Electronic Supplementary Material (ESI) for CrystEngComm.

The effect of substituents and their positions on the naphthalene ring towards intermolecular interactions and crystal packing

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Supplementary Information

Table S1: Structural formula of $DN1^{2+}$, $DN2^{2+}$ and $DN3^{2+}$ with labeling of atoms.

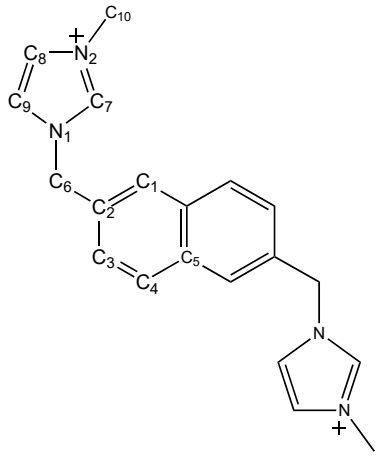
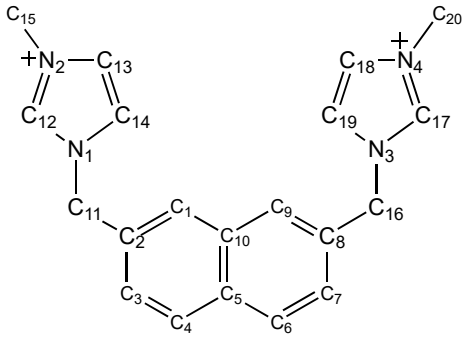
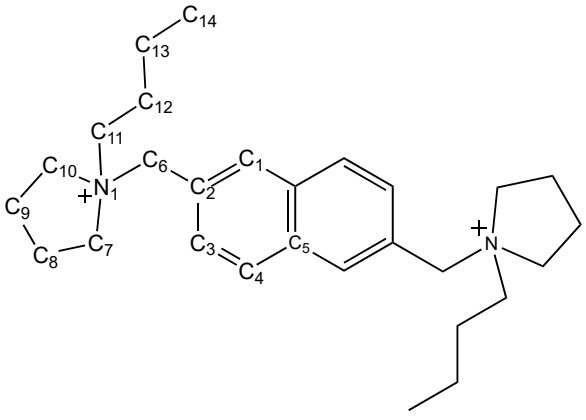
	Structural formula
$DN1^{2+}$	
$DN2^{2+}$	
$DN3^{2+}$	

Table S2: Selected bond lengths and bond angles for $DN1^{2+}$ in compound **1**.

	Crystal:	DFT Optimised Structure
Bond length, Å		
C7-N2	1.341(17)	1.352
N2-C8	1.384 (16)	1.401
C8-C9	1.336 (17)	1.365
C9-N1	1.394 (16)	1.398
N1-C7	1.310 (16)	1.352
C1-C2	1.346 (14)	1.420
C2-C3	1.454 (13)	1.423
C3-C4	1.356 (14)	1.385
C4-C5	1.442 (12)	1.423
C5-C1	1.460 (12)	1.438
C5-C5’	1.350 (14)	1.381
Bond angle, °		
C2-C6-N1	115.7 (10)	111.57
C3-C2-C6	113.4 (8)	119.78

Table S3: Selected bond lengths and bond angles for $DN2^{2+}$ in compound **2**.

	Crystal:	DFT Optimised Structure
Bond length, Å		
N1-C12	1.330 (2)	1.359
C12-N2	1.333 (2)	1.349
N2-C13	1.376 (2)	1.394
C13-C14	1.355 (2)	1.365
C14-N1	1.382 (2)	1.399
N3-C17	1.333 (2)	1.351
C17-N4	1.323 (2)	1.346
N4-C18	1.377 (2)	1.394
C18-C19	1.354 (2)	1.367
C19-N3	1.379 (2)	1.397
C1-C2	1.372 (2)	1.378
C2-C3	1.417 (2)	1.428
C3-C4	1.372 (2)	1.382
C4-C5	1.418 (2)	1.426
C5-C6	1.420 (2)	1.425
C6-C7	1.367 (2)	1.385
C7-C8	1.420 (2)	1.424
C8-C9	1.372 (2)	1.378
C9-C10	1.421 (2)	1.415
C10-C1	1.422 (2)	1.419
C5-C10	1.422 (2)	1.430
Bond angle, °		
C2-C11-N1	111.88 (12)	113.37
C8-C16-N3	113.54 (13)	111.32
C1-C2-C11	122.48 (14)	121.78
C9-C8-C16	123.60 (14)	118.95

Table S4: Selected bond lengths and bond angles for $DN3^{2+}$ in compound **3**.

