Supporting Information

for

Coordination Chemistry of Polynitriles, Part XII. Serendipitous Synthesis of the Octacyanofulvalenediide dianion and Study of its Coordination Chemistry with K^+ and Ag^+

Table of Contents

Es konnten keine Einträge für ein Abbildungsverzeichnis gefunden werden.

1. TABLES

Table S 1: Important bond parameters of compound **4** (room temperature determination)

Bond	**Length [Å]/ Angle[°]**	**Bond**	**Length [Å]/ Angle [°]**
Ag1–N1	2.261(5)	Ag1–N2′	2.268(4)
Ag1–N3′	2.339(5)	Ag1–N4′	2.345(5)
$(C–C)_{cp}$	1.400(6) – 1.422(6)	$C_{cp}–C_{CN}$	1.413(6) – 1.426(6)
(C–N)	1.124(7) – 1.138(6)	C4–C4′	1.461(7)
C1–C6–N1	178.0(6)	C2–C7–N2	178.5(6)
C3–C8–N3	176.8(7)	C5–C9–N4	177.3(7)
Ag1–N1–C6	170.5(5)	Ag1–N2–C7	170.6(5)
Ag1–N3–C8	165.9(6)	Ag1–N5–C9	165.7(6)
C3–C4–C4′–C3′	-122.4(5)		

2. FIGURES

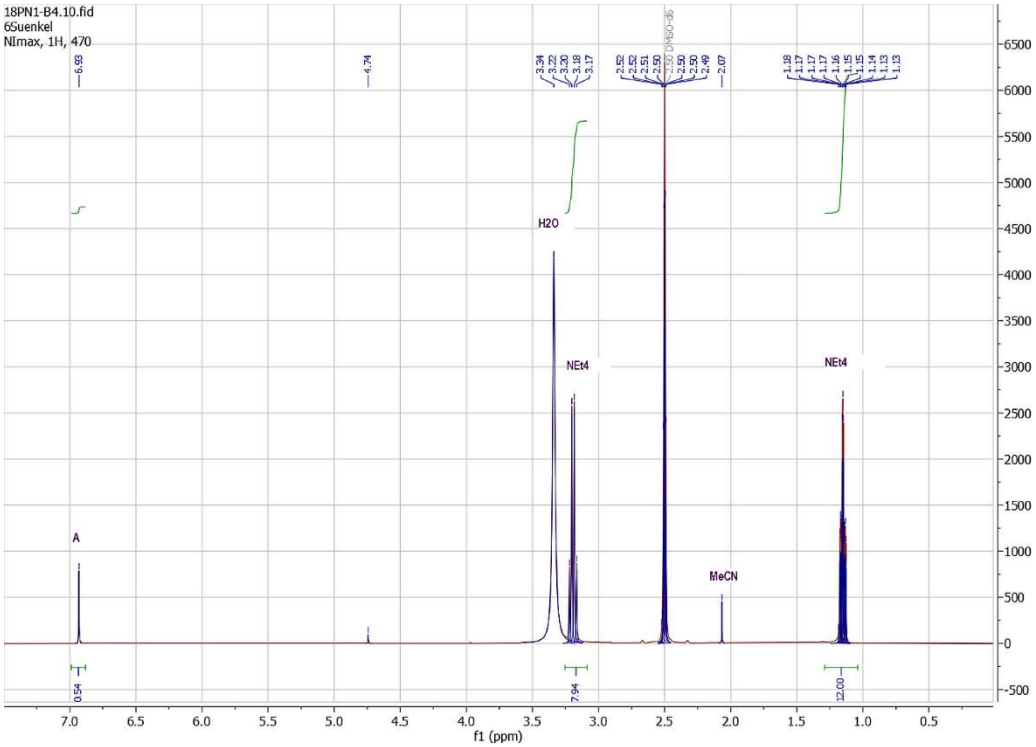

Figure S 1: ^{1}H-NMR (400 MHz, DMSO-d^{6}) of the crude reaction product of reaction 4.2.

