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Supporting Information

Zinc bromide voltammetry in dilute aqueous solutions of ionic liquid bromide salts: Mechanistic complications and the influence of complexation

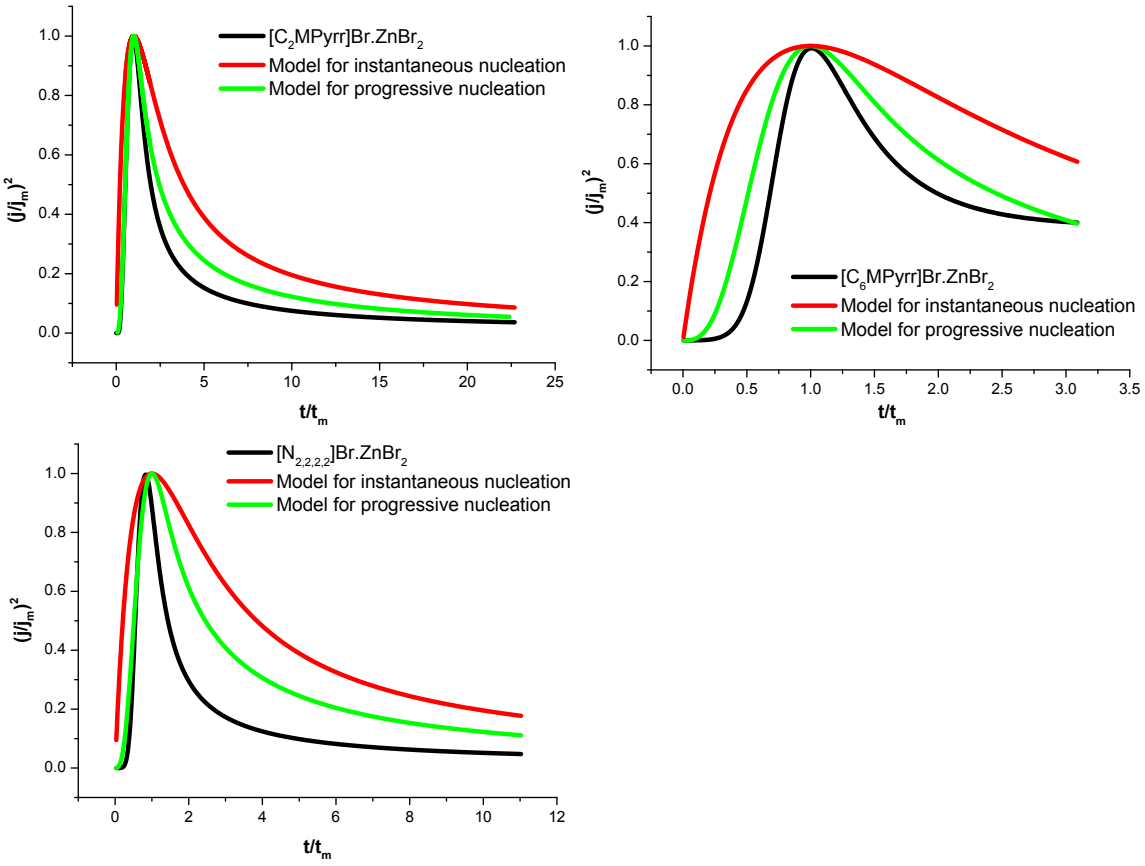
Additional Voltammetric Data

Dimensionless current-time transients for the chronoamperograms of Figure 4 in the main text are pictured in Figure S1, and compared to the theoretical responses for instantaneous and progressive nucleation as derived from the following equations –

$$\left(\frac{i}{i_m}\right)^2 = \frac{1.9542}{t/t_m}\{1 - \exp[-1.2564(t/t_m)]\}^2 \qquad (1)$$

$$\left(\frac{i}{i_m}\right)^2 = \frac{1.2254}{t/t_m}\left\{1 - \exp\left[-2.3367(t/t_m)^2\right]\right\}^2 \qquad (2)$$

– where i_m and t_m refer to the maximum current and time response from the experimental chronoamperogram respectively. See main text for brief discussion.



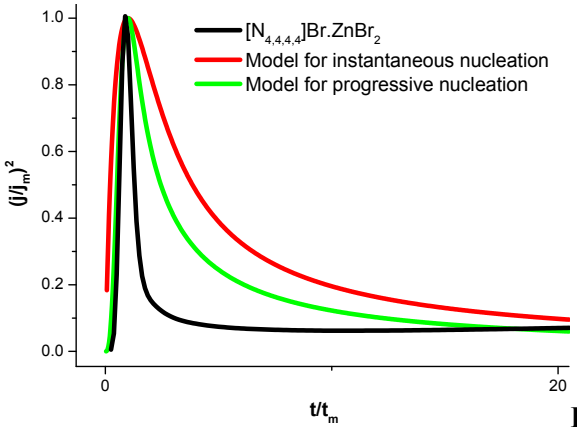


Figure S1. Dimensionless chronoamperograms for the four studied bromide salt additives comparewd to the modelled response for instantaneous or progressive nucleation (Eq 1 and 2).

EDX Data for Zinc electrodeposits

EDX analysis was performed using a Zeiss EVO scanning electron microscope operating at 17 kV. The resulting spectra for each electrodeposit are shown in Figures S2 – S5. The primary EDX signal arises from the zinc Kα line at 5 kV, with the next most abundant elements observed in the EDX spectrum belonging to tin, oxygen and silicon signals (summarised in Table S1) from the FTO glass substrate (see Experimental section for electrodeposition conditions). In the case of the more sparse zinc electrodeposits obtained from solutions containing the [C_6MPyrr]Br and [$N_{4,4,4,4}$]Br compounds, the response from the FTO glass was more prominent.

