TCNQ family - 3D transport

Experiment and theory: Adv Mater 27, 2453 (2015); J Phys Chem Lett 8, 2875 (2017)



	TCNQ	F ₂ -TCNQ	F ₄ -TCNQ
n-type mobility (cm^2/Vs)	0.1	6	0.2
hopping amplitude (eV·Å)	0.45	0.94	0.22 (2D)
half bandwidth (eV)	0.13	0.18	0.07
effective mass (m_e)	0.8-6	0.4-2	2-6 (2D)
energies of other polymorphs			
TCNQ-like (meV/mol)	0	130*	202*
F_2 -TCNQ-like (meV/mol)	113	0	242*
F_4 -TCNQ-like (meV/mol)	344*	157	0

^{*} structures unstable with respect to symmetry breaking