crystals

MDPI

SUPPLEMENTARY MATERIALS

Hydrogen-bonded chain of rings motif in *N*-(4-methoxy-phenyl)piperazin-1-ium salts with benzoate anions: supramolecular assemblies and their energy frameworks

Prabhakar Priyanka [1], Bidarur K. Jayanna [1], Thayamma R. Divakara [2], Gejjalagere P. Suresha [3], Vinaya [4], Yeriyur B. Basavaraju [4], Hemmige S. Yathirajan [4], Sean R. Parkin [5] and Lilianna Chęcińska [6,*]

[1] Department of Chemistry, B.N.M. Institute of Technology, Bengaluru 560 070, India;
[2] T. John Institute of Technology, Bengaluru 560 083, India;
[3] Honeychem Pharma Research Pvt. Ltd., Peenya Industrial Area, Bengaluru 560 058, India;
[4] Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysuru 570 006, India;
[5] Department of Chemistry, University of Kentucky, Lexington, KY 40506, USA;
[6] Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236 Łódź, Poland;
* Correspondence: lilianna.checinska@chemia.uni.lodz.pl

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Table S1. Geometry of C—H···π(arene) intermolecular interactions for (I) – (III).

Interaction	H···*Cg* [Å]	X···*Cg* [Å]	C—H···*Cg* [°]
(I)			
C6—H6···*Cg*3(−*x*+1, −*y*+1, −*z*+1)	2.63	3.4343(13)	143
C10—H10···*Cg*3(−*x*+2, −*y*+2, −*z*+1)	2.74	3.5109(13)	138
C19—H19A···*Cg*2(−*x*+2, −*y*+1, −*z*+1)	2.83	3.6385(13)	138
(II)			
C6—H6···*Cg*3(−*x*, −*y*+1, −*z*)	2.75	3.4813(15)	134
C10—H10···*Cg*3(−*x*+1, −*y*+1, −*z*+1)	2.66	3.4616(15)	143
C19—H19B···*Cg*2(−*x*, −*y*+1, −*z*+1)	2.88	3.7226(17)	145
(III)			
C6—H6···*Cg*3(−*x*+1, −*y*+1, −*z*+1)	2.60	3.3852(15)	140
C10—H10···*Cg*3(−*x*, −*y*+2, −*z*+1)	2.80	3.5329(15)	135

* *Cg* – centroid of the ring.

