Supporting Information

Imidazol-2-ylidene-N'-phenylureate Ligands in Alkali and Alkaline Earth Metal Coordination Sphere- Heterocubane Core to Polymeric Structural Motif Formation

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Table TS1. Crystallographic details and refinement parameters of compounds **1a, 1d, 2b, 2c, 3a**, **4a**, **5a**.

Crystal	**1a**	**1d**	**2b**
CCDC No.	1046050	1046051	1046052
Empirical formula	$C_{18}H_{26}N_4O$	$C_{22}H_{34}N_4OS$	$C_{128}H_{148}K_4N_{16}O_8$
Formula weight	314.43	402.59	2195.02
T (K)	293(2)	150(2)	150(2)
λ (Å)	1.54184	0.71070	1.54184
Crystal system	Monoclinic	Trigonal	Tetragonal
Space group	$P\ 2_1/c$	R -3	P 421/c
a (Å) b (Å) c (Å) α (°) β (°) γ (°)	9.0491(4) 12.7601(5) 16.7496(9) 90 109.9(4) 90	30.9905(15) 30.9905(15) 12.3331(6) 90 90 120	15.1711(6) 15.1711(6) 15.1711(6) 90 90 90
V (Å^3)	1818.04(15)	10257.9(9)	5857.8(6)
Z	4	18	2
D_{calc} Mg m^{-3}	1.149	1.173	1.245
μ (mm^{-1})	0.579	0.161	1.858
F (000)	680	3924.0	2336
Theta range for data collection	4.46 to 70.69º	1.817 to 25.806 º	3.391 to 70.661°
Limiting indices	-10<=h<=6, -15<=k<=13, -20<=l<=20	-37<=h<=37, -26<=k<=37, -14<=l<=14	-18<=h<= 12, -18<=k<=10, -30<=l<=28
Reflections collected / unique	6979 / 3395 [R(int) = 0.0260]	8326 / 4261 [R(int) = 0.0367]	12758 / 4870 [R(int) = 0.0315]
Completeness to theta	97.3 %	97.0 %	99.1 %
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.906 and 0.886	1.00000 and 0.89998	1.000 and 0.470
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3395 / 0 / 215	4261 / 2 / 259	4870 / 0 / 377
Goodness-of-fit on F^2	1.150	1.065	1.043
Final R indices [I>2sigma(I)]	R_1 = 0.0592, wR_2 = 0.1609	R_1 = 0.0728, wR_2 = 0.1833	R_1 = 0.0574, wR_2 = 0.1527
R indices (all data)	R_1 = 0.0784, wR_2 = 0.1735	R_1 = 0.0596, wR_2 = 0.1686	R_1 = 0.0749, wR_2 = 0.1727
Largest diff. peak and hole	0.133 and -0.157 e.A^{-3}	2.461 and -0.464 e.A^{-3}	0.228 and -0.303 e.A^{-3}

Table TS1. (contd)

