Electronic Supplementary Information for Dalton Transactions

Novel cyano-bridged mixed-valent copper complexes by the whole in situ synthetic method via the cleavage of C−C bond in acetonitrile

Feng Xu, Wei Huang, and Xiao-Zeng You

Electronic Supporting Information

Table ESI1. Intermolecular hydrogen bonding interactions (Å, °) in complexes **1-7**.

D−H···A	D−H	H−A	D···A	∠DHA	Sym. trans
1					
C4−H4···O5	0.93	2.41	3.313(8)	164.0	-1/2+x, 1/2-y, -1/2+z
C8−H8···O10	0.93	2.42	3.155(13)	136.0	-x, 1-y, -z
C28−H28···O4	0.93	2.51	3.361(10)	152.0	1/2+x, 1/2-y, 1/2+z
C33−H33···O7	0.93	2.54	3.263(9)	136.0	x, -y, -1/2+z
C41−H41···O1	0.93	2.56	3.289(8)	135.0	x, -y, 1/2+z
C45−H45···O12	0.93	2.49	3.112(14)	124.0	x, -y, -1/2+z
C50−H50···O8	0.93	2.39	3.171(9)	141.0	-x, y, 1/2-z
2					
C35−H35···O11	0.93	2.60	3.409(13)	146.0	-x, 2-y, 2-z
C40−H40···O11	0.93	2.48	3.299(14)	147.0	1-x, 2-y, 2-z
C49−H49···O10	0.93	2.42	3.308(15)	159.0	1-x, 1-y, 2-z
C50−H50···O12	0.93	2.59	3.336(14)	138.0	1-x, 1-y, 2-z
C52−H52···O9	0.93	2.51	3.242(13)	136.0	1+x, y, z
3					
C2−H2···F10	0.93	2.31	3.183(11)	156.0	1/2-x, 1/2-y, -z
C3−H3···F11	0.93	2.54	3.248(11)	133.0	1/2-x, 1/2-y, -z
C7−H7···F1	0.93	2.38	3.285(7)	165.0	-x, 1-y, -z
C20−H20···F6	0.93	2.52	3.269(7)	138.0	-1/2+x, 1/2-y, -1/2+z
C35−H35···F2	0.93	2.25	3.104(9)	152.0	-1/2+x, -1/2+y, z
C43−H43···F4	0.93	2.50	3.216(8)	134.0	1/2-x, 3/2-y, -z
C45−H45···F12	0.93	2.50	3.209(14)	133.0	1-x, y, 1/2-z
4					
O13−H13A···O6	0.95	2.58	3.138(15)	118.0	1+x, y, z
O13−H13A···O7	0.95	2.42	3.190(9)	139.0	1+x, y, z
C4−H4···O12	0.93	2.44	3.345(7)	163.0	1-x, 1-y, 1-z
C8−H8···O9	0.93	2.40	3.301(9)	163.0	x, -1+y, z
C12−H12···O4	0.93	2.57	3.263(12)	132.0	1+x, y, z

C17−H17···O8	0.93	2.50	3.431(9)	174.0	1-x, 1-y, -z
C18−H18···O13	0.93	2.55	3.317(10)	140.0	1-x, 1-y, -z
C24−H24···O6	0.93	2.57	3.254(10)	144.0	-x, 1-y, -z
C28−H28···O13	0.93	2.45	3.347(11)	161.0	1-x, 1-y, 1-z
C32−H32···O7	0.93	2.44	3.191(8)	138.0	x, 1+y, z
C33−H33···O4	0.93	2.56	3.319(11)	139.0	x, 1+y, z
C34−H34···O3	0.93	2.49	3.288(11)	144.0	x, 1+y, z
5					
C3−H3···O3	0.93	2.55	3.212(11)	128.0	2-x, 1-y, 1-z
C7−H7···O2	0.93	2.55	3.261(10)	133.0	2-x, -1/2+y, 1/2-z
C20−H20···O4	0.93	2.58	3.220(17)	127.0	x, 3/2-y, -1/2+z
6					
C18−H18A···O1	0.93	2.59	3.468(9)	157.0	2-x, 2-y, 2-z
C22−H22A···O9	0.93	2.44	3.176(10)	136.0	1+x, y, z
C52−H52A···O9	0.93	2.59	3.248(12)	128.0	1/2+x, 3/2-y, 1/2+z
7					
C5−H5···O2	0.93	2.47	3.38(2)	166.0	1-x, -y, 1-z
C10−H10···O4’	0.93	2.55	3.24(2)	132.0	1-x, 1-y, 1-z
C14−H14···O3	0.93	2.52	3.35(2)	149.0	-1+x, y, z
C35−H35···O2	0.93	2.49	3.31(3)	148.0	-1+x, y, z