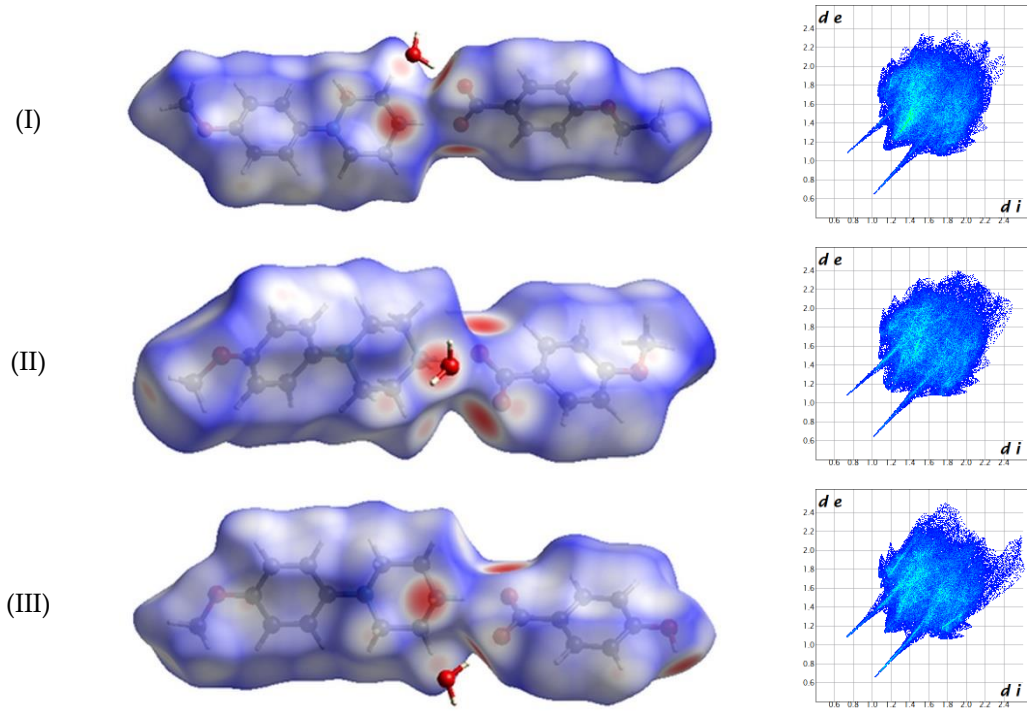

Figure S1. Hirshfeld surface of two ionic components mapped with d_{norm} function on it and corresponding fingerprint plot for (I) – (III).
The distances from a surface to the nearest interior/exterior atoms (d_i, d_e) are given in Å.

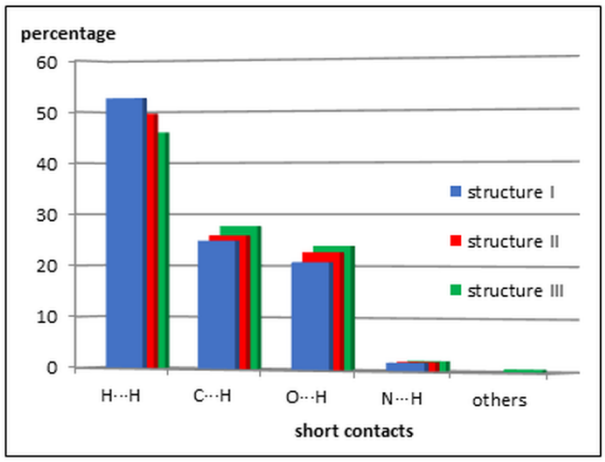

Figure S2. The percentage contributions of various intermolecular close contacts to the Hirshfeld surface area of two ionic components of (I) – (III).

(I)

(II)

(III)

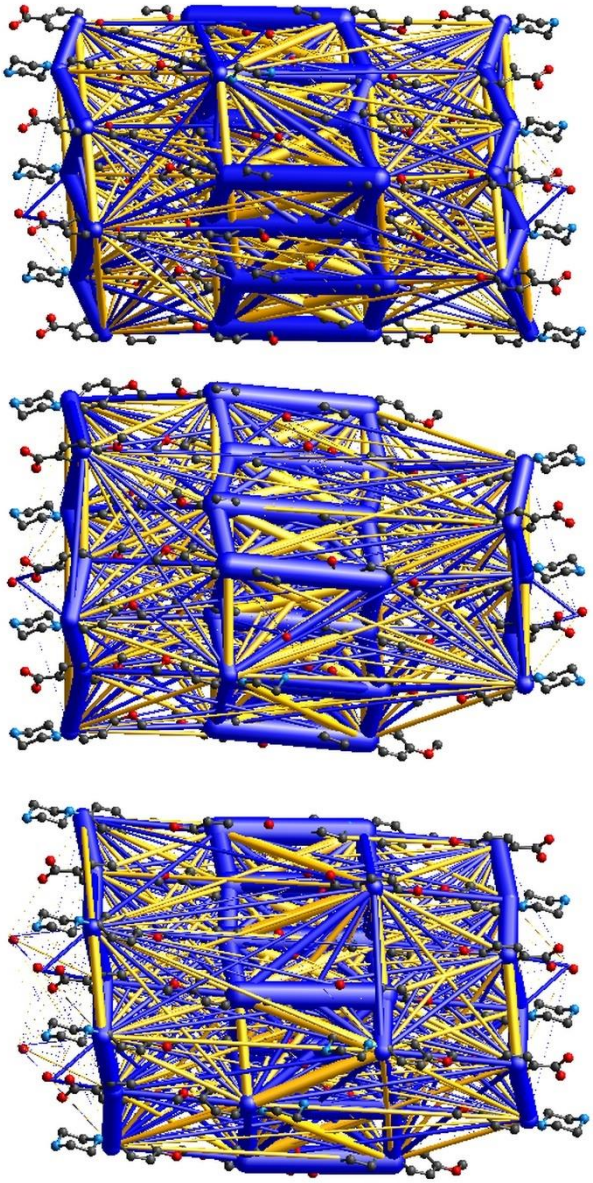

Figure S3. Diagrams of the total energy frameworks for 10Å cluster of (I) – (III);
drawn along the crystallographic *a* axis.
All diagrams use the same energy tube scale factor of 20 (no energy threshold).
The yellow cylinders represent destabilizing interactions.