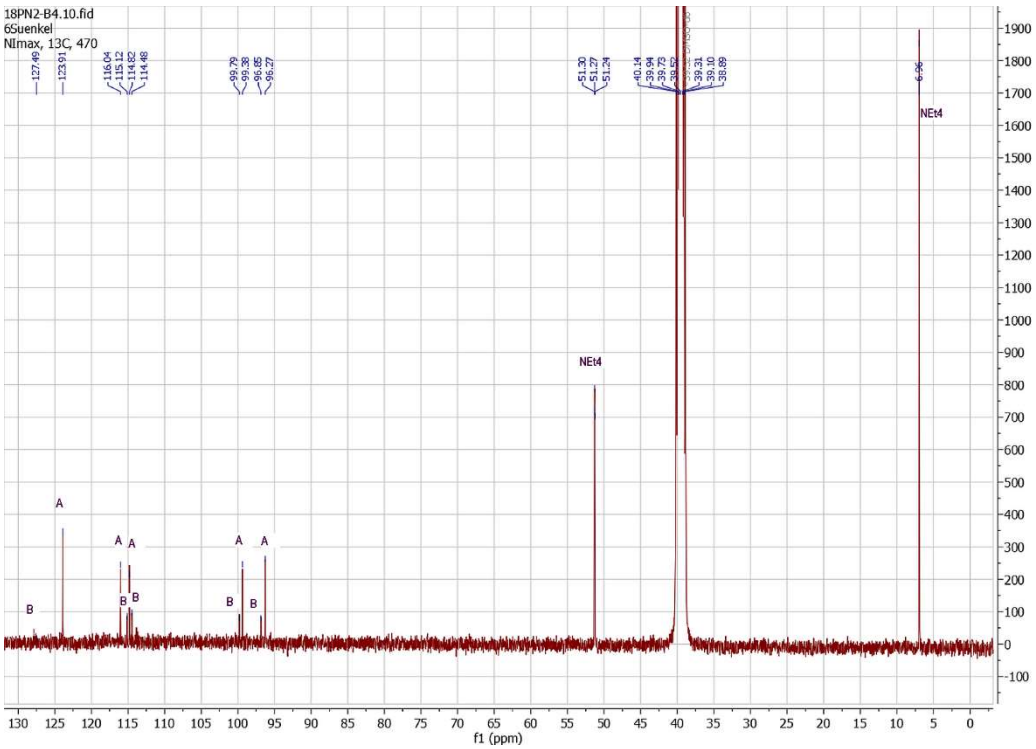

Figure S 2: ^{13}C{^{1}H}-NMR (101 MHz, DMSO-d^{6}) of the crude reaction product of reaction 4.2.

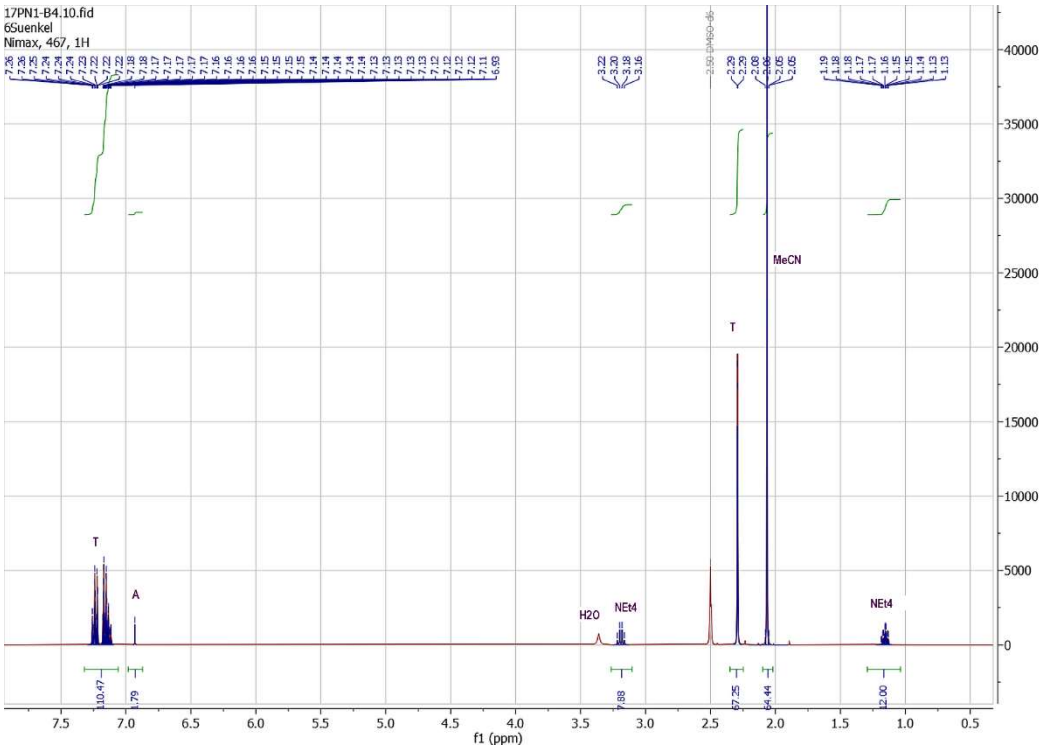

Figure S 3: ^{1}H-NMR (400 MHz, DMSO-d^{6}) of the crude reaction product of reaction 4.3. (T= toluene)

