Table S1. Exponents ζ_i and valence shell ionization potentials H_{ii} of Slater-type orbitals χ_i used for extended Hückel tight-binding calculation [a]

atom	χ_i	H_{ii} (eV)	ζ_i	C [b]	ζ'_i	C′ [b]
Cu	4s	-7.40 [c]	2.151	1.0		
Cu	4p	-2.06 [c]	1.370	1.0		
Cu	3d	-10.0 [c]	7.025	0.4473	3.004	0.6968
O	2s	-32.3	2.688	0.7076	1.675	0.3745
O	2p	-14.8	3.694	0.3322	1.659	0.7448
N	2s	-26.0	2.261	0.7297	1.425	0.3455
N	2p	-13.4	3.249	0.2881	1.499	0.7783
C	2s	-21.4	1.831	0.7931	1.153	0.2739
C	2p	-11.4	2.73	0.2595	1.257	0.8026
H	1s	-13.6	1.30	1.0		

a H_{ii}'s are the diagonal matrix elements $\langle\chi_i|H^{eff}|\chi_i\rangle$, where H^{eff} is the effective Hamiltonian. In our calculations of the off-diagonal matrix elements $H^{eff} = \langle\chi_i|H^{eff}|\chi_j\rangle$, the weighted formula was used. See: Ammeter, J.; Bürgi, H.-B.; Thibeault, J.; Hoffmann, R., *J. Am. Chem. Soc*. **1978**, *100*, 3686.

b Contraction coefficients used in the double-zeta Slater-type orbital.

c These H_{ii} values, higher than the usual ones by 4.0 eV, were employed to ensure that the frontier orbitals of the compounds that contain both organic and inorganic ligands are d-block levels.