

Electronic Supplementary Information

Insight into the Structure and Transport Properties of Pyrrolidinium-based Geminal Dicationic-Organic Ionic Crystals: Unravelling the Role of Alkyl-Chain Length

Amita Mahapatra,^{ab} Aneeya K. Samantara,^{ab} Sahadev Barik,^{ab} Malaya K. Sahoo,^{ab} J. N. Behera,^{ab} and Moloy Sarkar^{ab*}

Amita Mahapatra, Aneeya K. Samantara, Sahadev Barik, Malaya K. Sahoo, Dr. J. N. Behera and Dr. Moloy Sarkar*

^a School of Chemical Sciences, National Institute of Science Education and Research (NISER), Jatni, Khurda, Bhubaneswar 752050, Odisha, India. An OCC of Homi Bhabha National Institute (HBNI), Mumbai 400094.

^b Centre for Interdisciplinary Sciences (CIS), NISER, Jatni, Khurda, Bhubaneswar 752050, Odisha, India.

*E-mail: msarkar@niser.ac.in

Fig. S1 ^1H NMR Spectra of PMPYBr

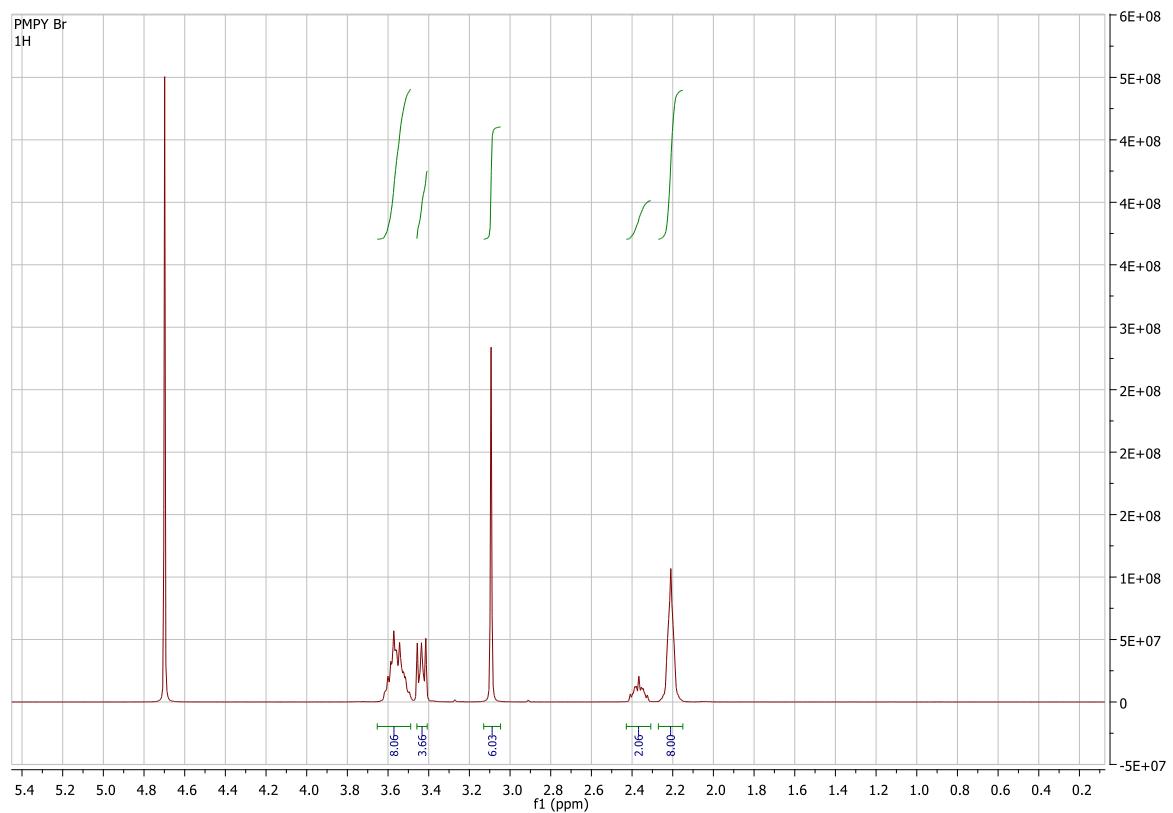


Fig. S2 ^1H NMR Spectra of HMPYBr

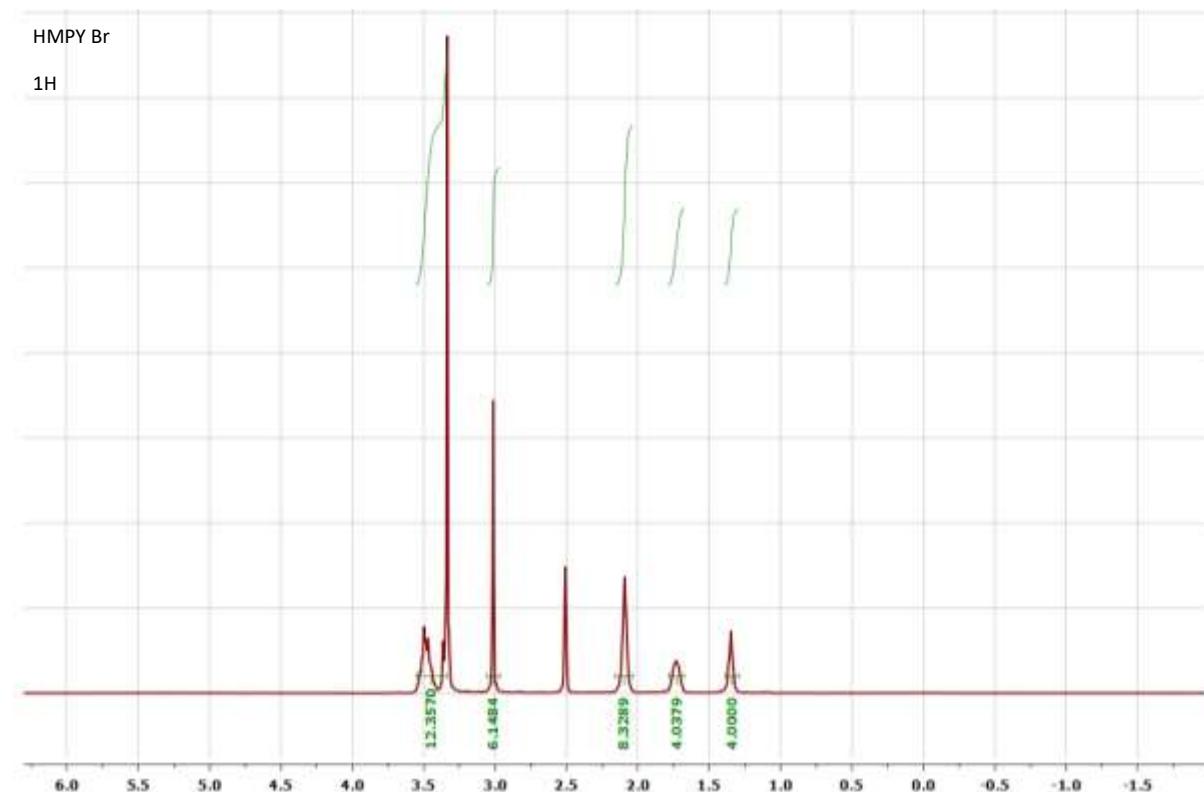


Fig. S3 ^1H NMR Spectra of OMPYBr

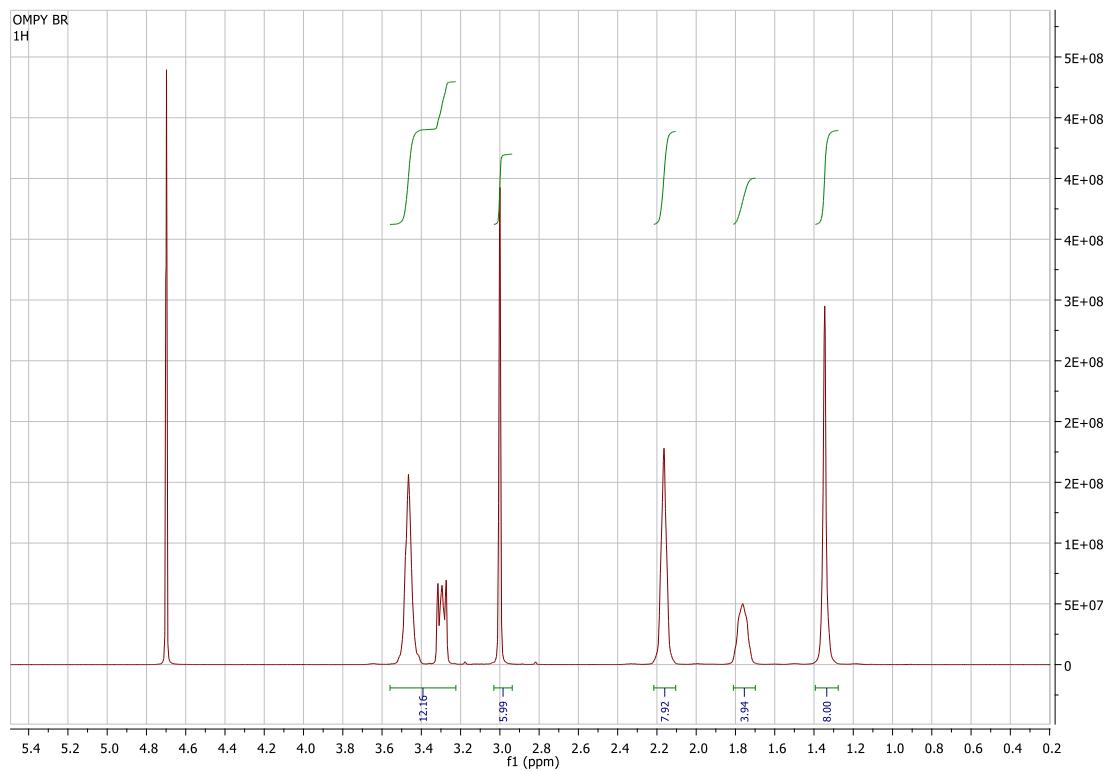


Fig. S4 ^1H NMR Spectra of NMPYBr

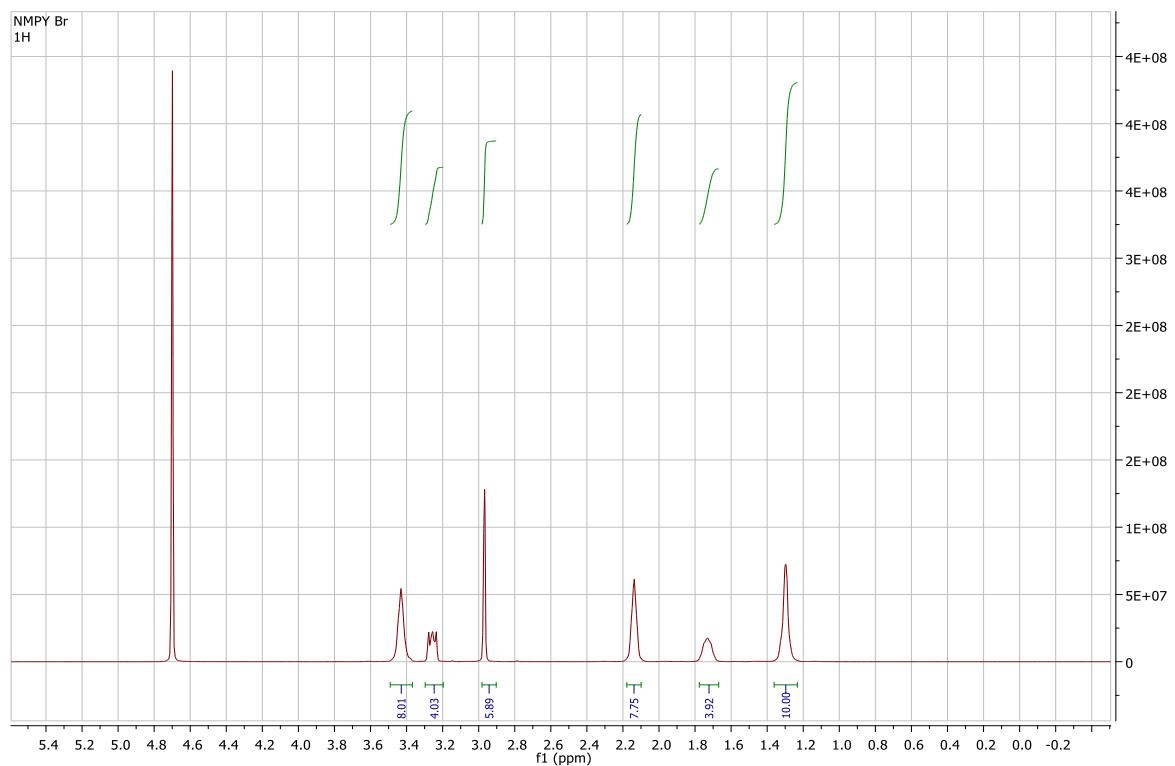


Fig. S5 ESI Mass spectra of HMPYBr with base peak value at 127.140 (m/z)

