Electronic Supplementary Information

Coordination Polymers Derived from Alkali Metal Complexes of Redox-Active Ligands

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Table S1. Crystallographic data and structure refinement details for **1**-**3**.

	1 (Li)	**2 (Na)**	**3 (K)**
Empirical Formula	$C_{46}H_{48}LiN_4$	$C_{56}H_{56}N_6Na$	$C_{46}H_{48}KN_4$
M	663.82	836.05	695.98
T [K]	150	100	100
λ [Å]	1.54184 (Cu)	0.71073 (Mo)	0.71073 (Mo)
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	$Pca2_1$	$P2_1/c$	$P2_1/n$
a [Å]	19.7085(8)	18.7293(11)	9.6059(3)
b [Å]	12.4030(6)	12.8174(8)	17.2348(6)
c [Å]	32.0285(14)	19.6609(12)	23.4133(8)
α [deg]	90	90	90
β [deg]	90	103.238(2)	100.2090(10)
γ [deg]	90	90	90
V [Å^3]	7829.2(6)	4594.4(5)	3814.8(2)
Z	8	4	4
d_{calc} [g/cm^3]	1.126	1.209	1.212
μ [mm^{-1}]	0.497	0.079	0.177
F_{000}	2840	1780	1484
Crystal dimensions [mm]	0.44 × 0.27 × 0.11	0.34×0.19×0.15	0.41×0.12×0.08
θ range [deg]	2.76 – 66.60	2.23–26.11	2.13 – 28.70
HKL indices	-23 ≤ h ≤ 20 -14 ≤ k ≤ 11 -38 ≤ l ≤ 37	–23 ≤ h ≤ 23 –15 ≤ k ≤ 15 –24 ≤ l ≤ 24	–12 ≤ h ≤ 12 –23 ≤ k ≤ 23 –31 ≤ l ≤ 31

	1 (Li)	2 (Na)	3 (K)
Reflections collected	31124	57742	61367
Independent reflns (I > 2σ(I))	10118	6986	7703
R_{int}	0.0660	0.0913	0.0466
Completeness to θ, %	100.0	99.4	100.0
Data / Restraints / Parameters	13320/194/1058	9086/0/576	9843/0/652
$S(F^2)$	1.061	1.044	1.015
Flack parameter	0.0(3)		
R_1 / wR_2 ($I > 2\sigma(I)$)	0.0883 / 0.1957	0.0482 / 0.1012	0.0447 / 0.0978
R_1 / wR_2 (all data)	0.1121 / 0.2116	0.0707 / 0.1112	0.0646 / 0.1068
Largest diff. peak and hole [e/Å^3]	0.23 / -0.24	0.23 / –0.29	0.52 / –0.34

Table S2. Selected bond lengths [Å] and angles [°] for complexes **1-3**.

	1 (Li)	2 (Na)	3 (K)
	Bond		
M(1)–N(1)	2.078(17)	2.3974(15)	2.7310(11)
M(1)–N(2)	2.022(16)	2.4775(14)	2.7453(12)
M(1)–N(3)	2.054(16)	2.5338(15)	2.8020(13)
M(1)–N(4)	1.99(3)	2.4946(15)	2.8792(12)
M(1)–N(5)	-	2.4697(16)	-
N(1)–C(1)	1.329(10)	1.330(2)	1.3244(17)
N(2)–C(2)	1.344(10)	1.325(2)	1.3171(17)
C(1)–C(2)	1.445(12)	1.456(2)	1.4552(18)
N(3)–C(37)	1.337(11)	1.333(2)	1.340(2)
N(3)–C(41)	1.341(10)	1.342(2)	1.340(2)
N(4)–C(42)	-	1.334(2)	-
N(4)–C(46)	-	1.332(2)	-
C(37)–C(38)	1.390(11)	1.383(2)	1.386(2)
C(38)–C(39)	1.392(11)	1.390(2)	1.3933(19)
C(39)–C(39')	1.484(10)	1.487(3)	1.4840(19)