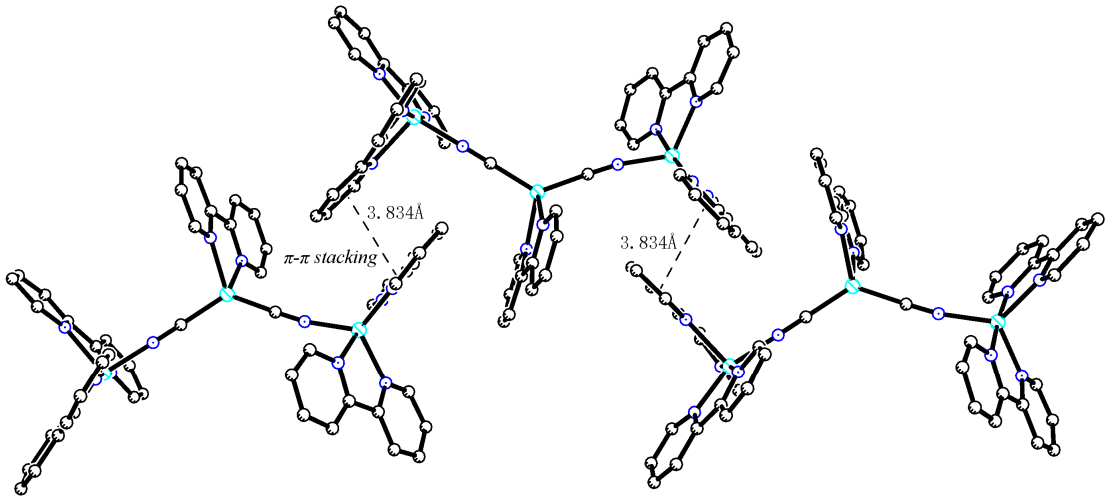

Fig. ESI1. View of the π-π stacking interactions in the crystal packing of **1** with labeling of the centroid-to-centroid distance. Hydrogen atoms and percholate anions are omitted for clarity.