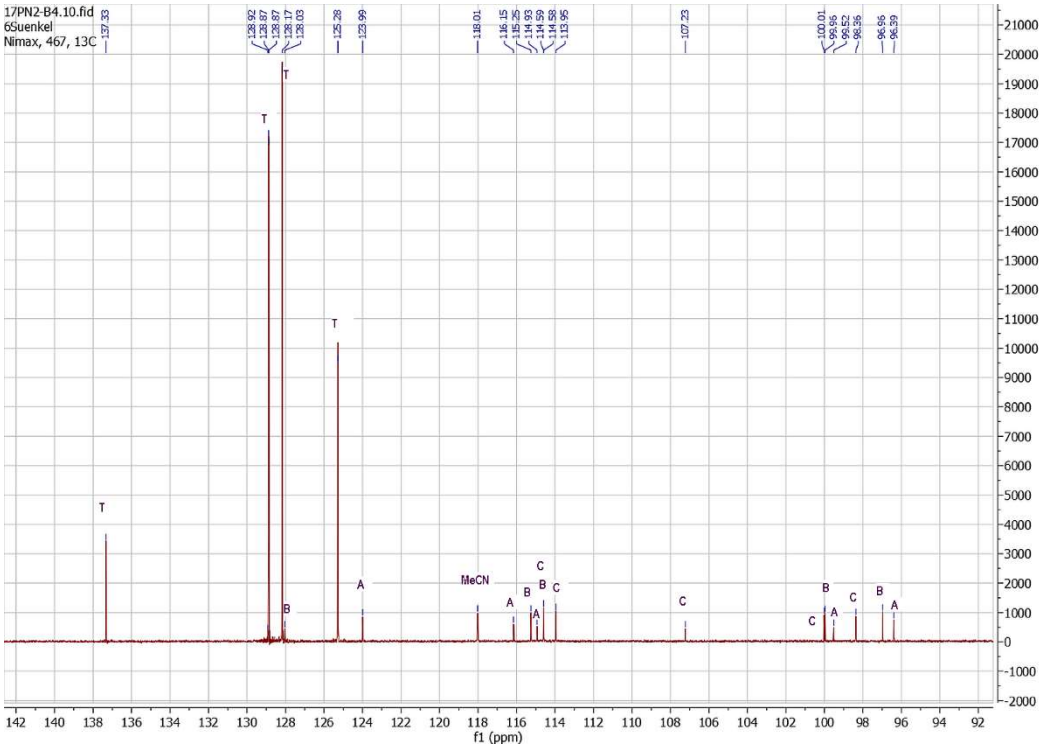

Figure S 4: ^{13}C{^{1}H}-NMR (101 MHz, DMSO-d^{6}) of the crude reaction product of reaction 4.3. (T=toluene)

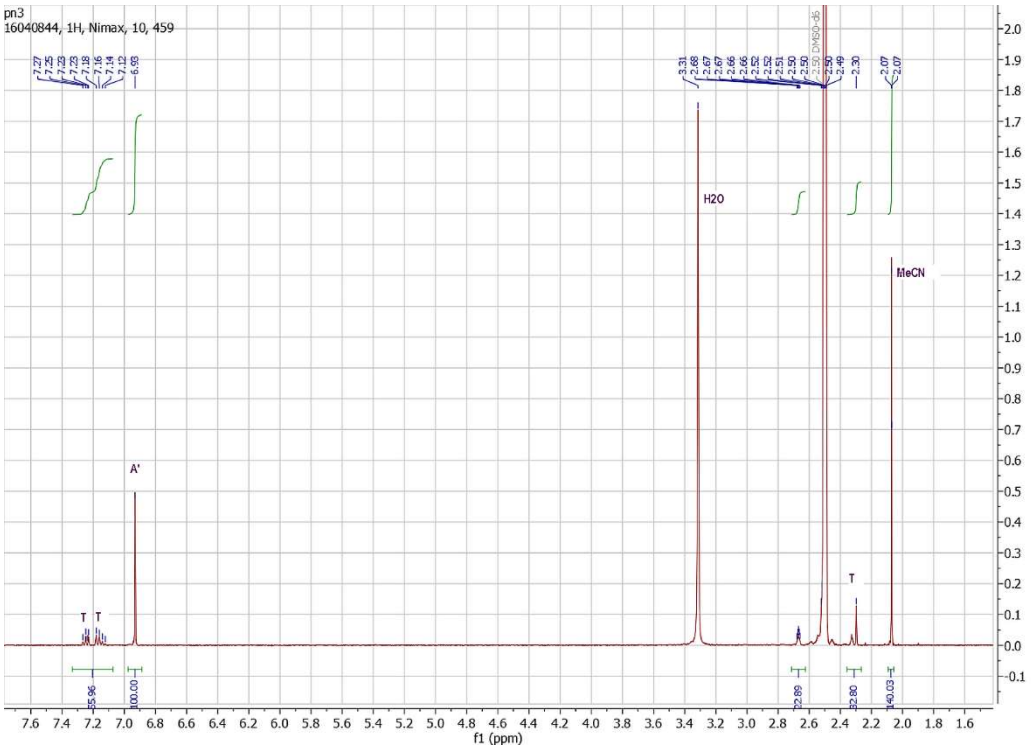

Figure S 5: ^{1}H-NMR (400 MHz, DMSO-d^{6}) of the first chromatography fraction of reaction 4.4. (T= toluene)

