

Table 1. Energy Band Calculations of Organic Conductors

Compounds	Calculation	Ref.
(TTF)(TCNQ)	Geometry dependence	1
	semimetallic	2
(TMTSF) ₂ X	Transfers for various anions	3
	open (Fig. 1)	4,5
β -phase		
β -(ET) ₂ I ₃	close (Fig. 2)	6,7
	open+semimetal (Xa)	8
(ET) ₂ SF ₅ CH ₂ CF ₂ SO ₃	open + close	49
(ET) ₂ BrO ₄	κ -like	9
(ET) ₂ ReO ₄	κ -like	9
(ET) ₄ Cu(C ₂ O ₄) ₂	Semimetal	10
(ET) ₅ Hg ₃ Br ₁₁	Transfers	11
(ET) ₃ Li _{0.5} Hg(SCN) ₄ (H ₂ O) ₂	β -like	12
β' -phase		
(ET) ₂ AuCl ₂	open (Fig. 3)	13
(ET) ₂ ICl ₂	open	14
(ET)(TCNQ)	close(ET)+open(TCNQ) (Fig. 4)	15
BETS salts		
λ -(BETS) ₂ GaCl ₄	κ -like	16
λ -(BETS) ₂ FeCl ₄	κ -like	16
β'' -phase		
(ET) ₂ Cl(DIA)	close	17
DIA: diiodoacetylene		
β'' -(ET) ₂ AuBr ₂	open+close (Fig. 5)	18
(ET) ₂ (ClO ₄)(TCE) _{0.5}	semimetal	19
(ET) ₂ Pd(CN) ₄	semimetal	20
(ET) ₂ Pt(CN) ₄	semimetal	21
(ET) ₂ Pd(CN) ₄ (H ₂ O)	semimetal (Fig. 6)	20
(ET) ₂ Pt(CN) ₄ (H ₂ O)	semimetal	21
(ET) ₃ Cl ₂ (H ₂ O) ₂	semimetal (Fig. 7)	22
β'' -phase BO salts		
(BO) ₂ Br(H ₂ O) ₃	close	23

$(BO)_2.4I_3$	close		39
$(BO)_{10}(CF)_4(H_2O)_3$	close	(Fig. 8)	39
$(BO)_3Cu_2(NCS)_3$	close		39
$(BO)_2AuBr_2$	close		39
$(BO)_2ClO_4$	close + open		39
$(BO)_2ReO_4H_2O$	semimetal	(Fig. 9)	39,41
$(BO)_5(HCTMM)(PhCN)_2$	close		39
$(BO)_4(SQR)(H_2O)_6$	semimetal		39
θ -Phase			
$(ET)_2Cu_2(CN)[N(CN)_2]_2$	close		24
$(ET)Cd_{0.66}(SCN)_2$	close		25
$(ET)_2TiZn(SCN)_4$	close		26
$(ET)_2TiCo(SCN)_4$	close		26
$(ET)_2RbZn(SCN)_4$	close		25
$(ET)_2RbCo(SCN)_4$	close		25
$(ET)_2CsZn(SCN)_4$	close	(Fig. 10)	27
$(ET)_2CsCo(SCN)_4$	close		27
$\theta-(ET)_2I_3$	close		28
$(BO)_2Cl(H_2O)_x$	close		29
$\alpha-(ET)_2I_3$	semimetal		6,30
$(ET)_2KHg(SCN)_4$	close + open	(Fig. 11)	31
$(ET)_2NH_4Hg(SCN)_4$	close + open		32
$(ET)_2RbHg(SCN)_4$	close + open		33
$(ET)_2KHg(SeCN)_4$	close + open		34
$(ET)_2TIHg(SeCN)_4$	close + open		34
$(BETS)_2Cu_2Cl_6$	close + open		35
$\alpha-(ET)_4Ni(CN)_4$	close + open		36
α'' -Phase			
$(ET)_2KCu(SCN)_4$	open		37
$(ET)_2Cu_5I_6$	open		38
$(ET)_2CsHg(SCN)_4$	open	(Fig. 12)	12
$(ET)_2K_{1.4}Co(SCN)_4$	open		25
$(BO)_5(HCP)(PhCN)_{0.2^a}$	open		39
$(BO)_6(HCDAH)^b$	open		40
κ -Phase			

κ -(ET) ₂ Cu(CN) ₃	κ -type		42,46,50
κ -(ET) ₂ Cu(NCS) ₂	κ -type	(Fig. 13)	43,44
(ET) ₂ Cu(CF ₃) ₄ (TCE)	κ -type		45
κ -(ET) ₂ Cu[N(CN) ₂]Br	κ -type		46
κ -(ET) ₂ I ₃	κ -type		46,47
κ -(ET) ₂ Cu(CN)[N(CN) ₂]	κ -type		46
κ -(ET) ₂ Ag(CN) ₂ H ₂ O	κ -type		48
(BO) ₂ CF ₃ SO ₃	κ -type		51
(BETS) ₂ Cu[N(CN) ₂]Br	κ -type		52
(MDT-TTF) ₂ AuI ₂	κ -type		44
(MT) ₂ Au(CN) ₂	κ -type		44
δ -phase			
β -(ET) ₂ PF ₆	open(transverse)		53
β -(ET) ₂ AsF ₆	open(transverse)		53
δ -(ET) ₂ Ni(CN) ₄ (H ₂ O) ₄	open(transverse)		36
(ET) ₂ Br(H ₂ O) ₃	κ -like		54
δ -(ET) ₂ AuBr ₂	open(transverse)	(Fig. 14)	55
δ -(ET) ₂ AuI ₂	open(stack)		56,57
α' -Phases			
α' -(ET) ₂ Ag(CN) ₂	open(stack)		58
α' -(ET) ₂ Au(CN) ₂	open(stack)		58
α' -(ET) ₂ AuBr ₂	open(stack)		58
γ' -(ET) ₂ AuI ₂	open(stack)		59