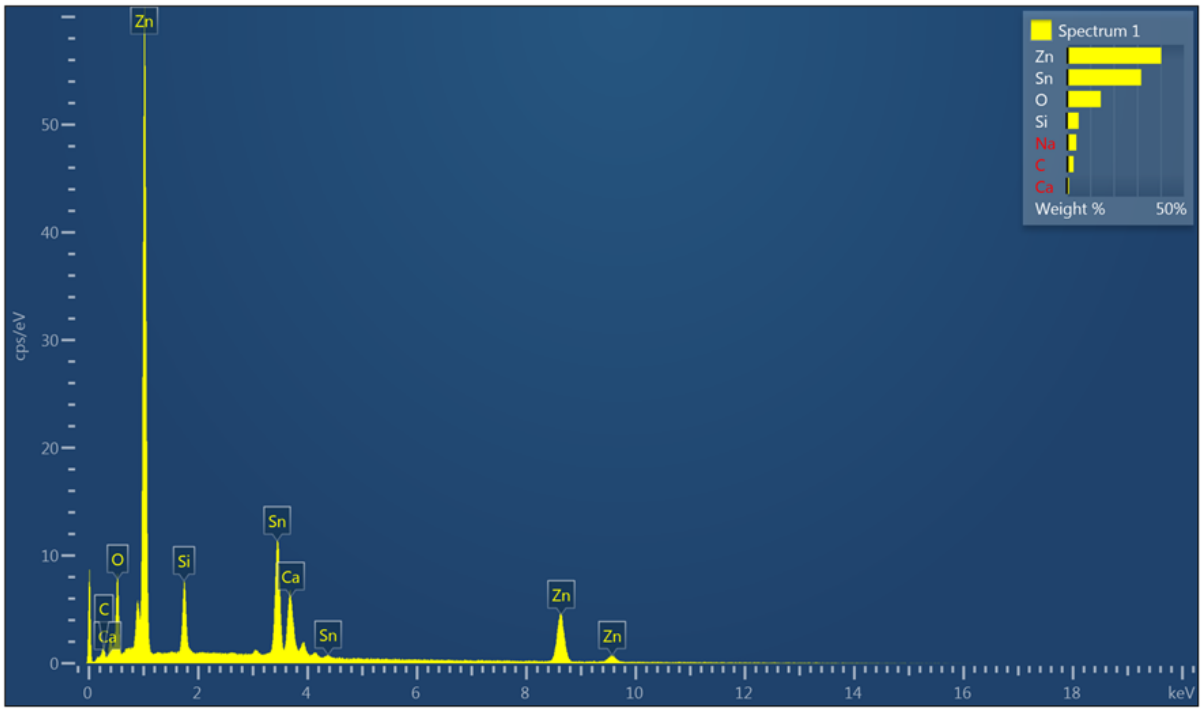


Figure S2. EDX spectra obtained from the zinc electrodeposit performed in 50 mM ZnBr2 : 50 mM [C_2MPyrr]Br

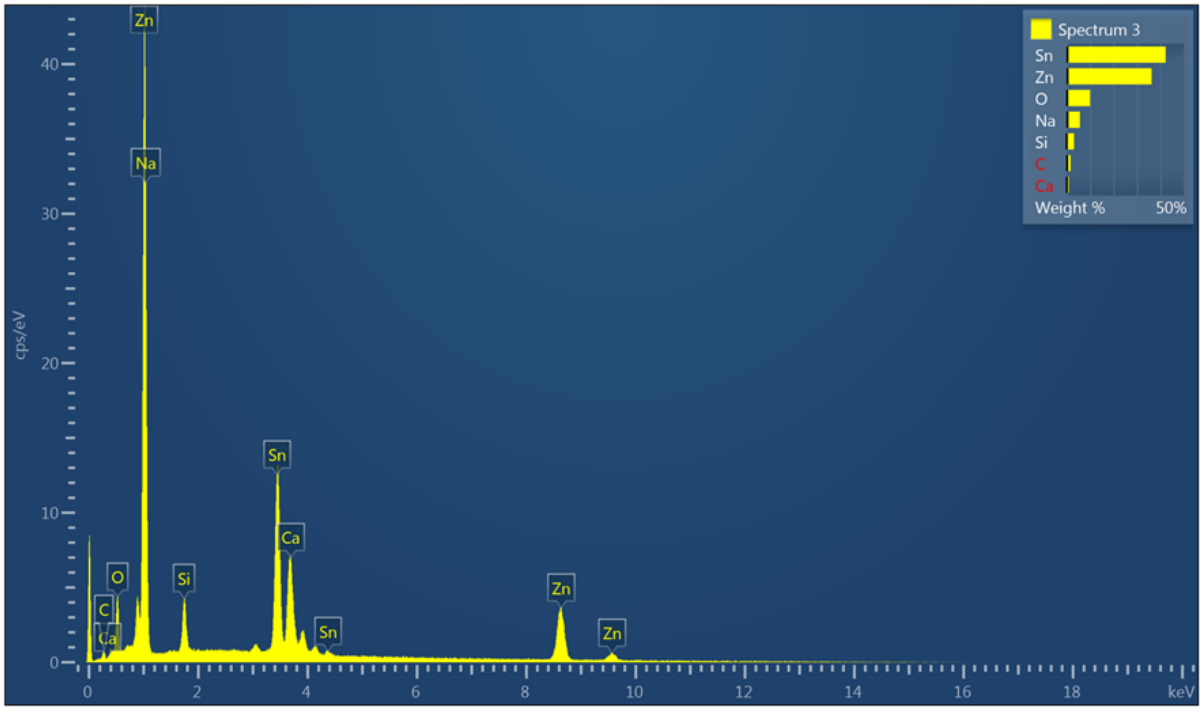


Figure S3. EDX spectra obtained from the zinc electrodeposit performed in 50 mM ZnBr2 : 50 mM $[C_6MPyrr]Br$