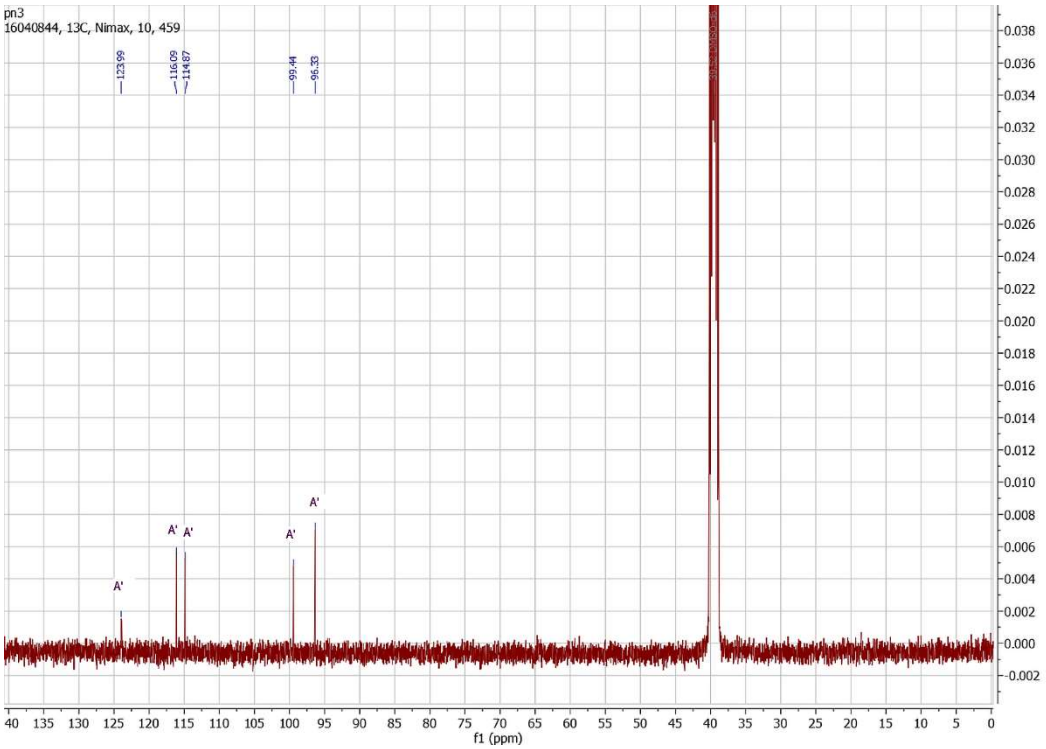

Figure S 6: ^{13}C{^{1}H}-NMR (101 MHz, DMSO-d^{6}) of the first chromatography fraction of reaction 4.4.

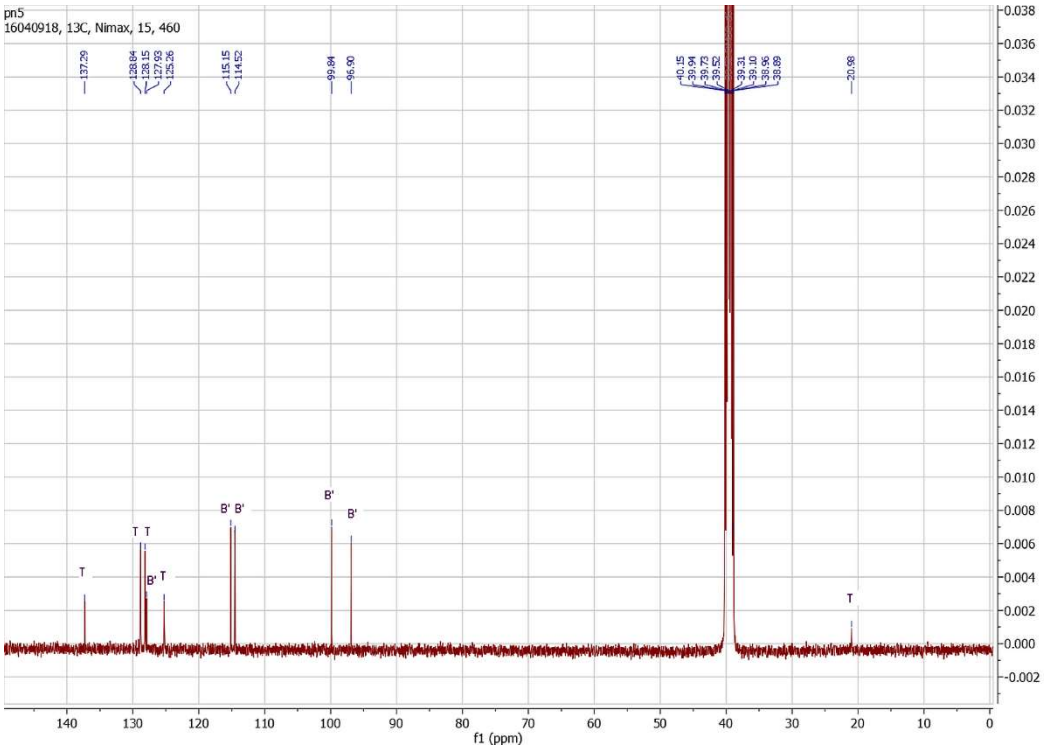

Figure S 7: $^{13}C\{^{1}H\}$-NMR (101 MHz, DMSO-d^6) of the second chromatography fraction of reaction 4.4 (T= toluene)