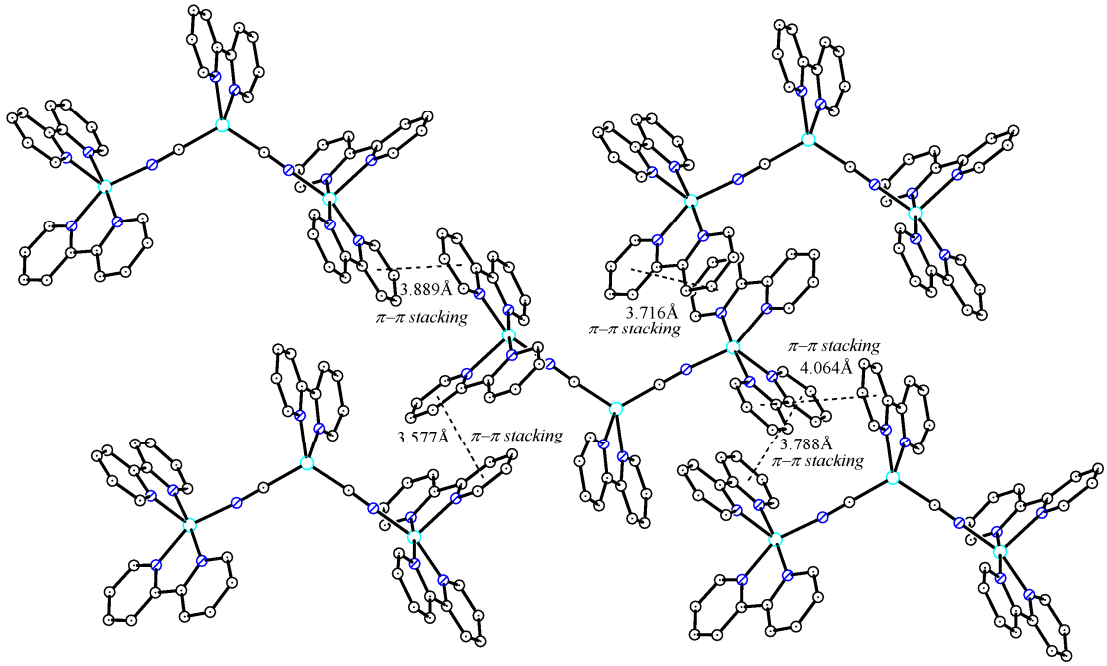

Fig. ESI2. View of the π-π stacking interactions in the crystal packing of **2** with labeling of the centroid-to-centroid distance. Hydrogen atoms and percholate anions are omitted for clarity.

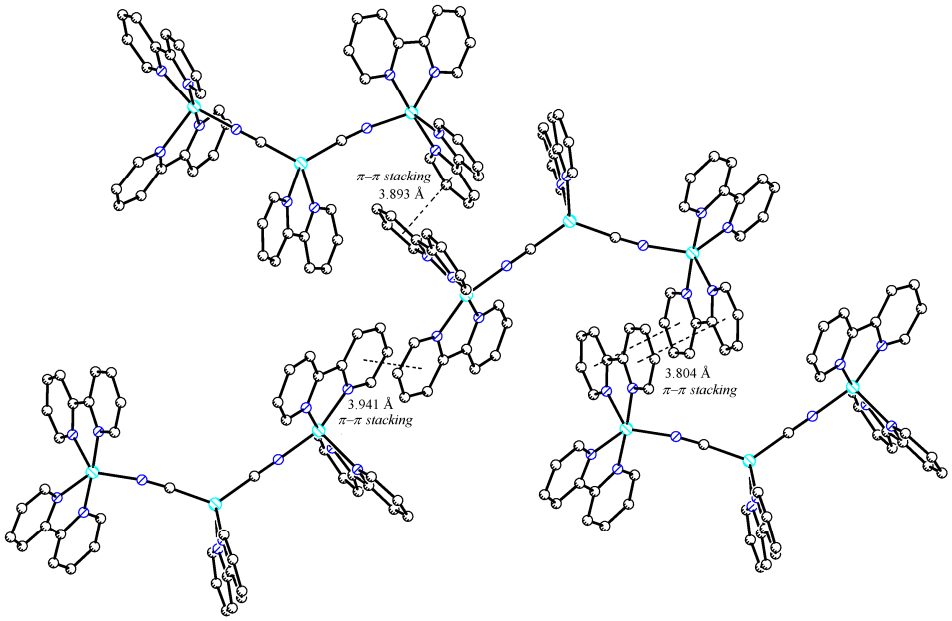

Fig. ESI3. View of the π-π stacking interactions in the crystal packing of **3** with labeling of the centroid-to-centroid distance. Hydrogen atoms and tetrafluoroborate anions are omitted for clarity.