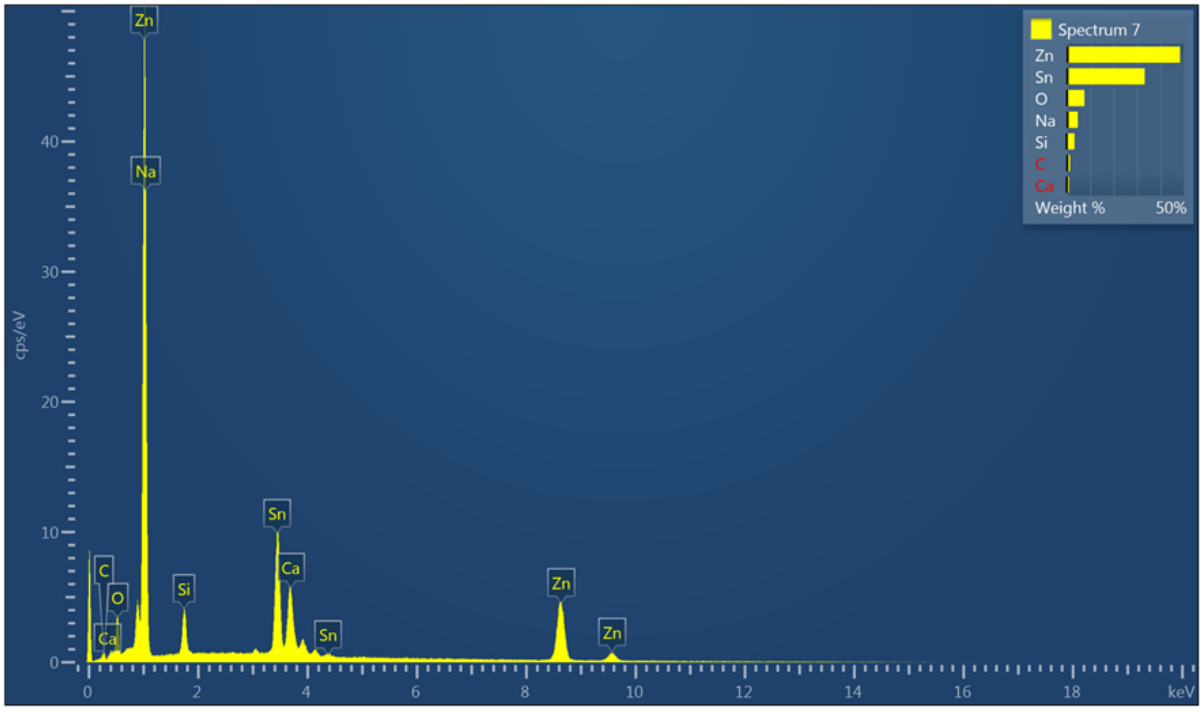


Figure S4. EDX spectra obtained from the zinc electrodeposit performed in 50 mM ZnBr2 : 50 mM $[N_{2,2,2,2}]Br$

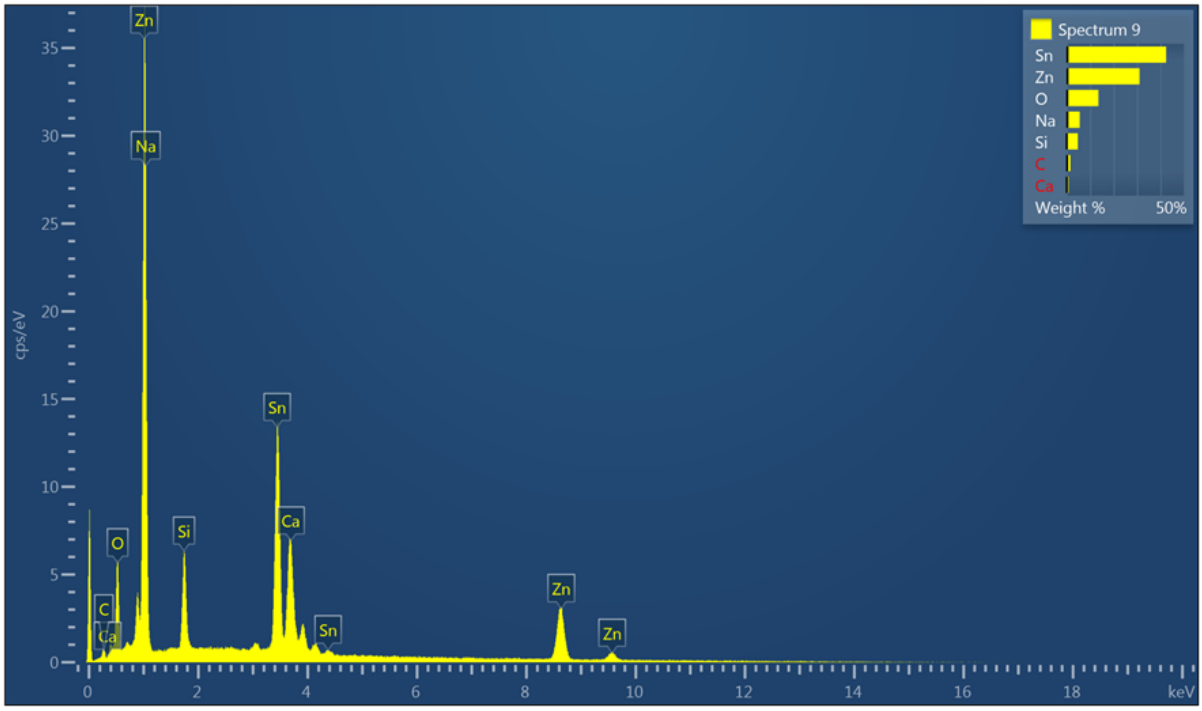


Figure S4. EDX spectra obtained from the zinc electrodeposit performed in 50 mM ZnBr2 : 50 mM $[N_{4,4,4,4}]Br$

Table S1. Relative abundance (wt %) of elements observed in the EDX spectrum of Zn electrodeposits

BSA:	$[C_2MPyrr]Br$	$[C_6MPyrr]Br$	$[N_{2,2,2,2}]Br$	[N4,4,4,4]Br
Zn (K series)	40.32	36.22	48.36	31.11
Sn (L series)	31.77	42.22	33.30	42.42
O (K series)	14.59	10.01	7.61	13.57
Si (K series)	5.14	3.20	3.41	4.79
Na (K series)	4.16	5.67	4.80	5.60
C (K series)	2.98	1.72	1.47	1.62
Ca (K series)	1.04	0.96	1.05	0.89

Crystallographic Details

1) $[N_{2,2,2,2}]_2[Zn_2Br_6]$

A colourless prismatic crystal was attached with Exxon Paratone N to a Hampton Research nylon loop. The crystal was quenched in a cold nitrogen gas stream from an Oxford Cryosystems Cryostream. An APEXII-FR591 diffractometer employing mirror monochromated MoKα radiation generated from a rotating anode was used for the data collection. Cell constants were obtained from a least squares refinement against 8162

reflections located between 6 and 56° 2θ. Data were collected at 150(2) Kelvin with ω+ϕ scans to 57° 2θ. Data were collected at 150(2) Kelvin with ω+ϕ scans to 62° 2θ. The data processing was undertaken with APEX, SAINT and XPREP[1] and subsequent computations were carried out with WinGX[2] and ShelXle.[3] An empirical absorption correction determined with SADABS[4] was applied to the data.