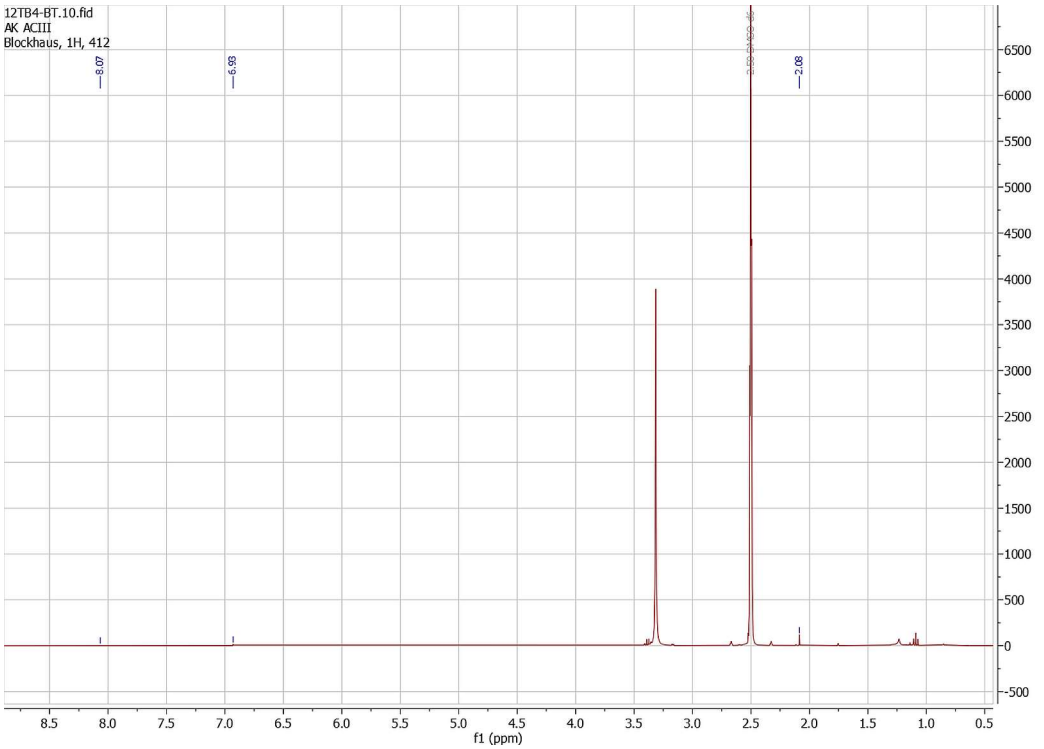

Figure S 8: ^{1}H-NMR (400 MHz, DMSO-d^6) of the purified product of reaction 4.6.

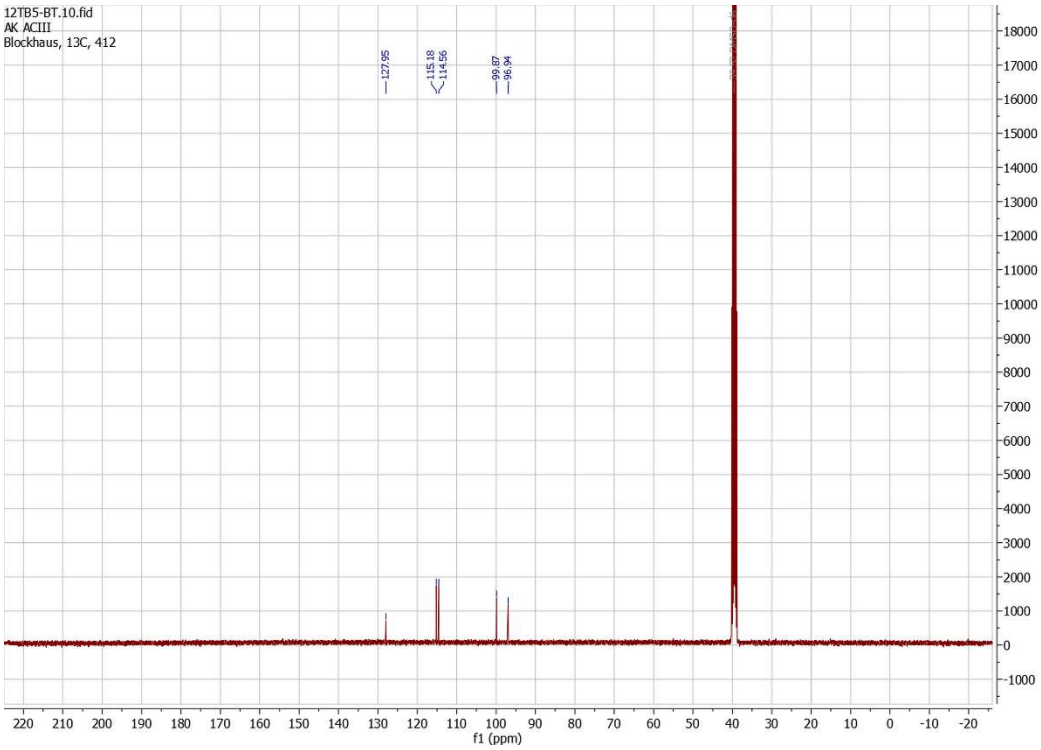

Figure S 9: $^{13}C\{^{1}H\}$-NMR spectrum (101 Mhz, DMSO-d^6) of the purified product of reaction 4.6.