	Crystal:	DFT Optimised Structure
Bond length, Å		
N1-C7	1.534 (2)	1.536
C7-C8	1.505 (3)	1.530
C8-C9	1.534 (3)	1.541
C9-C10	1.516 (3)	1.532
C10-N1	1.543 (2)	1.553
C1-C2	1.377 (3)	1.388
C2-C3	1.419 (3)	1.426
C3-C4	1.370 (3)	1.380
C4-C5	1.422 (3)	1.424
C5-C1	1.418 (3)	1.418
C5-C5’	1.412 (3)	1.437
Bond angle, °		
C2-C6-N1	115.67 (15)	114.24
C1-C2-C6	119.80 (18)	121.42

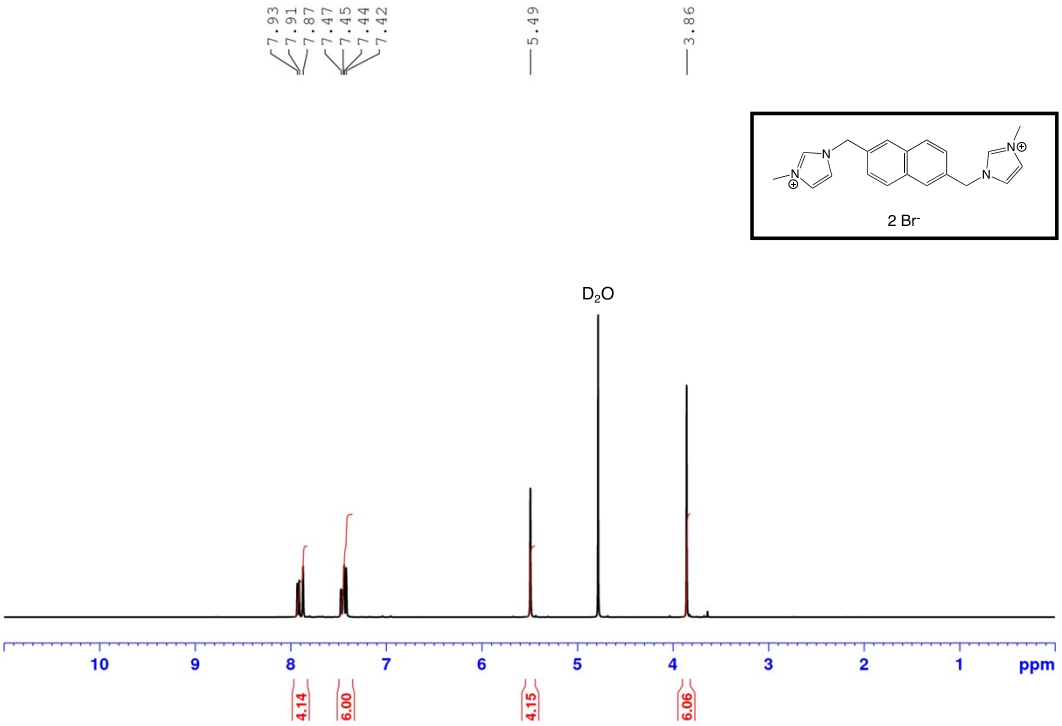


Figure S1. ^{1}H NMR spectrum of Compound **1** ($DN1^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.