The structure was solved in the space group $P2_1/n$ (#14) by direct methods with SIR97[5], and extended and refined with SHELXL-14.[6] The asymmetric unit contains half a dizinchexabromide anion centred about an inversion site and a tertraethylammonium cation. The non-hydrogen atoms in the asymmetric unit were modelled with anisotropic displacement parameters and a riding atom model with group displacement parameters was used for the hydrogen atoms. An ORTEP[7] depiction of the molecule with 50% displacement ellipsoids is provided in Figure S6 (the asterix denotes inversion related sites with 1-x, -y, -z).

Table S2. Crystallographic details for the $[N_{2,2,2,2}]_2[Zn_2Br_6]$ crystal

Formula of the Refinement Model	$C_{16}H_{40}Br_6N_2Zn_2$
Model Molecular Weight	870.7
Crystal System	monoclinic
Space Group	$P2_1/n$ (#14)
a	8.9131(10) Å
b	10.4346(12) Å
c	15.6895(19) Å
β	104.580(7)º
V	1412.2(3) Å3
*D*c	2.048 g cm-3
Z	2
Crystal Size	0.089x0.070x0.053 mm
Crystal Colour	colourless
Crystal Habit	prismatic
Temperature	150(2) Kelvin
λ(MoKα)	0.71073 Å
μ(MoKα)	10.192 mm-1
T(SADABS)min,max	0.846, 1.00
2θmax	56.85º
hkl range	-11 11, -13 13, -20 20
N	61940
*N*ind	3528(*R*merge 0.0911)
*N*obs	2915(I > 2σ(I))
*N*var	122
Residuals* *R*1(*F*), *wR*2(*F*2)	0.0412, 0.1637
GoF(all)	1.143

Residual Extrema	-2.962, 1.579 e- Å-3

$^{*}R1 = \Sigma||F_O| - |F_C||/\Sigma|F_O|$ for $F_O > 2\sigma(F_O)$; $wR2 = (\Sigma w(F_O^2 - F_C^2)^2/\Sigma(wF_C^2)^2)^{1/2}$ all reflections $w=1/[\sigma^2(F_O^2)+(0.1P)^2+5.0P]$ where $P=(F_O^2+2F_C^2)/3$

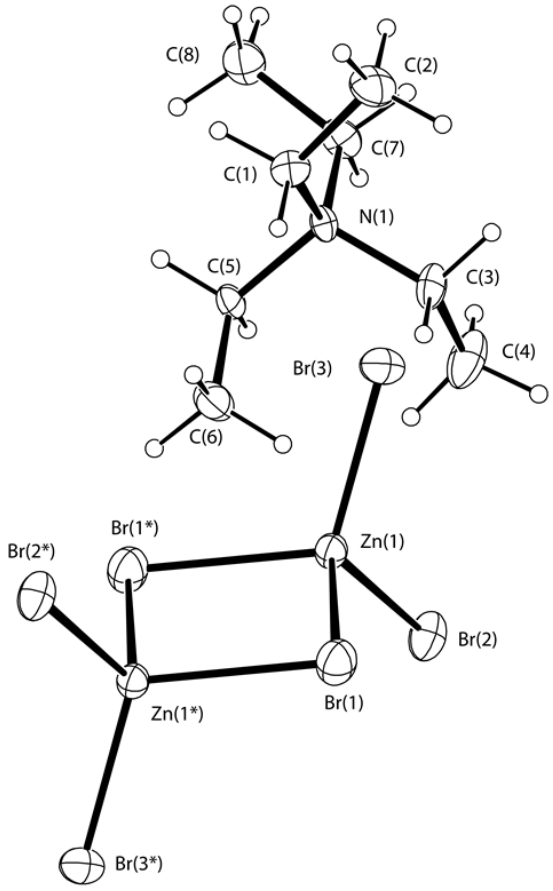


Figure S6. ORTEP representation of the $[N_{2,2,2,2}]_2[Zn_2Br_6]$ crystal.

Table S3. Non-Hydrogen Atom Coordinates,Isotropic Thermal Parameters and Occupancies

atom	x	y	z	Ueq(Å2)	Occ
Br(1)	0.64944(8)	0.11278(6)	-0.00972(4)	0.02948(19)	1
Br(2)	0.23381(7)	0.25563(6)	-0.00887(4)	0.02775(19)	1
Br(3)	0.51645(7)	0.12403(6)	0.21185(4)	0.02517(18)	1
Zn(1)	0.42744(7)	0.10915(6)	0.05746(4)	0.01782(18)	1
N(1)	0.0555(5)	0.0781(4)	0.2778(3)	0.0148(8)	1
C(1)	0.2050(6)	0.0142(5)	0.3261(4)	0.0196(11)	1

C(2)	0.2970(7)	0.0836(7)	0.4072(4)	0.0282(13)	1
C(3)	0.0919(6)	0.2097(5)	0.2471(4)	0.0225(11)	1
C(4)	-0.0445(8)	0.2781(6)	0.1863(5)	0.0359(16)	1
C(5)	-0.0231(6)	-0.0059(5)	0.1997(3)	0.0179(10)	1
C(6)	0.0662(7)	-0.0161(6)	0.1284(4)	0.0278(13)	1
C(7)	-0.0547(6)	0.0939(6)	0.3368(4)	0.0219(11)	1
C(8)	-0.0926(7)	-0.0280(6)	0.3786(4)	0.0284(13)	1

Table S4. Hydrogen Atom Coordinates,Isotropic Thermal Parameters and Occupancies

atom	x	y	z	Ueq(Å2)	Occ
H(1A)	0.2715	0.0043	0.2846	0.024	1
H(1B)	0.1803	-0.0728	0.3437	0.024	1
H(2A)	0.2323	0.0954	0.4487	0.042	1
H(2B)	0.3298	0.1674	0.3902	0.042	1
H(2C)	0.3886	0.0328	0.4353	0.042	1
H(3A)	0.1754	0.2008	0.2162	0.027	1
H(3B)	0.1322	0.2642	0.2996	0.027	1
H(4A)	-0.1289	0.2865	0.2157	0.054	1
H(4B)	-0.0807	0.2284	0.132	0.054	1
H(4C)	-0.012	0.3635	0.172	0.054	1
H(5A)	-0.1276	0.0292	0.1729	0.021	1
H(5B)	-0.0368	-0.0931	0.2216	0.021	1
H(6A)	0.1679	-0.0548	0.1535	0.042	1
H(6B)	0.08	0.0697	0.1061	0.042	1
H(6C)	0.0078	-0.0696	0.08	0.042	1
H(7A)	-0.0085	0.1555	0.3841	0.026	1
H(7B)	-0.1526	0.1318	0.3016	0.026	1
H(8A)	0.0009	-0.06	0.4204	0.043	1
H(8B)	-0.1304	-0.0924	0.3329	0.043	1
H(8C)	-0.1728	-0.0106	0.4099	0.043	1