Table S2. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase neutral pair of (I) optimized at the ωB97XD /6-311++G(d,p) level of theory.

Atom	X	Y	Z
O	-1.85482400	0.82116600	0.84306100
O	-2.07590100	-1.16313200	-0.16543300
O	-8.13180700	0.64756300	0.03635200
C	-4.03330600	0.09489100	0.22699500
C	-4.81813800	-0.88353300	-0.37271300
H	-4.34503400	-1.77009900	-0.77643500
C	-6.19771400	-0.73752100	-0.46098300
H	-6.78244900	-1.51464400	-0.93473900
C	-6.80278700	0.40582200	0.06234400
C	-6.01785800	1.39507600	0.66534400
H	-6.50913900	2.27412700	1.06453400
C	-4.65038500	1.23796400	0.74444700
H	-4.03307900	1.99710000	1.21004300
C	-2.55731000	-0.03429400	0.33718200
C	-8.99876600	-0.32057400	-0.53573800
H	-8.87679200	-1.27875000	-0.01583400
H	-8.74313700	-0.46877600	-1.59227400
C	-10.41431300	0.19234200	-0.39174800
H	-11.11685600	-0.52849700	-0.81691500
H	-10.53402000	1.14413600	-0.91291700
H	-10.66221500	0.33984500	0.66121400
O	8.78813600	1.00256400	-0.12316400
N	3.38541300	-0.44184900	-0.21711400
N	0.56201900	-0.79294300	0.22872000
H	0.32724600	-0.10684300	0.94464100
H	-1.07460000	-1.15876100	-0.04846400
C	2.44092400	0.56182300	-0.67971500
H	2.81770300	1.00590800	-1.60420000
H	2.31270600	1.37493800	0.05968900
C	1.08262900	-0.07980400	-0.94003100
H	0.35489800	0.68247700	-1.22741600
H	1.17173200	-0.79786700	-1.76123000
C	1.54429400	-1.74670000	0.74289700
H	1.65355400	-2.54809400	0.00519500
H	1.15928300	-2.18687100	1.66587700
C	2.90337100	-1.10388700	0.99344700
H	2.81853000	-0.37587200	1.82212000
H	3.61953000	-1.86613900	1.30251400
C	4.75265500	-0.06345300	-0.18414100
C	5.73002200	-1.05228900	-0.08140800
H	5.42977000	-2.09392500	-0.04987600
C	7.08339100	-0.74052300	-0.04495000
H	7.80365700	-1.54456100	0.03320000
C	7.49209900	0.58900300	-0.13591200
C	6.52846200	1.58554100	-0.25510400
H	6.85329300	2.61689800	-0.32648200
C	5.17963000	1.26599900	-0.26853100
H	4.45943000	2.07107800	-0.34280700
C	9.79362800	0.02636100	0.02109200
H	10.74060800	0.56379200	0.01829000
H	9.78424700	-0.68860200	-0.80991300
H	9.69111400	-0.51721000	0.96777700

Table S3. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase neutral pair of (II) optimized at the ωB97XD /6-311++G(d,p) level of theory.

