Electronic Supplementary Material (ESI) for *CrystEngComm*

$[MeNC_5H_5]_2[TCNE]_2$ (TCNE = tetracyanoethylene). Single Crystal X-Ray and Neutron Diffraction Characterization of an Exceptionally Long 2.8 Å C-C Bond

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Supporting Information

Table S1. Intra $[TCNE]_2^{2-}$ bond distances (Å) and torsion angles (°) for $[Mepy]_2[TCNE]_2$ as determined by neutron diffraction at 50 K.

Table S2. Intermolecular contacts between methyl pyridine H and TCNE N atoms less than 3 Å for $[Mepy]_2[TCNE]_2$ as determined by neutron diffraction

Table S1. Intra $[TCNE]_2^{2-}$ bond distances (Å) and torsion angles (°) for $[Mepy]_2[TCNE]_2$ as determined by neutron diffraction at 50 K.

Atoms	Angle, °	Distance, Å
C2 – C2		3.157(5)
C4 – C4		3.126(5)
C2 – C4_2		2.801(4)
C2'-C4-C2-C1	96.70(25)	
C2'-C4-C2-C3	-96.72(26)	
C4'-C2-C4-C5	93.14(25)	
C4'-C4-C2-C6	-100.27(25)	

Table S2. Intermolecular contacts between methyl pyridine H and TCNE N atoms less than 3 Å for $[Mepy]_2[TCNE]_2$, as determined by neutron diffraction at 50 K.

Atoms	Distance	Atoms	Distance
H7 - N1	2.913(6)	H11 - N3	2.910(7)
H7 - N4	2.774(7)	H12a - N1	2.882(9)
H8 - N1	2.524(7)	H12a - N3	2.630(8)
H8 - N4	2.757(6)	H12b - N4	2.949(9)
H9 - N2	2.454(7)	H12c - N2	2.913(11)
H9 - N4	2.650(7)	H12c - N4	2.895(9)
H10 - N2	2.597(7)		