Table S5. Anisotropic Thermal Parameters ($Å^2$)

atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Br(1)	0.0316(4)	0.0251(3)	0.0346(4)	-0.0028(2)	0.0134(3)	0.0000(2)
Br(2)	0.0234(3)	0.0203(3)	0.0373(4)	0.0006(2)	0.0035(2)	0.0030(2)
Br(3)	0.0234(3)	0.0321(3)	0.0201(3)	-0.0032(2)	0.0057(2)	0.0003(2)
Zn(1)	0.0186(3)	0.0160(3)	0.0197(3)	-0.0007(2)	0.0064(2)	-0.0001(2)
N(1)	0.0130(19)	0.0126(19)	0.019(2)	0.0007(16)	0.0041(16)	-0.0038(16)
C(1)	0.014(2)	0.023(3)	0.020(3)	0.003(2)	0.0011(19)	0.002(2)
C(2)	0.024(3)	0.035(3)	0.022(3)	-0.003(2)	-0.002(2)	-0.002(2)
C(3)	0.019(3)	0.014(2)	0.032(3)	-0.004(2)	0.002(2)	0.000(2)

C(4)	0.028(3)	0.020(3)	0.052(4)	0.002(2)	-0.004(3)	0.010(3)
C(5)	0.020(2)	0.015(2)	0.016(2)	-0.0035(19)	0.0003(19)	-0.0038(19)
C(6)	0.034(3)	0.029(3)	0.022(3)	-0.009(3)	0.009(2)	-0.007(2)
C(7)	0.018(3)	0.026(3)	0.024(3)	0.000(2)	0.010(2)	-0.005(2)
C(8)	0.030(3)	0.029(3)	0.032(3)	-0.004(2)	0.018(3)	-0.005(3)

Table S6. Non-hydrogen bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br(1)	Zn(1)	2.4653(9)	Br(1)	Zn(1)	2.4768(9)
Br(2)	Zn(1)	2.3439(9)	Br(3)	Zn(1)	2.3566(9)
Zn(1)	Br(1)	2.4769(9)	N(1)	C(1)	1.512(6)
N(1)	C(3)	1.518(7)	N(1)	C(7)	1.518(7)
N(1)	C(5)	1.525(6)	C(1)	C(2)	1.514(8)
C(3)	C(4)	1.521(8)	C(5)	C(6)	1.531(8)
C(7)	C(8)	1.508(9)			

Table S7. Non-hydrogen bond angles (°)

atom	atom	atom	angle
Zn(1)	Br(1)	Zn(1)	85.66(3)
Br(2)	Zn(1)	Br(3)	115.67(3)
Br(2)	Zn(1)	Br(1)	112.37(3)
Br(3)	Zn(1)	Br(1)	109.86(3)
Br(2)	Zn(1)	Br(1)	111.02(3)
Br(3)	Zn(1)	Br(1)	111.62(3)
Br(1)	Zn(1)	Br(1)	94.35(3)
C(1)	N(1)	C(3)	109.0(4)
C(1)	N(1)	C(7)	111.5(4)
C(3)	N(1)	C(7)	108.5(4)
C(1)	N(1)	C(5)	108.5(4)
C(3)	N(1)	C(5)	110.9(4)
C(7)	N(1)	C(5)	108.4(4)
N(1)	C(1)	C(2)	115.7(5)
N(1)	C(3)	C(4)	115.0(5)
N(1)	C(5)	C(6)	114.1(4)
C(8)	C(7)	N(1)	115.1(5)

Table S8. Hydrogen bond lengths (Å)

atom	atom	Distance	atom	atom	Distance
C(1)	H(1A)	0.99	C(1)	H(1B)	0.99
C(2)	H(2A)	0.98	C(2)	H(2B)	0.98
C(2)	H(2C)	0.98	C(3)	H(3A)	0.99

C(3)	H(3B)	0.99	C(4)	H(4A)	0.98
C(4)	H(4B)	0.98	C(4)	H(4C)	0.98
C(5)	H(5A)	0.99	C(5)	H(5B)	0.99
C(6)	H(6A)	0.98	C(6)	H(6B)	0.98
C(6)	H(6C)	0.98	C(7)	H(7A)	0.99
C(7)	H(7B)	0.99	C(8)	H(8A)	0.98
C(8)	H(8B)	0.98	C(8)	H(8C)	0.98

Table S9. Hydrogen bond angles (°)

atom	**atom**	**atom**	**angle**
N(1)	C(1)	H(1A)	108.4
C(2)	C(1)	H(1A)	108.4
N(1)	C(1)	H(1B)	108.4
C(2)	C(1)	H(1B)	108.4
H(1A)	C(1)	H(1B)	107.4
C(1)	C(2)	H(2A)	109.5
C(1)	C(2)	H(2B)	109.5
H(2A)	C(2)	H(2B)	109.5
C(1)	C(2)	H(2C)	109.5
H(2A)	C(2)	H(2C)	109.5
H(2B)	C(2)	H(2C)	109.5
N(1)	C(3)	H(3A)	108.5
C(4)	C(3)	H(3A)	108.5
N(1)	C(3)	H(3B)	108.5
C(4)	C(3)	H(3B)	108.5
H(3A)	C(3)	H(3B)	107.5
C(3)	C(4)	H(4A)	109.5
C(3)	C(4)	H(4B)	109.5
H(4A)	C(4)	H(4B)	109.5
C(3)	C(4)	H(4C)	109.5
H(4A)	C(4)	H(4C)	109.5
H(4B)	C(4)	H(4C)	109.5
N(1)	C(5)	H(5A)	108.7
C(6)	C(5)	H(5A)	108.7
N(1)	C(5)	H(5B)	108.7
C(6)	C(5)	H(5B)	108.7
H(5A)	C(5)	H(5B)	107.6
C(5)	C(6)	H(6A)	109.5
C(5)	C(6)	H(6B)	109.5
H(6A)	C(6)	H(6B)	109.5
C(5)	C(6)	H(6C)	109.5
H(6A)	C(6)	H(6C)	109.5
H(6B)	C(6)	H(6C)	109.5