Display Report

Analysis Info

Analysis Name D:\Data\DEC-2020\MS\28122020_MS_HMPY_BR2.d

Method Pos_tune_low.m

Sample Name Tmix-131118

Comment

Acquisition Date 12/28/2020 11:49:01 AM

Operator Amit S.Sahu

Instrument micrOTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

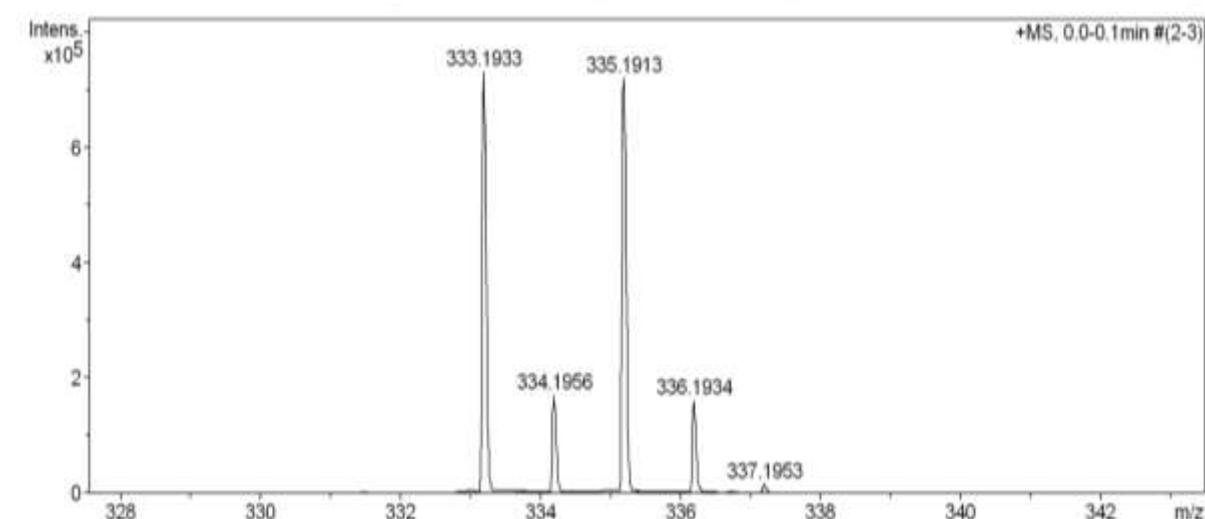
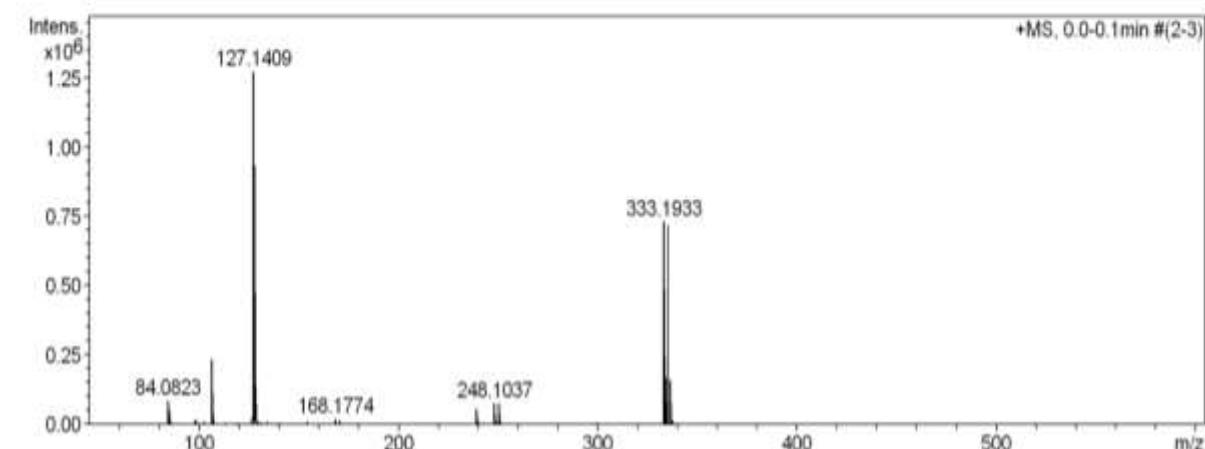
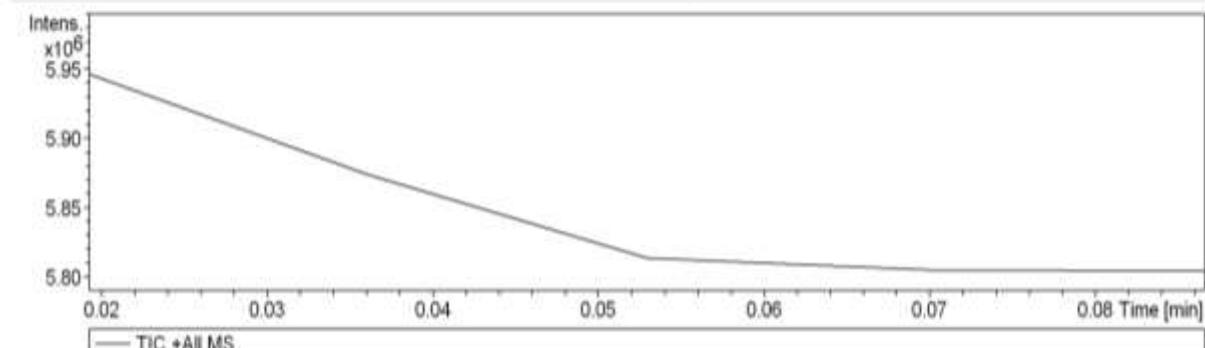