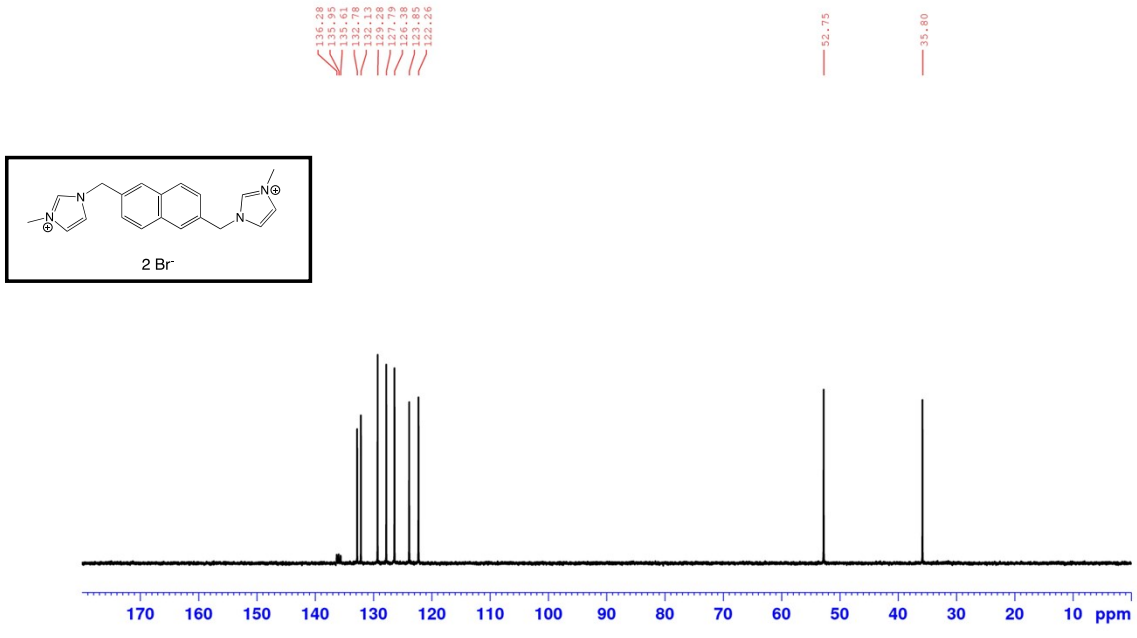


Figure S2. ^{13}C NMR spectrum of Compound **1** ($DN1^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.