C(8)	C(7)	H(7A)	108.5
N(1)	C(7)	H(7A)	108.5
C(8)	C(7)	H(7B)	108.5
N(1)	C(7)	H(7B)	108.5
H(7A)	C(7)	H(7B)	107.5
C(7)	C(8)	H(8A)	109.5
C(7)	C(8)	H(8B)	109.5
H(8A)	C(8)	H(8B)	109.5
C(7)	C(8)	H(8C)	109.5
H(8A)	C(8)	H(8C)	109.5
H(8B)	C(8)	H(8C)	109.5

2) $[C_6MPyrr]_3[Zn_2Br_7]$

A colourless tablet was attached with Exxon Paratone N to a nylon loop and quenched in a cold nitrogen gas stream from an Oxford Cryosystems Cryostream. A SuperNova Dual equipped with an Atlas detector and employing mirror monochromated Cu (Kα) radiation from a micro-source was used for the data collection. Cell constants were obtained from a least squares refinement against 15448 reflections located between 10 and 147° 2θ. Data were collected at 150(1) Kelvin with ω scans to 154° 2θ. The data processing was undertaken with CrysAlis Pro[8] and subsequent computations were carried out with WinGX[2] and ShelXle.[3] A multi-scan absorption correction was applied[8] to the data.

The structure was solved in the space group *P*31c(#159) by direct methods with SHELXT[9] and extended and refined with SHELXL-2014/7.[6] The data were treated as being twinned about a two-fold axis parallel to the *c*-axis and additionally twinned by inversion, with the minor rotation twin fraction refining to 0.18, with the inversion twin fractions refining to 0.19 and 0.32. The asymmetric unit contains one third of a dizincheptabromo anion and a disordered N-hexyl-N-methylpyrrolidine cation. A rigid body was used to refine the methylpyrrolidine moiety and restraints were required for the hexyl residue. The hexyl residue is disordered over at least two orientations. Unresolved disorder is reflected in large displacement parameters. The occupancies of the resolved disorder sites were refined and then fixed. The metal sites of the anion are located on a threefold axis, whereas the bridging bromo is slightly displaced from, and accordingly disordered about this axis. Presumably reflecting steric constraints, the bromo displacement is not towards the nitrogen of the nearest N-hexyl-N-methylpyrrolidine cation. Instead the bromo is slightly displaced from the plane defined by the metal sites and the unique terminal bromo sites.

The non-hydrogen atoms in the asymmetric unit were modelled with anisotropic displacement parameters, while a riding atom model with group displacement parameters was used for the hydrogen atoms. An ORTEP[10] depiction of the molecule with 50% displacement ellipsoids is provided in Figure S7. The symmetry operators indicated by the atom label superscripts are (i) -y+1, x-y, z and (ii) -x+y+1, -x+1, z.

Table S10. Crystallographic details for the $[C_6MPyrr]_3[Zn_2Br_7]$ crystal

Formula of the Refinement Model	$C_{33}H_{72}Br_7N_3Zn_2$
Model Molecular Weight	1201.04

Crystal System	trigonal
Space Group	*P*31c(#159)
a	14.7234(2) Å
b	14.7234(2) Å
c	12.4759(3) Å
γ	120º
V	2342.17(8) Å^3
D_c	1.703 g cm^{-3}
Z	2
Crystal Size	0.110x0.074x0.033 mm
Crystal Colour	colourless
Crystal Habit	tablet
Temperature	150(1) Kelvin
λ(Cu Kα)	1.5418 Å
μ(Cu Kα)	8.429 mm^{-1}
$T_{min,max}$	0.616, 1.00
$2\theta_{max}$	153.69º
hkl range	-18 18, -18 18, -15 15
N	50065
N_{ind}	3280(R_{merge} 0.0443)
N_{obs}	2634(I > 2σ(I))
N_{var}	141
Residuals* *R*1(*F*), *wR*2(F^2)	0.0536, 0.1646
GoF(all)	1.234
Residual Extrema	-0.756, 0.971 e$^-$ Å^{-3}

*$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ for $F_o > 2\sigma(F_o)$; $wR2 = (\Sigma w(F_o^2 - F_c^2)^2/\Sigma(wF_c^2)^2)^{1/2}$ all reflections