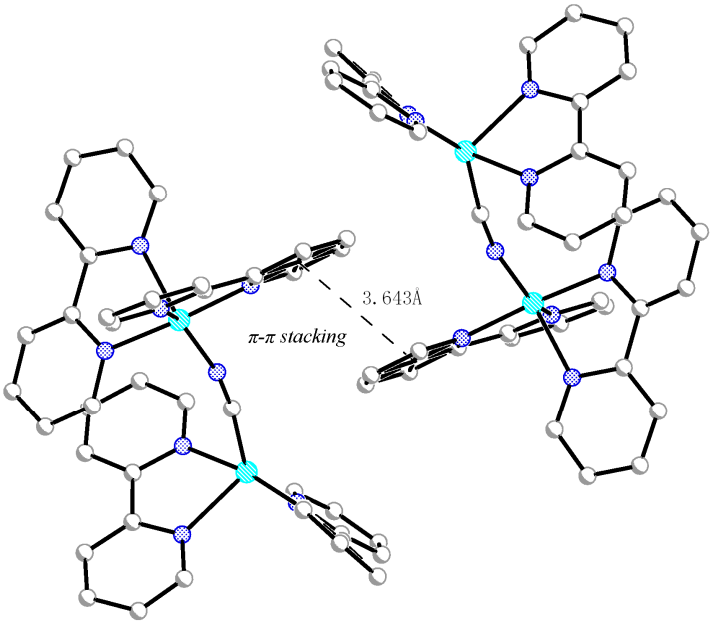

Fig. ESI4. View of the π-π stacking interactions in the crystal packing of **4** with labeling of the centroid-to-centroid distance. Hydrogen atoms, solvent molecules and percholate anions are omitted for clarity.

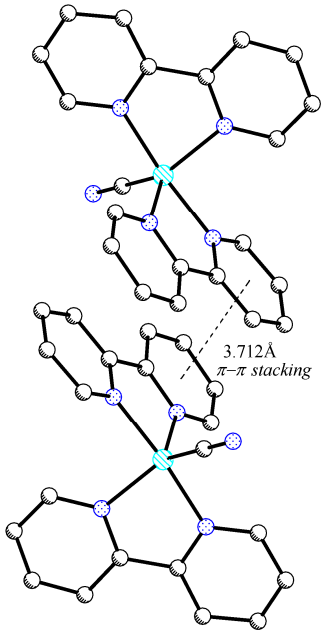

Fig. ESI5. View of the π-π stacking interactions in the crystal packing of **5** with labeling of the centroid-to-centroid distance. Hydrogen atoms, solvent molecules and percholate anions are omitted for clarity.

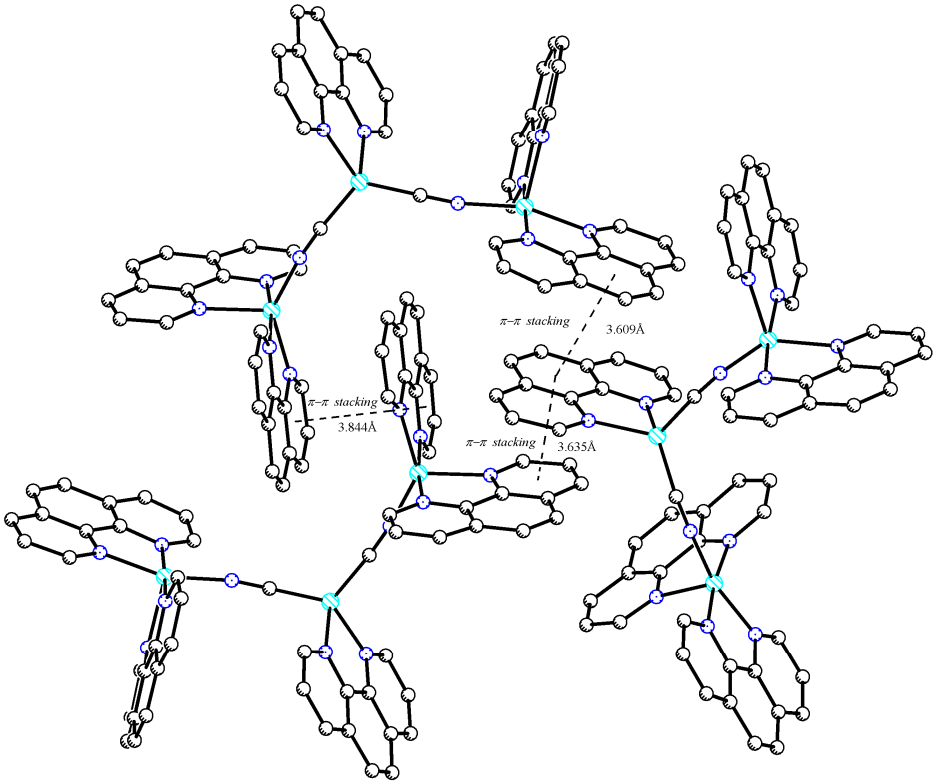

Fig. ESI6. View of the π-π stacking interactions in the crystal packing of **6** with labeling of the centroid-to-centroid distance. Hydrogen atoms, solvent molecules and percholate anions are omitted for clarity.