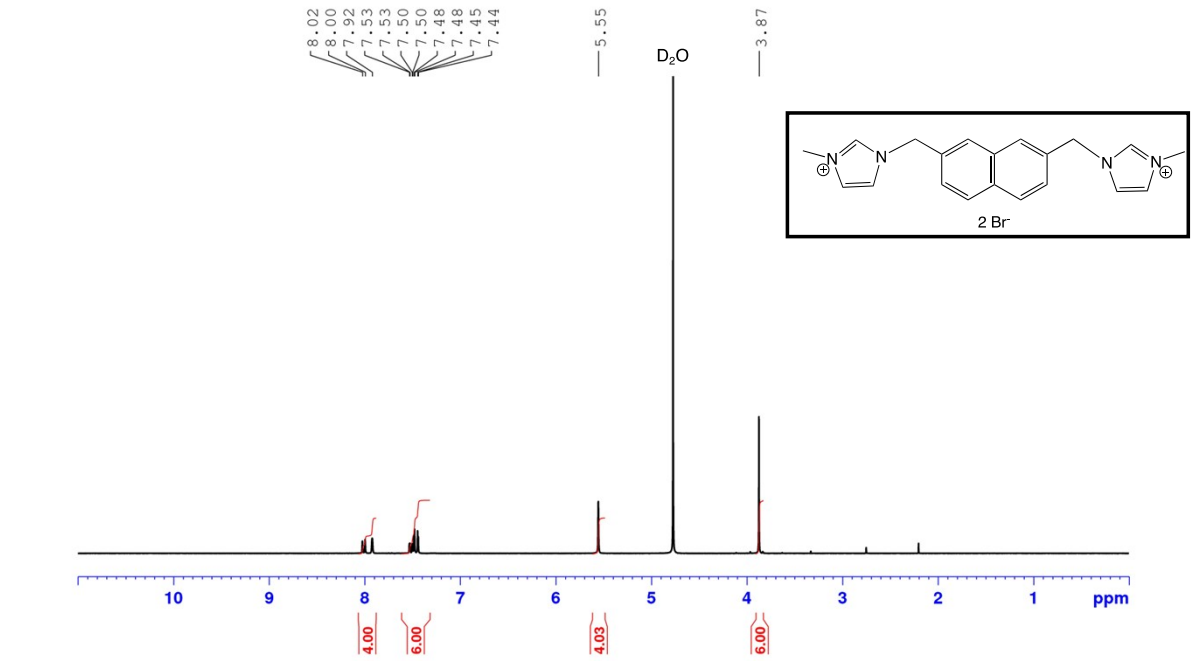


Figure S3. ^{1}H NMR spectrum of Compound **2** ($DN2^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.

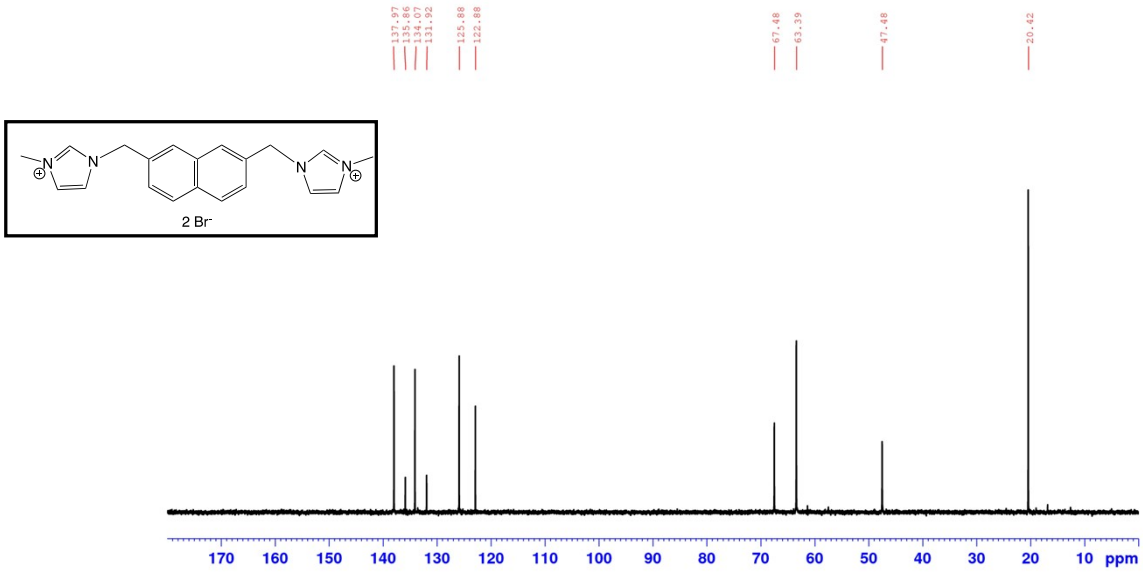


Figure S4. ^{13}C NMR spectrum of Compound **2** ($DN2^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.

