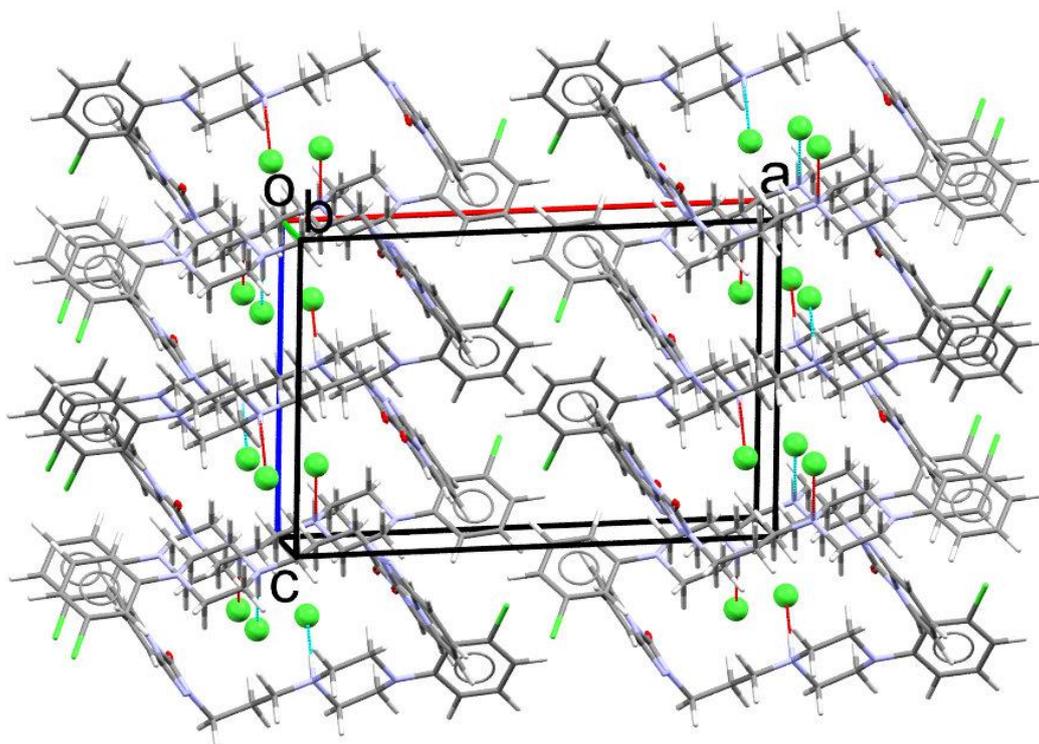


Fig 5S. Packing diagram for **T:HCl** crystal. View along [010] direction.