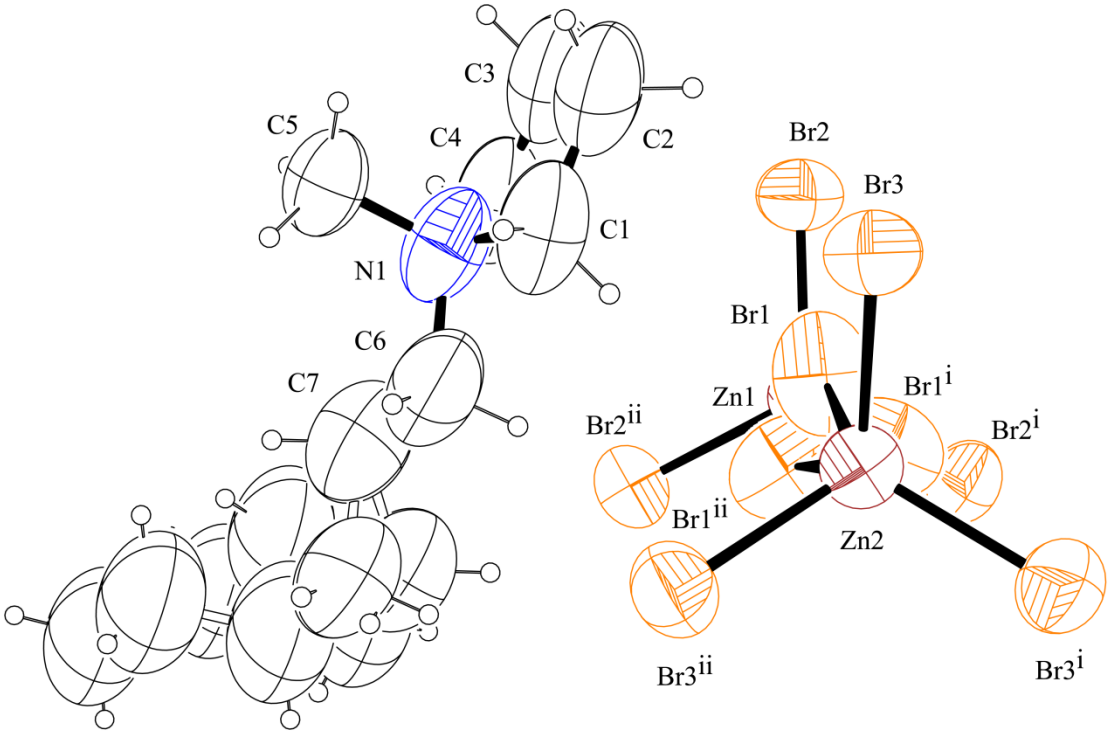


Figure S7. ORTEP representation of the $[C_2MPyrr]_2[Zn_2Br_7]$ crystal.

Table S11. Non-Hydrogen Atom Coordinates,Isotropic Thermal Parameters and Occupancies

atom	x	y	z	Ueq(Å2)	Occ
Br(1)	0.6177(4)	0.3131(10)	0.3430(9)	0.1222(18)	0.3333
Br(2)	0.4884(2)	0.2345(3)	0.5857(3)	0.1020(9)	1
Br(3)	0.4881(2)	0.2332(3)	0.0988(3)	0.0996(9)	1
Zn(1)	0.6667	0.3333	0.5361(5)	0.0703(15)	1
Zn(2)	0.6667	0.3333	0.1497(5)	0.0724(18)	1
N(1)	0.4839(16)	0.5178(15)	0.3458(19)	0.117(3)	1
C(1)	0.466(3)	0.440(2)	0.2571(19)	0.142(5)	1
C(2)	0.358(4)	0.338(3)	0.294(3)	0.165(7)	1
C(3)	0.354(4)	0.365(4)	0.410(4)	0.165(7)	1
C(4)	0.460(3)	0.463(3)	0.451(2)	0.142(5)	1
C(5)	0.4229(18)	0.5717(17)	0.335(2)	0.103(4)	1
C(6)	0.600(2)	0.592(2)	0.309(2)	0.151(8)	1
C(7)	0.654(2)	0.677(3)	0.391(3)	0.180(12)	1
C(8A)	0.769(3)	0.712(9)	0.389(6)	0.22(3)	0.4
C(9A)	0.827(3)	0.775(7)	0.485(6)	0.246(17)	0.4
C(10A)	0.760(4)	0.799(7)	0.557(5)	0.246(17)	0.4
C(11A)	0.823(8)	0.888(7)	0.633(7)	0.246(17)	0.4
C(8B)	0.766(3)	0.751(3)	0.358(5)	0.203(17)	0.6
C(9B)	0.826(3)	0.835(3)	0.440(7)	0.246(17)	0.6
C(10B)	0.791(5)	0.915(4)	0.445(5)	0.246(17)	0.6
C(11B)	0.837(8)	0.988(6)	0.539(6)	0.246(17)	0.6

Table S12. Hydrogen Atom Coordinates, Isotropic Thermal Parameters and Occupancies

atom	x	y	z	U_{eq}(Å2)	Occ
H(1A)	0.5243	0.4251	0.253	0.17	1
H(1B)	0.4578	0.4663	0.1867	0.17	1
H(2A)	0.2971	0.33	0.2532	0.198	1
H(2B)	0.3621	0.2728	0.2873	0.198	1
H(3A)	0.3383	0.3037	0.4546	0.198	1
H(3B)	0.2964	0.3804	0.4185	0.198	1
H(4A)	0.4482	0.502	0.5089	0.17	1
H(4B)	0.5129	0.4442	0.4732	0.17	1
H(5A)	0.3542	0.5235	0.3041	0.155	1
H(5B)	0.4605	0.6329	0.2883	0.155	1
H(5C)	0.4136	0.5946	0.406	0.155	1
H(6A)	0.6366	0.552	0.301	0.181	1
H(6B)	0.6003	0.6238	0.2385	0.181	1
H(7A)	0.6251	0.65	0.4634	0.216	1
H(7B)	0.6435	0.737	0.3751	0.216	1
H(8A1)	0.7774	0.6494	0.3837	0.266	0.4
H(8A2)	0.8007	0.7547	0.3233	0.266	0.4
H(9A1)	0.8537	0.7357	0.5269	0.295	0.4
H(9A2)	0.8887	0.8417	0.4616	0.295	0.4
H(10A)	0.7127	0.736	0.5988	0.295	0.4
H(10B)	0.7158	0.8174	0.5119	0.295	0.4
H(11A)	0.7756	0.901	0.6774	0.369	0.4
H(11B)	0.8658	0.8705	0.6788	0.369	0.4
H(11C)	0.869	0.9519	0.5918	0.369	0.4
H(8B1)	0.8016	0.7096	0.3469	0.244	0.6
H(8B2)	0.766	0.7837	0.2891	0.244	0.6
H(9B1)	0.9017	0.8706	0.4214	0.295	0.6
H(9B2)	0.8171	0.8023	0.5111	0.295	0.6
H(10C)	0.8124	0.9568	0.3778	0.295	0.6
H(10D)	0.714	0.8786	0.4497	0.295	0.6
H(11D)	0.8125	1.0387	0.5385	0.369	0.6
H(11E)	0.8157	0.9477	0.6055	0.369	0.6
H(11F)	0.9142	1.0259	0.5337	0.369	0.6

Table S13. Anisotropic Thermal Parameters (Å2)

atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)
Br(1)	0.193(4)	0.136(7)	0.0533(11)	0.093(8)
Br(2)	0.0738(15)	0.0979(18)	0.123(2)	0.0347(15)
Br(3)	0.0785(16)	0.0976(18)	0.115(2)	0.0379(15)