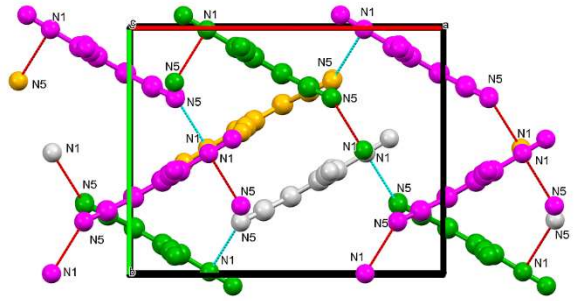

Figure S 10: The infinite 1D-chain in the structure of compound **1.** MERCURY plot, color "by symmetry operation", standard settings

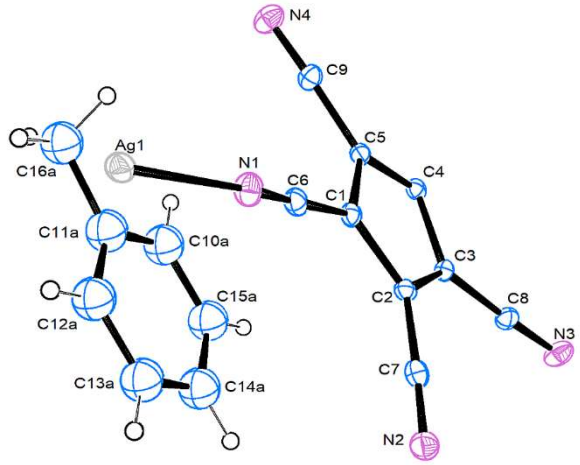

Figure S 11: ORTEP3 plot of the asymmetric unit of **4**, at r.t.

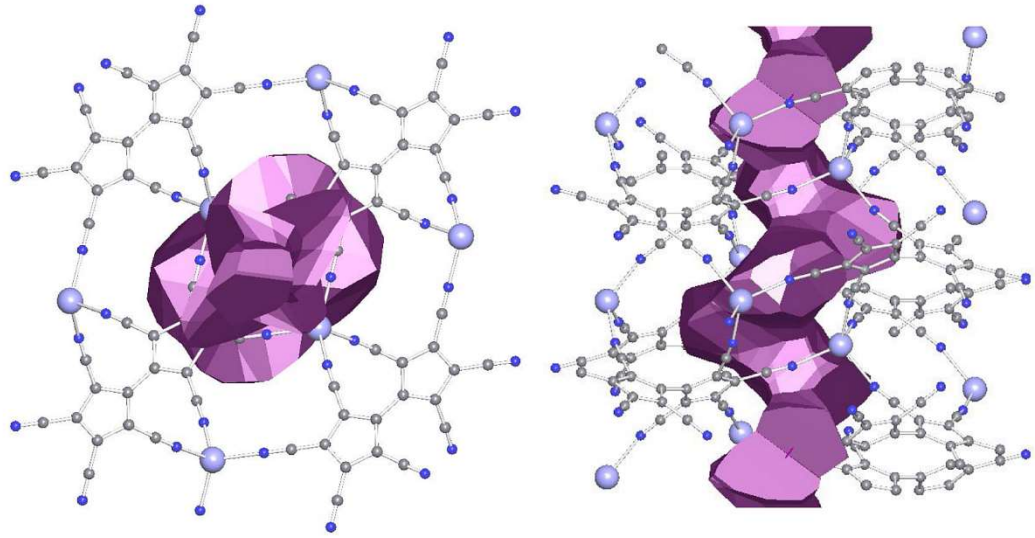

Figure S 12: Two views of the pore structure of **4**, generated by virtual removing the disordered toluenes.