Crystal	**2c**	**3a**	**4a**	**5a**
CCDC No.	1046053	1046054	1046055	1046056
Empirical formula	$(C_{80}H_{118}K_4N_{10}O_2Si_4)n$	$C_{102}H_{150}Li_2N_{16}O_6$	$C_{37}H_{69}CaKN_6OSi_4$	$C_{118}H_{212}Ca_5K_4N_{20}O_{10}Si_{12}$
Formula weight	1520.61	1710.26	805.52	2764.96
T (K)	150(2)	150(2)	150(2)	150(2)
λ (Å)	1.54184	1.54184	1.54184	1.54184
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	P 2/c	P $2_1/c$	P -1
a (Å) b (Å) c (Å) α (°) β (°) γ (°)	28.2189(18) 10.5566(7) 31.0868(17) 90 108.476(6) 90	16.8744(6) 14.2505(6) 23.1944(13) 90 140.678(4) 90	13.3821(4) 18.2812(3) 18.9510(5) 90 103.948(2) 90	13.5505(8) 14.8203(10) 20.0745(14) 95.918(6) 96.395(5) 101.199(5)
V (Å^3)	8783.3(9)	5068.1(4)	4499.49(19)	3897.7(4)
Z	4	2	4	1
D_{calc} Mg m^{-3}	1.150	1.121	1.111	1.178
μ (mm^{-1})	2.691	0.547	3.315	3.771
F (000)	3264	1856	1744	1484
Theta range for data collection	2.93 to 71.17 º	3.0979 to 70.8318 º	3.40 to 70.67 º	3.06 to 70.8º
Limiting indices	-34<=h<=34, -11<=k<=12, -27<=l<=37	-20<=h<=19, -17<=k<=17, -28<=l<=17	-15<=h<=15, -14<=k<=22, -21<=l<=22	-16<=h<=13, -16<=k<=18, -18<=l<=24
Reflections collected / unique	38894 / 16591 [R(int) = 0.0667]	22833 / 9435 [R(int) = 0.0419]	17614 / 8468 [R(int) = 0.0402]	29900 / 14690 [R(int) = 0.0737]
Completeness to theta	97.5 %	96.2 %	97.8	97.9 %
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	1.00000 and 0.63659	1.00000 and 0.74586	1.00000 and 0.62213	1.00000 and 0.66635
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	16320 / 0 / 955	9435 / 0 / 587	8468 / 0 / 389	14690 / 0 / 792
Goodness-of-fit on F^2	1.036	1.075	0.997	1.064
Final R indices [I>2sigma(I)]	R_1 = 0.1036, wR_2 = 0.2367	R_1 = 0.0826, wR_2 = 0.2410	R_1 = 0.0549, wR_2 = 0.1128	$R1$ = 0.0533 wR2 = 0.1649
R indices (all data)	R_1 = 0.0830, wR_2 = 0.2127	R_1 = 0.1014, wR_2 = 0.2402	R_1 = 0.0418, wR_2 = 0.1041	R1 = 0.0965 wR2 = 0.1758
Largest diff. peak and hole	0.715 and -0.342 e.A^{-3}	0.368 and -0.335 e.A^{-3}	0.779 and -0.477 e.A^{-3}	0.359 and -0.404 e.A^{-3}

Figure of compounds **1d**:

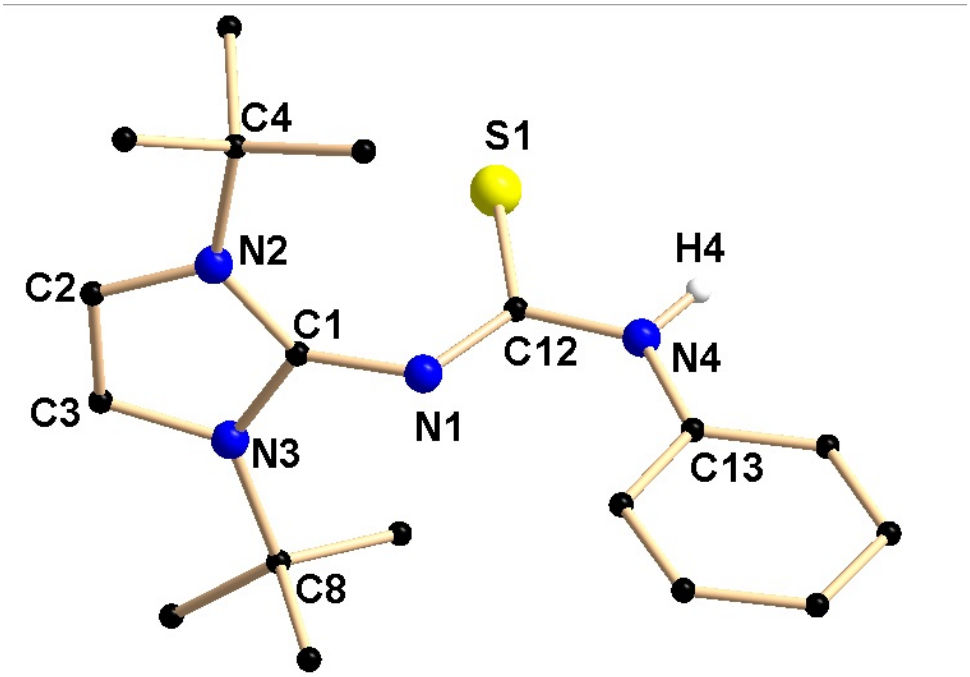

Figure S1. Solid-state structures of complexes **1d**. Selected bond lengths [Å] and bond angles[°]: N1-C12 1.311(6), N4-C12 1.373(6), C12-S1 1.725(4), N4-C13 1.406(6), N1-C1 1.353(6), C1-N2 1.366(6), C1-N3 1.359(6), C2-C3 1.337(7), N4-H4 0.858, N1-C12-N4 118.09(4), N1-C12-S1 126.16(4), N4-C12-S1 115.73(3), C1-N1-C12 120.46(2), C12-N4-C13 131.11(2).