	1 (Li)	2 (Na)	3 (K)
C(39)–C(40)	1.400(10)	1.393(2)	1.391(2)
C(40)–C(41)	1.385(11)	1.379(3)	1.382(2)
N(5)–C(47)		1.337(2)	
N(5)–C(51)		1.341(2)	
C(47)–C(48)		1.382(2)	
C(48)–C(49)		1.392(2)	
C(49)–C(50)		1.389(2)	
C(50)–C(51)		1.383(2)	
C(49)–C(52)		1.389(2)	
	Angle		
N(1)–M(1)–N(2)	86.3(6)	71.44(5)	62.03(3)
N(1)–M(1)–N(3)	102.4(9)	109.83(5)	151.36(4)
N(1)–M(1)–N(4)	110.0(7)	91.23(5)	88.85(3)
N(2)–M(1)–N(3)	109.3(8)	100.15(5)	121.14(4)
N(2)–M(1)–N(4)	119.8(10)	161.26(5)	148.29(3)
N(4)–M(1)–N(3)		92.29(5)	78.24(4)
N(5)–M(1)–N(2)		101.32(5)	-
N(5)–M(1)–N(3)		83.83(5)	-
N(5)–M(1)–N(4)		93.87(5)	-
N(1)–M(1)–N(5)		165.23(6)	-

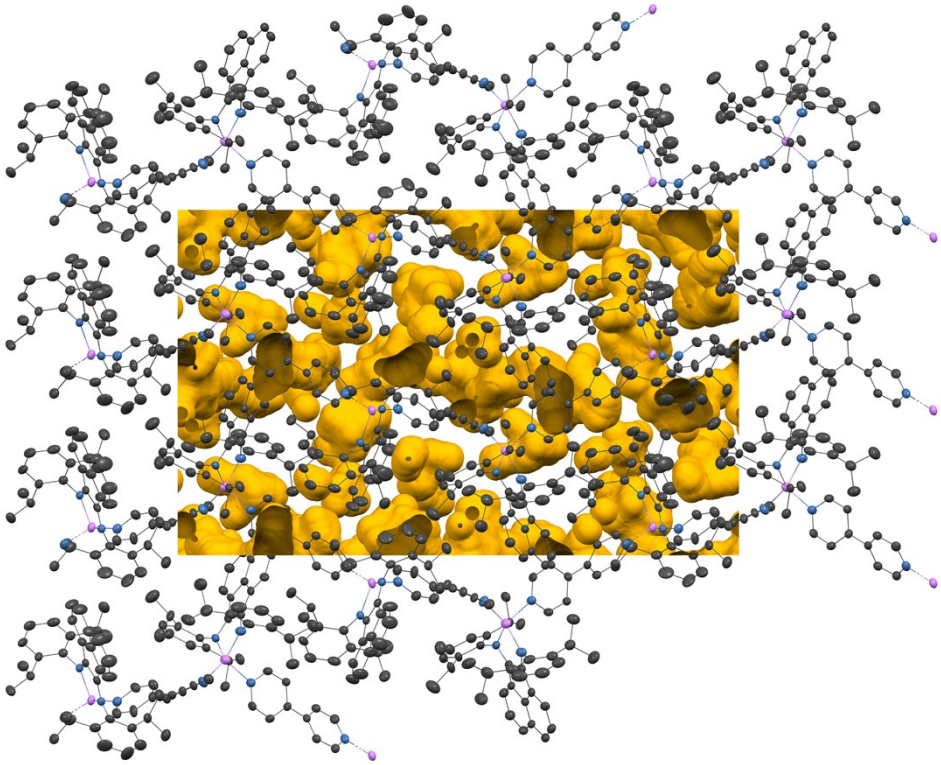

Figure S1. The Mercury visualization of voids volume (probe radius is 0.8 Å, approximating grid spacing is 0.1 Å) in **1**.