Fig. S6 ESI Mass spectra of OMPYBr with base peak value at 141 (m/z)

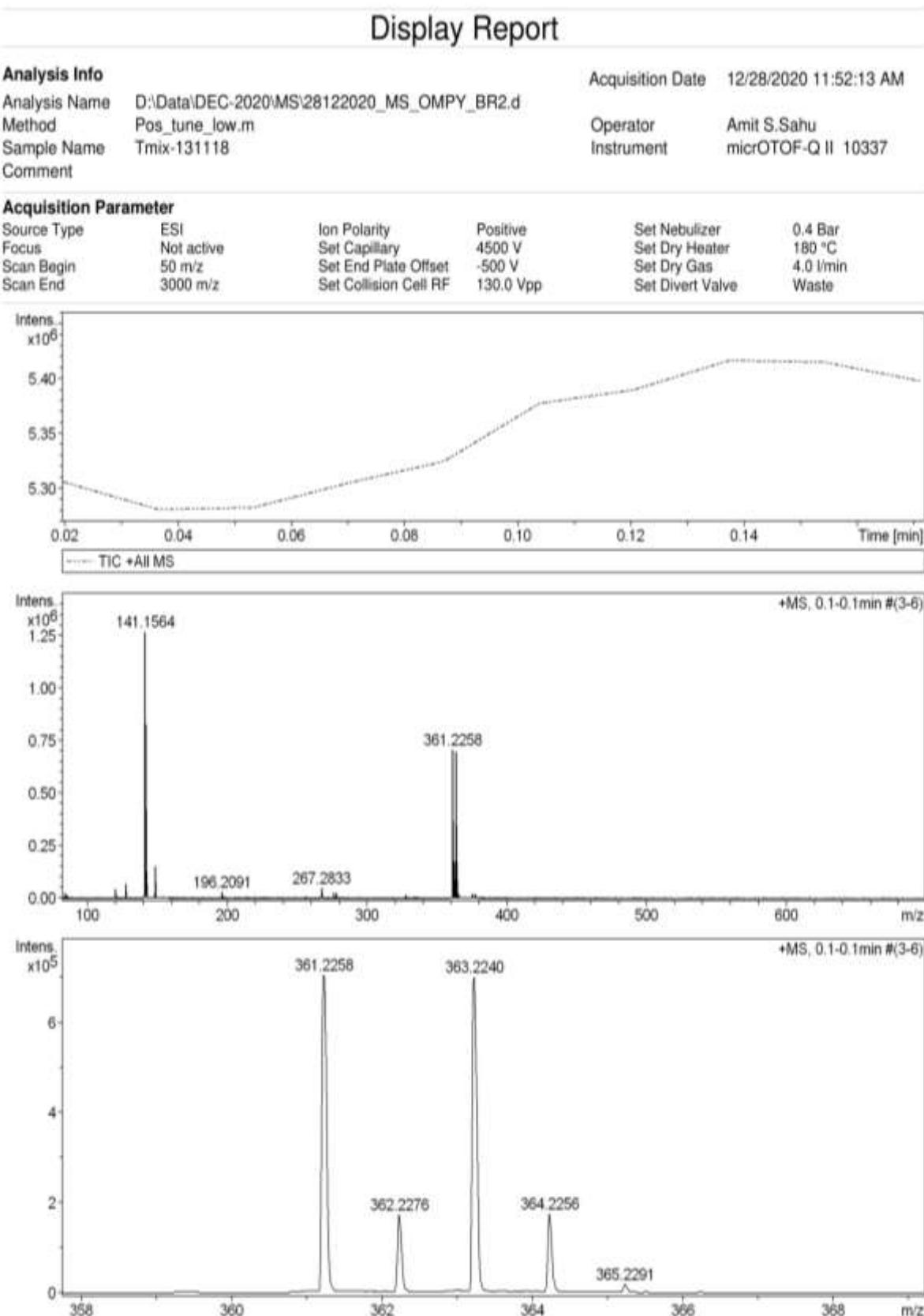


Fig. S7 ESI Mass spectra of NMPYBr with base peak value at 148 (m/z)

Display Report

Analysis Info

Analysis Name D:\Data\DEC-2020\MS\28122020_MS_NMPY_BR2.d
Method Pos_tune_low.m
Sample Name Tmix-131118
Comment

Acquisition Date 12/28/2020 11:50:35 AM

Operator Amit S.Sahu
Instrument micrOTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