Atom	X	Y	Z
O	-2.53825500	-1.15223200	0.16552100
O	-2.31964900	0.82769000	-0.85221400
O	-8.58272800	0.70230200	0.06554900
C	-4.49295700	0.11792000	-0.19959000
C	-5.27355900	-0.85194900	0.41891600
H	-4.79961900	-1.73992500	0.81845900
C	-6.65027500	-0.69494600	0.53145700
H	-7.23224500	-1.46545600	1.01947200
C	-7.25526900	0.45045700	0.01402700
C	-6.47551700	1.43070800	-0.60922500
H	-6.96769200	2.31126100	-1.00387400
C	-5.11086400	1.26277900	-0.71225600
H	-4.49652400	2.01481000	-1.19303400
C	-3.01956800	-0.02180900	-0.33317700
C	-9.42942900	-0.25519200	0.66543900
H	-9.18664600	-0.39718100	1.72425400
H	-9.37394200	-1.21801400	0.14593500
H	-10.43874900	0.14312100	0.57879500
O	8.32515200	0.99059700	0.12074200
N	2.91977900	-0.44427100	0.20432200
N	0.09686300	-0.79242200	-0.24663000
H	-1.53799300	-1.15313400	0.03749500
H	-0.13552200	-0.10843600	-0.96530800
C	2.43946300	-1.10946600	-1.00513700
H	3.15513400	-1.87381200	-1.31013600
H	2.35758400	-0.38402100	-1.83636500
C	1.07882000	-1.74939700	-0.75559000
H	0.69515400	-2.19190800	-1.67799500
H	1.18514100	-2.54857200	-0.01506600
C	0.61616900	-0.07603500	0.92084300
H	0.70236400	-0.79153000	1.74458300
H	-0.11102200	0.68830500	1.20409600
C	1.97598200	0.56253800	0.66134200
H	1.85068300	1.37337800	-0.08107900
H	2.35140900	1.00913700	1.58514900
C	4.28779800	-0.06841000	0.17361700
C	4.71673800	1.26063000	0.25428000
H	3.99762300	2.06713700	0.32346900
C	6.06611800	1.57789100	0.24365600
H	6.39249700	2.60895200	0.31216100
C	7.02841000	0.57928800	0.13105400
C	6.61774000	-0.74988300	0.04371300
H	7.33695700	-1.55534400	-0.02933800
C	5.26374600	-1.05927300	0.07732300
H	4.96177400	-2.10050700	0.04881800
C	9.32949000	0.01216700	-0.01643500
H	9.22921900	-0.53485000	-0.96137000
H	9.31621100	-0.69957900	0.81728100
H	10.27733200	0.54806100	-0.01255900

Table S4. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase neutral pair of (III) optimized at the ωB97XD /6-311++G(d,p) level of theory.

Atom	X	Y	Z
O	7.88188300	1.02830700	0.06166400
N	2.48756500	-0.44182300	0.20959500
N	-0.33601000	-0.81550600	-0.21551900
H	-1.96027700	-1.18380300	0.09357000
H	-0.57993700	-0.14486200	-0.94293900
C	1.54065400	0.56527800	0.65889600
H	1.40452600	1.36486600	-0.09384400
H	1.91975600	1.02726200	1.57359000
C	0.18732500	-0.07873700	0.93748800
H	0.28455100	-0.78179900	1.77061300
H	-0.54284400	0.68451700	1.21620000
C	0.64868000	-1.77303600	-0.71856600
H	0.26124000	-2.23009100	-1.63220400
H	0.76539400	-2.56162100	0.03166300
C	2.00316600	-1.12754000	-0.98667000
H	2.72195100	-1.89140600	-1.28553500
H	1.91073300	-0.41477600	-1.82773100
C	3.85282100	-0.05691400	0.16270800
C	4.83478200	-1.04289000	0.07919100
H	4.53953100	-2.08643600	0.07358000
C	6.18637500	-0.72515000	0.03030300
H	6.91054400	-1.52706000	-0.03170900
C	6.58828600	0.60830400	0.08878000
C	5.61986000	1.60242500	0.18848200
H	5.93959600	2.63680700	0.23460400
C	4.27281000	1.27633500	0.21455500
H	3.54866600	2.07915600	0.27329100
C	8.89253100	0.05422300	-0.05967800
H	8.88755000	-0.64020700	0.78861100
H	9.83660400	0.59662600	-0.07089800
H	8.79236800	-0.51278600	-0.99275000
O	-2.78161700	0.74751700	-0.87068200
O	-2.95854400	-1.18510500	0.24204300
O	-9.01973300	0.50577500	0.34147300
H	-9.33682100	1.30589700	-0.08096500
C	-4.93028500	0.05674200	-0.12177900
C	-5.56637800	1.16467600	-0.67676800
H	-4.97180000	1.88914200	-1.22054700
C	-6.93364900	1.33638700	-0.53699700
H	-7.42256700	2.20226100	-0.97381400
C	-7.67913200	0.39227000	0.16826700
C	-7.05349100	-0.72000200	0.72800900
H	-7.65188500	-1.43978800	1.27295900
C	-5.68747900	-0.88345800	0.58012700
H	-5.19474000	-1.74552100	1.01197000
C	-3.46002700	-0.08175100	-0.29338800