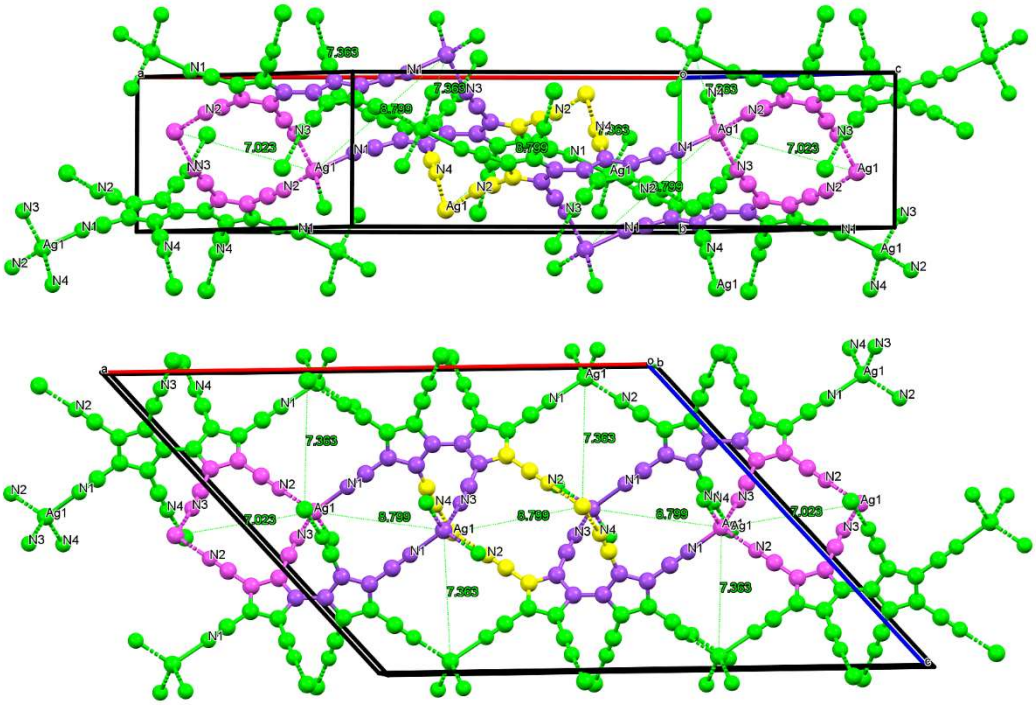

Figure S 13: Two packing views of compound **4**, showing the formation of 14-membered rings involving nitrile nitrogens N2 and N3 (lilac) and 20-membered rings involving N3 and N4 (lilac + purple) or N2 and N4 (yellow + purple), with Ag…Ag distances across the rings given.

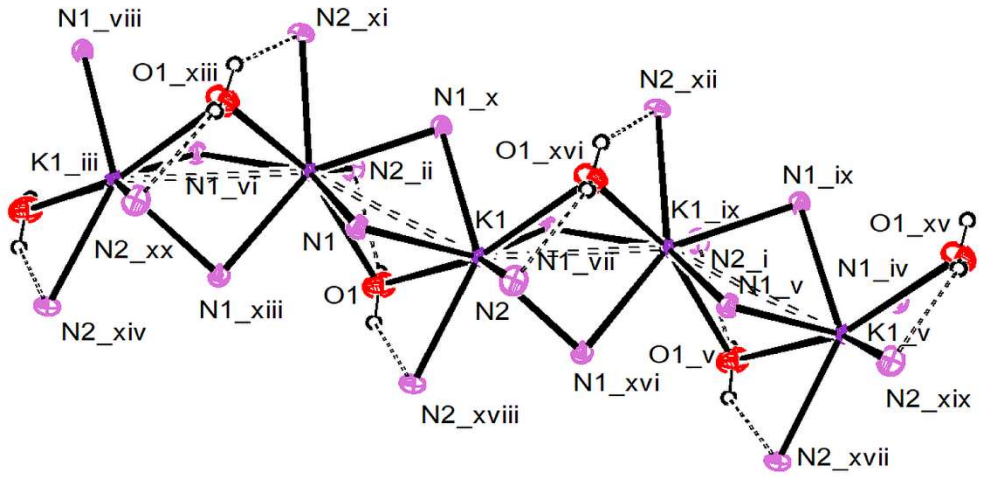

Figure S 14: ORTEP3 view of the zigzag chain of face-fused KN_4O_2 octahedra along the *x*-direction.

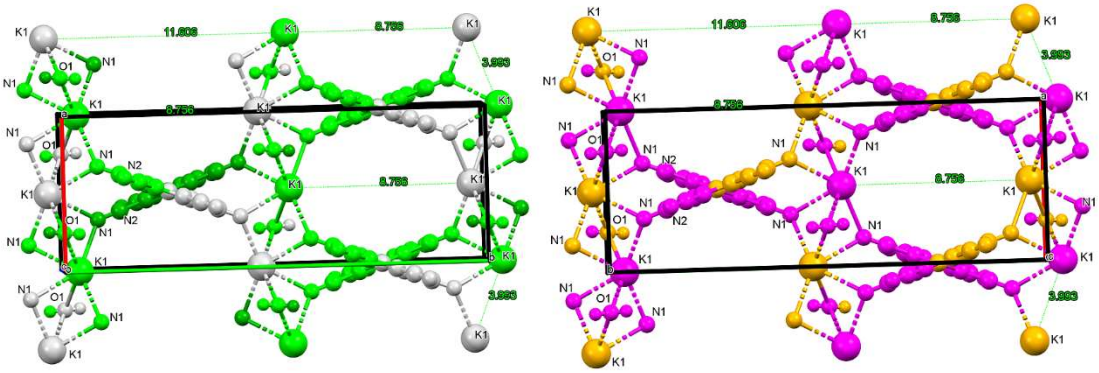

Figure S 15: Packing plots of compound **6** (MERCURY, watched along *c*) showing the two separated independent systems of zig-zag chains of octahedra of Figure 15, together with the K…K distances between them in *y* direction. Color coding as in Figure 15.