Zn(1)	0.080(3)	0.080(3)	0.051(2)	0.0401(13)
Zn(2)	0.080(3)	0.080(3)	0.057(3)	0.0400(15)
N(1)	0.158(9)	0.162(9)	0.085(5)	0.120(7)
C(1)	0.209(12)	0.160(11)	0.113(7)	0.136(10)
C(2)	0.211(13)	0.163(13)	0.181(12)	0.138(11)
C(3)	0.211(13)	0.163(13)	0.181(12)	0.138(11)
C(4)	0.209(12)	0.160(11)	0.113(7)	0.136(10)
C(5)	0.137(10)	0.129(10)	0.078(8)	0.092(7)
C(6)	0.168(11)	0.176(15)	0.160(19)	0.125(11)
C(7)	0.190(16)	0.20(2)	0.19(3)	0.129(14)
C(8A)	0.19(2)	0.21(7)	0.31(5)	0.13(2)
C(9A)	0.25(2)	0.22(3)	0.32(4)	0.16(2)
C(10A)	0.25(2)	0.22(3)	0.32(4)	0.16(2)
C(11A)	0.25(2)	0.22(3)	0.32(4)	0.16(2)
C(8B)	0.180(18)	0.21(2)	0.27(4)	0.133(17)
C(9B)	0.25(2)	0.22(3)	0.32(4)	0.16(2)
C(10B)	0.25(2)	0.22(3)	0.32(4)	0.16(2)
C(11B)	0.25(2)	0.22(3)	0.32(4)	0.16(2)

Table S14. Non Hydrogen Bond Lengths (Å)

atom	atom	Distance	atom	atom	Distance
Br(1)	Br(1)	1.086(8)	Br(1)	Br(1)	1.086(8)
Br(1)	Zn(1)	2.490(11)	Br(1)	Zn(2)	2.492(11)
Br(2)	Zn(1)	2.360(3)	Br(3)	Zn(2)	2.369(3)
Zn(1)	Br(2)	2.360(3)	Zn(1)	Br(2)	2.360(3)
Zn(1)	Br(1)	2.490(11)	Zn(1)	Br(1)	2.490(11)
Zn(2)	Br(3)	2.369(3)	Zn(2)	Br(3)	2.369(3)
Zn(2)	Br(1)	2.492(11)	Zn(2)	Br(1)	2.492(11)
N(1)	C(5)	1.471(15)	N(1)	C(4)	1.49(3)
N(1)	C(1)	1.5169	N(1)	C(6)	1.57(3)
C(1)	C(2)	1.62(6)	C(2)	C(3)	1.50(5)
C(3)	C(4)	1.59(7)	C(6)	C(7)	1.504(7)
C(7)	C(8A)	1.505(10)	C(7)	C(8B)	1.505(10)
C(8A)	C(9A)	1.504(10)	C(9A)	C(10A)	1.504(10)
C(10A)	C(11A)	1.504(10)	C(8B)	C(9B)	1.504(10)
C(9B)	C(10B)	1.504(10)	C(10B)	C(11B)	1.504(10)

Table S15. Non Hydrogen Bond Angles (º)

atom	atom	atom	angle	atom	atom	atom	angle
Br(1)	Br(1)	Br(1)	60.003(4)	Br(3)	Zn(2)	Br(1)	110.1(3)
Br(1)	Br(1)	Zn(1)	77.40(10)	Br(3)	Zn(2)	Br(1)	91.17(19)
Br(1)	Br(1)	Zn(1)	77.40(10)	Br(1)	Zn(2)	Br(1)	25.2(2)

Br(1)	Br(1)	Zn(2)	77.41(12)	Br(3)	Zn(2)	Br(1)	110.1(3)
Br(1)	Br(1)	Zn(2)	77.41(12)	Br(3)	Zn(2)	Br(1)	91.17(19)
Zn(1)	Br(1)	Zn(2)	150.8(2)	Br(3)	Zn(2)	Br(1)	114.5(3)
Br(2)	Zn(1)	Br(2)	113.38(13)	Br(1)	Zn(2)	Br(1)	25.2(2)
Br(2)	Zn(1)	Br(2)	113.38(13)	Br(1)	Zn(2)	Br(1)	25.2(2)
Br(2)	Zn(1)	Br(2)	113.38(13)	C(5)	N(1)	C(4)	109(2)
Br(2)	Zn(1)	Br(1)	109.9(3)	C(5)	N(1)	C(1)	114.7(18)
Br(2)	Zn(1)	Br(1)	90.80(17)	C(4)	N(1)	C(1)	109(2)
Br(2)	Zn(1)	Br(1)	114.1(3)	C(5)	N(1)	C(6)	109.9(18)
Br(2)	Zn(1)	Br(1)	90.80(17)	C(4)	N(1)	C(6)	121(2)
Br(2)	Zn(1)	Br(1)	114.1(3)	C(1)	N(1)	C(6)	92(2)
Br(2)	Zn(1)	Br(1)	109.9(3)	N(1)	C(1)	C(2)	102(2)
Br(1)	Zn(1)	Br(1)	25.20(19)	C(3)	C(2)	C(1)	100(4)
Br(2)	Zn(1)	Br(1)	114.1(3)	C(2)	C(3)	C(4)	114(5)
Br(2)	Zn(1)	Br(1)	109.9(3)	N(1)	C(4)	C(3)	94(3)
Br(2)	Zn(1)	Br(1)	90.80(17)	C(7)	C(6)	N(1)	109(2)
Br(1)	Zn(1)	Br(1)	25.20(19)	C(6)	C(7)	C(8A)	108(3)
Br(1)	Zn(1)	Br(1)	25.20(19)	C(6)	C(7)	C(8B)	110(3)
Br(3)	Zn(2)	Br(3)	113.09(13)	C(9A)	C(8A)	C(7)	112.8(14)
Br(3)	Zn(2)	Br(3)	113.09(13)	C(10A)	C(9A)	C(8A)	112.6(14)
Br(3)	Zn(2)	Br(3)	113.09(13)	C(9A)	C(10A)	C(11A)	112.8(15)
Br(3)	Zn(2)	Br(1)	91.17(19)	C(9B)	C(8B)	C(7)	112.9(14)
Br(3)	Zn(2)	Br(1)	114.5(3)	C(8B)	C(9B)	C(10B)	112.7(14)
Br(3)	Zn(2)	Br(1)	110.1(3)	C(11B)	C(10B)	C(9B)	112.8(14)
Br(3)	Zn(2)	Br(1)	114.5(3)				

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