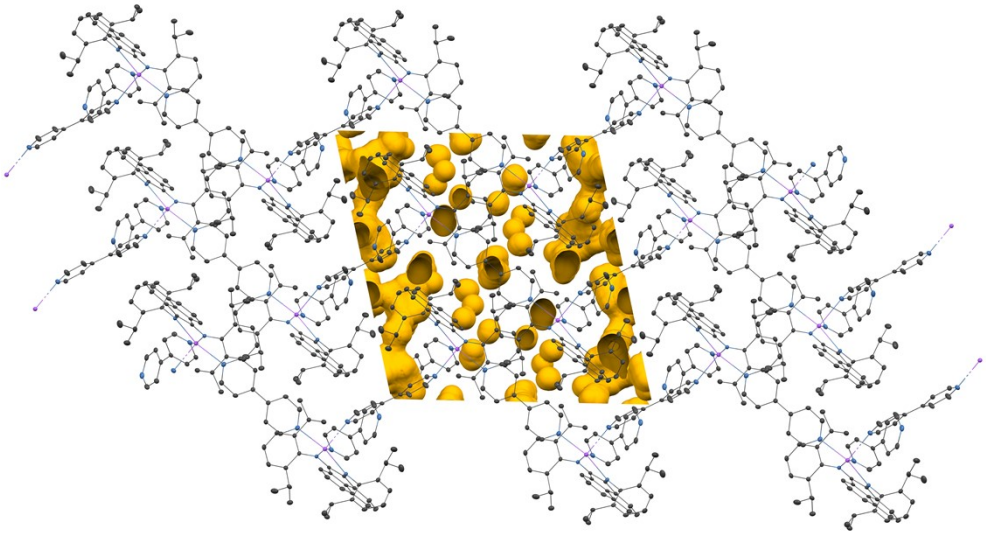

Figure S2. The Mercury visualization of voids volume (probe radius is 0.8 Å, approximating grid spacing is 0.1 Å) in **2**.

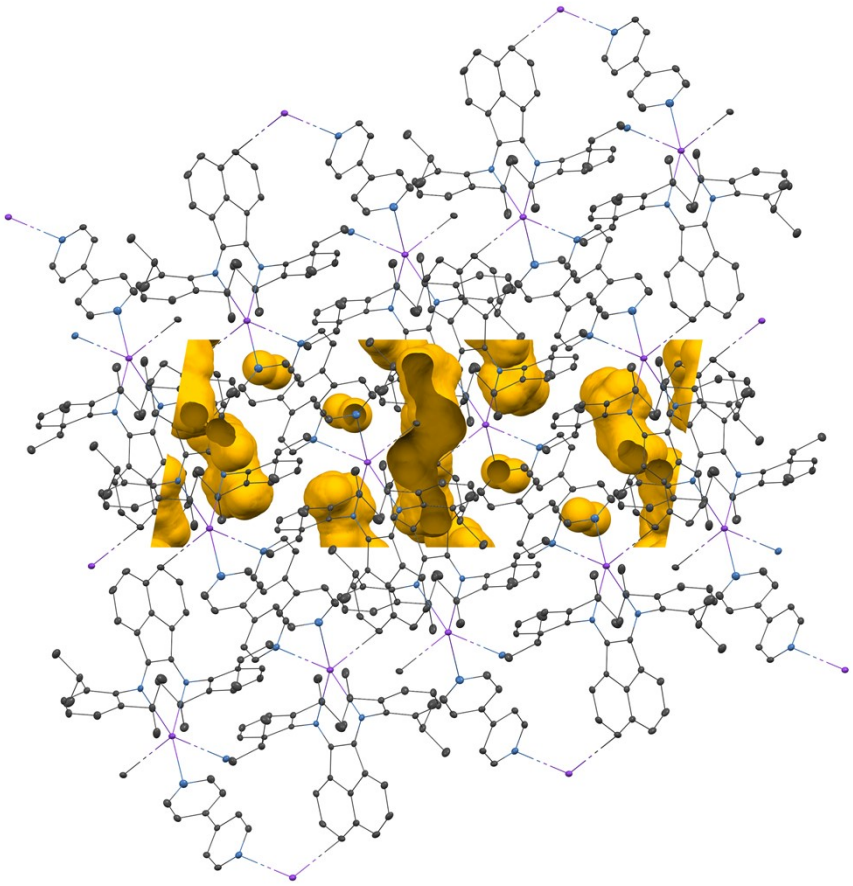

Figure S3. The Mercury visualization of voids volume (probe radius is 0.8 Å, approximating grid spacing is 0.1 Å) in **3**.