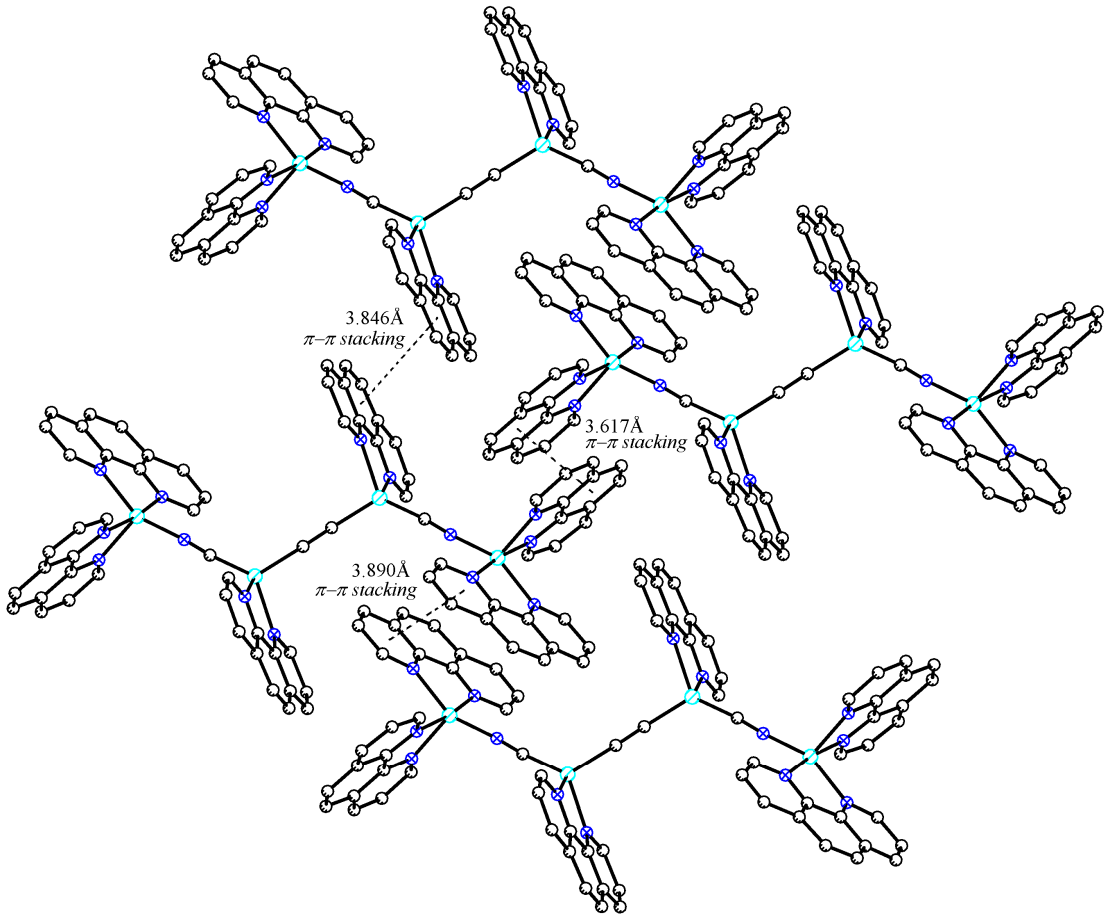

Fig. ESI7. View of the π-π stacking interactions in the crystal packing of **7** with labeling of the centroid-to-centroid distance. Hydrogen atoms, solvent molecules and percholate anions are omitted for clarity.