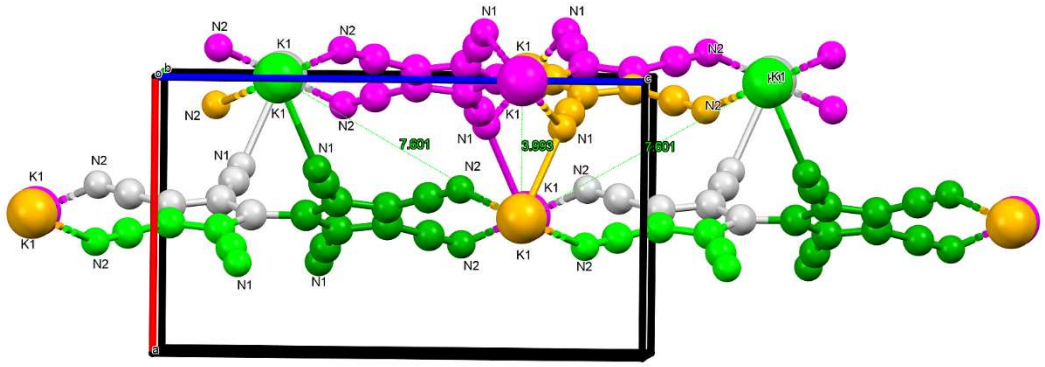

Figure S 16: Packing plot of compound **6** (MERCURY, watched along *b*) showing the connection of the octahedra chains in *z* direction via nitrile nitrogens N2.

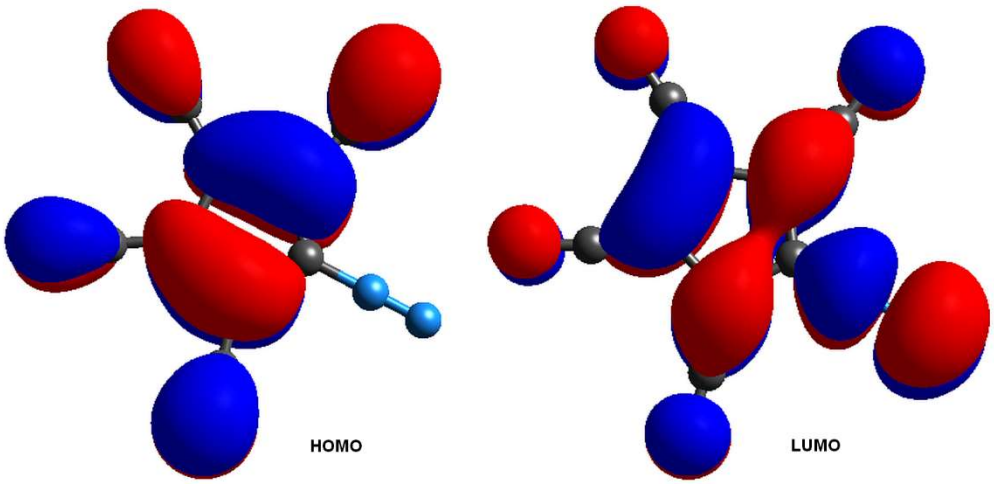

Figure S 17: HOMO and LUMO of compound **1**, as calculated with *CrystalExplorer*

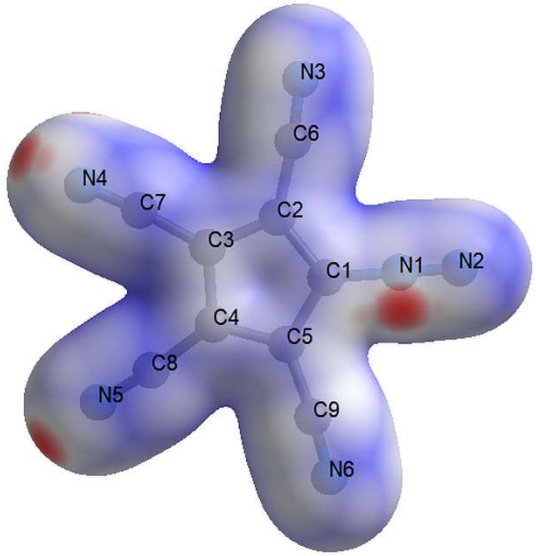

Figure S 18: Electron Density plot of compound **1 (**red patches correspond to positive charges)

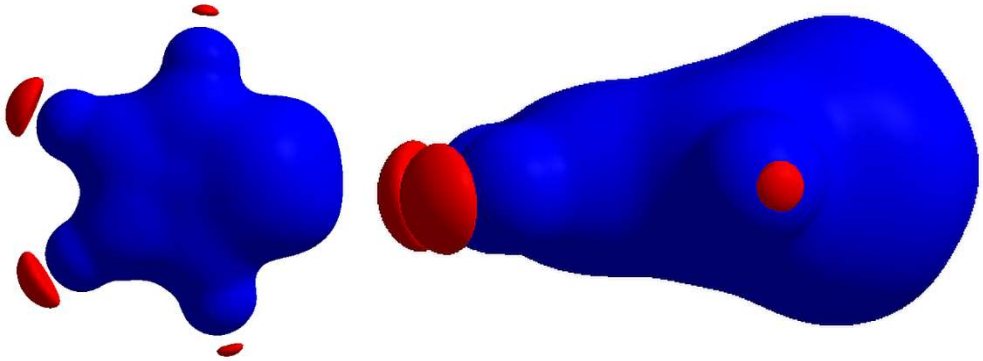

Figure S 19: Two views of the electrostatic potential distribution in compound **1**