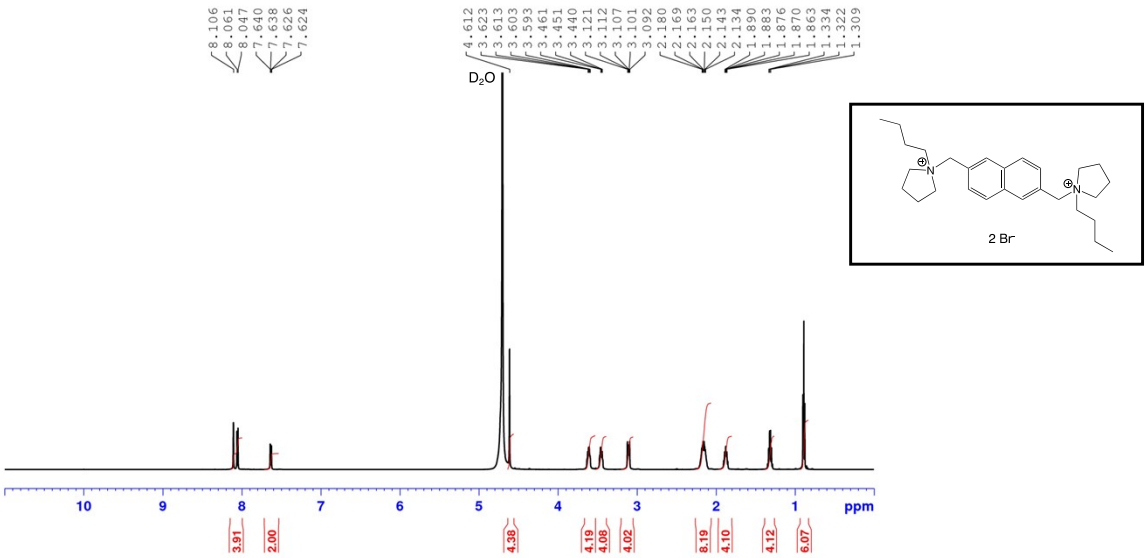


Figure S5. ^{1}H NMR spectrum of Compound **3** ($DN3^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.

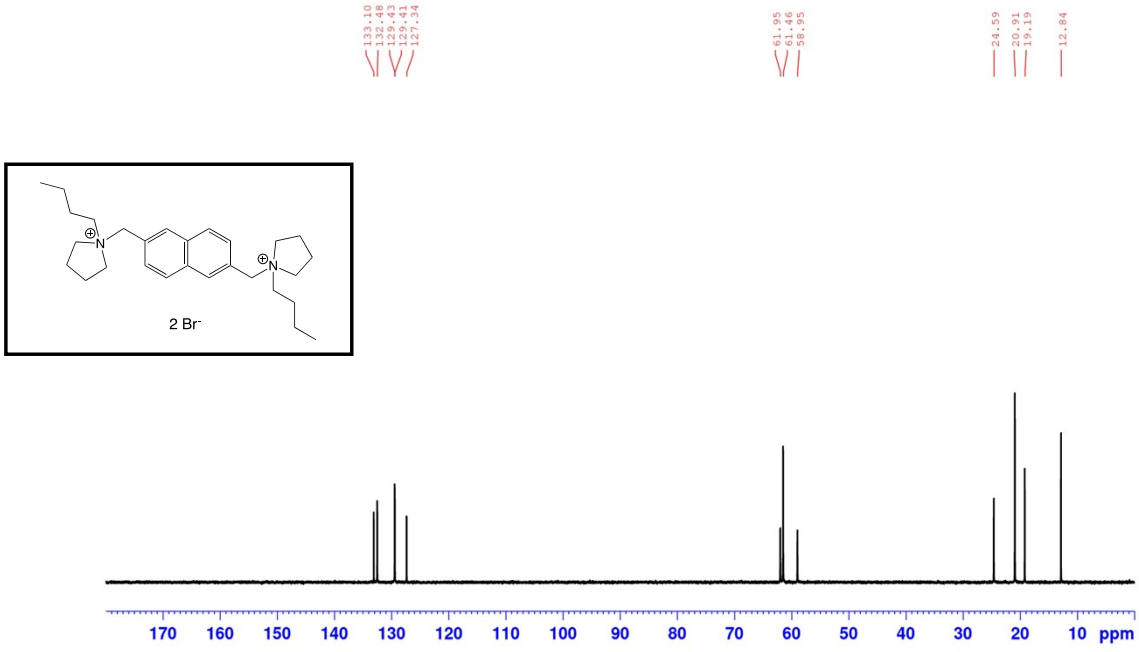


Figure S6. ^{13}C NMR spectrum of Compound **3** ($DN3^{2+}\cdot 2Br^{-}$) in D_2O at 25 °C.