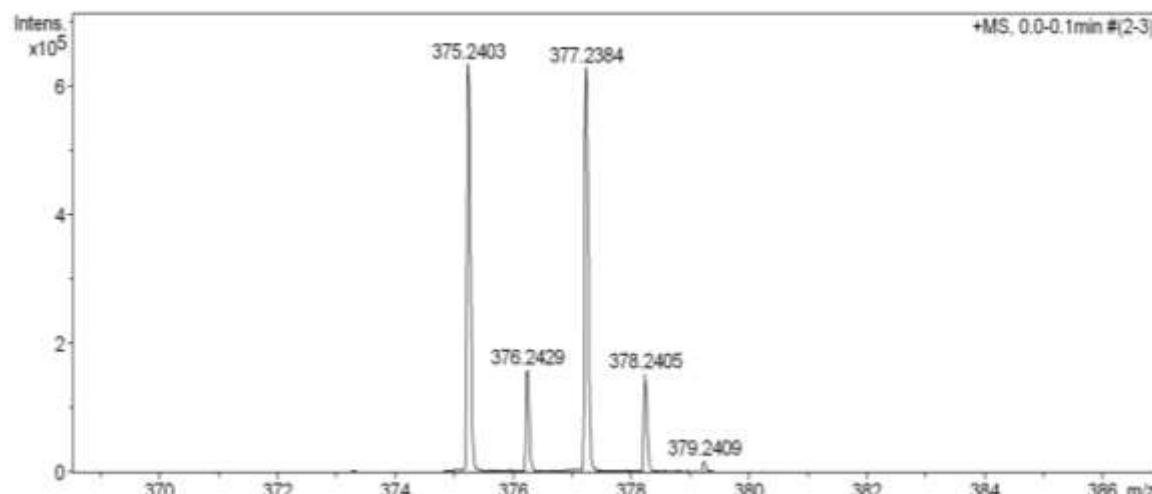
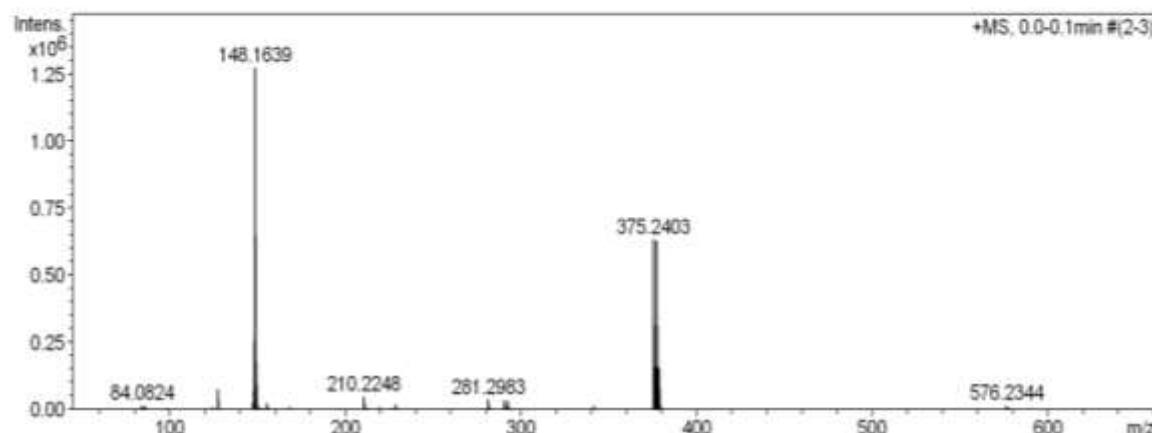
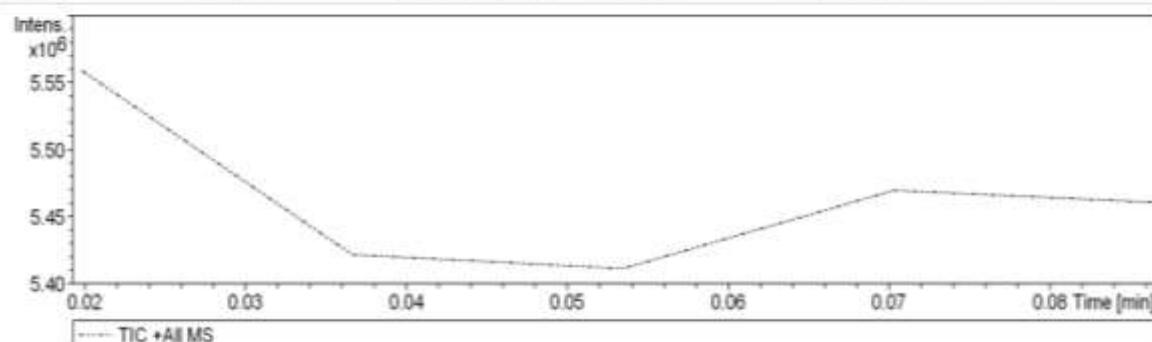


Table S1. Crystallographic information on PMPYBr.³⁹

Formula	C ₁₃ H ₂₈ Br ₂ N2
fw (g)	372.19
T (K)	193(2)
Lattice cell	orthorhombic
space group	Pbca
a (Å)	21.367(6)
b (Å)	19.888(5)
c (Å)	23.787(6)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å ³)	10108(5)
Z	24
d (calc d) (Mg/m ³)	1.467
abs coeff. (mm ⁻¹)	4.798
F(000)	4560
θ range (deg)	1.64-20.82
Reflections collected	45036
GOF	1.067
R1, ^a wR2 ^b [I > 2σ(I)]	0.0702, 0.1628

