Electronic Supplementary Material (ESI) for Dalton Transactions.

Structural diversity in the alkaline earth metal compounds of tetra- and pentacyanocyclopentadienide

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SUPPORTING INFORMATION

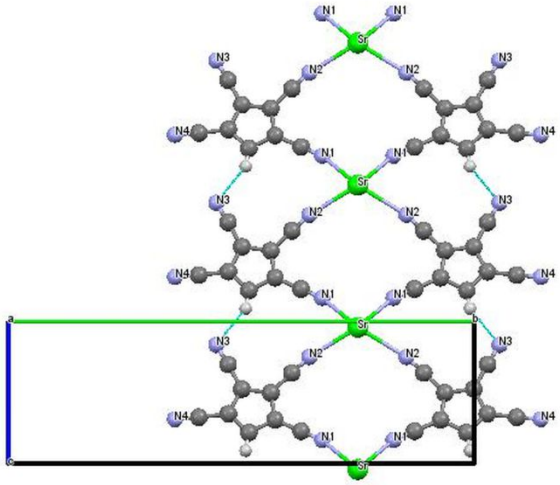

Figure SI 1: $Sr(TCC)_{4/2}$ ribbon in **2c'**, shown with y= 0.75, viewed down the *a*-axis.

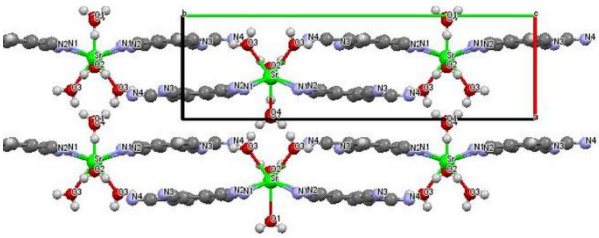

Figure SI 2: The H-bond network connecting the different $Sr(TCC)_{4/2}$ ribbons, viewed down the *c*-axis.

compound	**1a'**	**1b**	**2b'**	**2c'**	**2d'**
Temperature (K)	100	173	293	100	100
Empirical formula	C_{20} H_{20} Mg N_{10} O_{10}	C_{20} H_{12} Ca N_{10} O6	C_{18} H_{12} Ca N_8 O_5	C_{18} H_{12} N_8 O_5 Sr	C_{18} H_8 Ba N_8 O_3
M	584.77	528.48	460.44	507.98	521.66
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_12_12_1$	$P2_1/m$	$P2_1/m$	$Pnb2_1$
Crystal size (mm)	0.1 x 0.09 x 0.08	0.1 x 0.1 x 0.05	0.07 x 0.05 x 0.04	0.1 x 0.09 x 0.08	0.04 x 0.02 x 0.02
a (Å)	12.1470(3)	11.0319(5)	7.1830(2)	7.2643(2)	6.8320(2)
b (Å)	6.6285(2)	12.4908(5)	21.9235(8)	22.2182(7)	13.8221(4)
c (Å)	17.9227(5)	17.7452(8)	7.4531(3)	7.5502(2)	21.1263(5)
ß [°]	97.4580(10)°.	90	115.6950(10)	116.1240(10)	90
V [$Å^3$]	1430.86(7)	2445.24(18)	1057.63(7)	1094.11(5)	1995.01(9)
Z	2	4	2	2	4
D_c [g/dm^3]	1.357	1.436	1.446	1.542	1.737
F (000)	604	1080	472	508	1008
μ (MoKα) [mm-1]	0.130	0.314	0.345	2.510	2.028
Absorption correction	Semi-empirical from equivalents				
T_{max}/ T_{min}	0.7454/ 0.7147	0.7452/ 0.7039	0.7456/ 0.6696	0.6468/ 0.5896	0.7456/ 0.6851
no. of total reflections	24200	39685	18543	21595	36043
Data / restraints / parameters	2935 / 0 / 227	4490 / 0 / 382	2430 / 0 / 177	2588 / 0 / 173	4557 / 16 / 299
R1 [I>2σ(I)]	0.0318	0.0239	0.0492	0.0205	0.0154
wR2 (all data)	0.0970	0.0544	0.0800	0.0520	0.0363
GOOF	1.252	1.054	1.132	1.183	1.039
Largest diff. peak and hole [e Å-3]	0.358 and -0.195	0.179 and -0.172	0.334 and -0.278	0.421 and -0.391	0.275 and -0.419
CCDC-#	1569428	1569429	1569430	1569431	1569432

Table SI1: Experimental details for the crystal structure determinations.