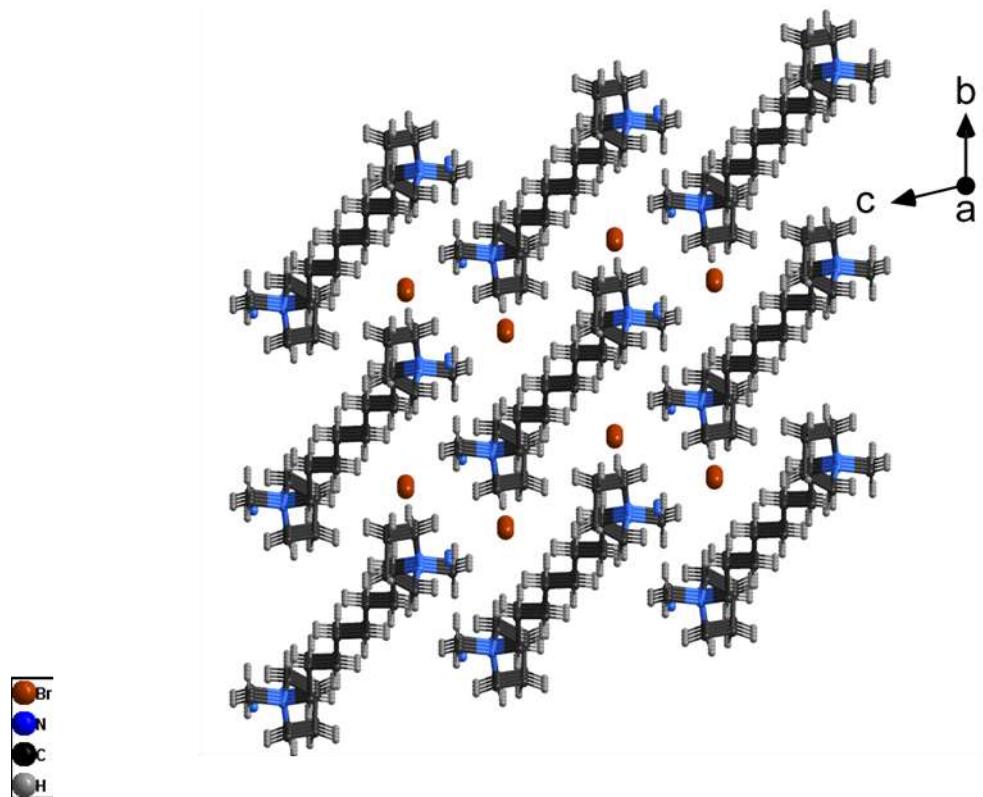


Fig. S8 Crystal packing of OMPYBr along the crystallographic *a*-axes.

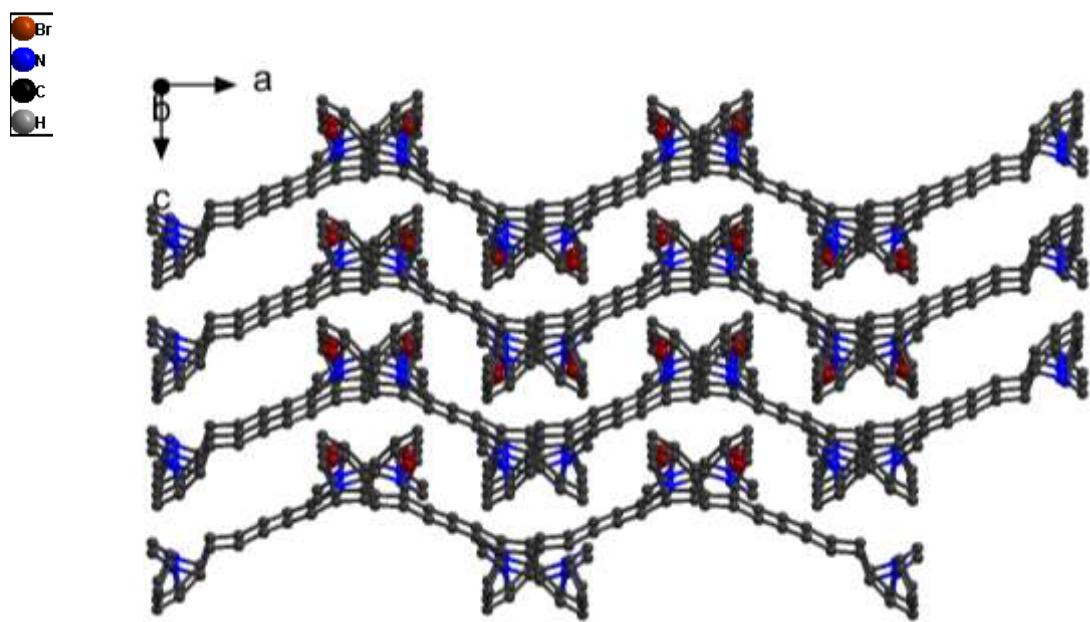


Fig. S9 Crystal packing of NMPYBr along the crystallographic *b*-axes.