BEDT-TTF and BETS Salts

The following tables are a compilation of BEDT-TTF (ET) and BETS salts. We confine ourselves to the salts whose crystal structures have been determined. The entries are arranged in two different ways.

Method A In the order of the central atoms of the anions according to the periodic table.

Table 1 ET salts in the order of the central atoms of the anions
Table 2 BETS salts in the order of the central atoms of the anions

Here the periodic table is scanned from the upper right (starting from Cl) to the lower left. If the definition of the central atom is obscure, we adopted the heavier atoms, for example, Se in Cl_2SeCN. Salts with organic anions and acceptors are located at the end of the table. In the column of the conductivity, "I" stands for an insulator even at room temperature, and "M" means a metal down to helium temperatures. The classification of the structure, particularly subscript system in β and β" phases, follows the description in Refs. I - III. In some cases the reported information is not enough to specify the structure type, in which the column of the structure is empty. Other cases where the structures are not specified are some complicated structures.

Method B Lists according to the structures with lattice parameters.

Table 3 β-phase ET and BETS salts
Table 4 β"-phase ET and BETS salts
Table 5 θ-phase ET and BETS salts
Table 6 α-phase ET and BETS salts
Table 7 Multiple θ-phase ET and BETS salts
Table 8 α"-phase ET and BETS salts
Table 9 κ-phase ET and BETS salts
Table 10 δ- and α'-phase ET and BETS salts

In principle each table is arranged in the order of axis ratio, for demonstrating the systematic change of the physical properties. The salts whose structures are not specified in Tables 1 and 2 or designated as "Mixed" do not appear in these tables.

The articles are searched up to 1998, including Chemical Abstracts Vol. 128, and International Conference of Synthetic Metals, 1998, Montpelier.

[I] T. Mori, *Bull. Chem. Soc. Jpn.*, **71**, 2509 (1998).
[II] T. Mori, H. Mori, and S. Tanaka, *Bull. Chem. Soc. Jpn.*, **72** (1999).
[III] T. Mori, *Bull. Chem. Soc. Jpn.*, **72**, 2011 (1999).

(by Takehiko MORI, Tokyo Institute of Technology, January 2000)

Table 1 ET Salts in the Order of the Central Atoms of the Anions

Compound	Conductivity	Structure	Ref.
$(ET)_2Cl(H_2O)_2$	T_{MI}=20K	143	
$(ET)_2Cl(H_2O)_3$	T_{MI}=120K	δ-type	123
$(ET)_3Cl_2(H_2O)_2$	T_{MI}=100K T_{SC}=2K(16kbar)	β''_{321x2}	51
$(ET)_3Cl_{2.5}(H_5O_2)$	T_{MI}=170K	β''_{321}	39
$(ET)_2ClO_4(TCE)_{0.5}$	M	β''_{41242}	
$(ET)_2ClO_4$(Dioxane)	I($10^{-2}Scm^{-1}$)	δ-type	135
$(ET)_3(ClO_4)_2$	T_{MI}=170K	β''_{311}	35
$(ET)(ClO_4)_2$	I		180
$(ET)_2Br(H_2O)_3$	T_{MI}=150K	δ-type	122
$(ET)_3Br_2(H_2O)_2$	T_{MI}=185K	β''_{311}	37
(ET)Br	I	Dimer	36
$(ET)_2Br[C_2H_4(OH)_2]$	T_{MI}=200K	δ'-type	131
$(ET)_2BrO_4$	T_{MI}=150K	β_{21x2}	8
$(ET)_2BrO_4(TCE)_{0.5}$	M	β''_{412}	36
$(ET)_3(BrO_4)_2$	T_{MI}=210K	β''_{311}	36
α-$(ET)_2I_3$	T_{MI}=135K	α-type	68
β-$(ET)_2I_3$	T_{SC}=1.5K T_{SC}=8K(0.3kbar)	β_{21}	2
γ-$(ET)_3(I_3)_{2.5}$	T_{SC}=2.5K	Mixed	145
δ-(ET).$I_3(TCE)_{0.33}$	T_{MI}=130K	Mixed	146
ε-$(ET)_2I_3(I_8)$0.5	I	Mixed	147
ζ-$(ET)_2I_2I_8$	I	Mixed	148
η-(ET).I_3	I($10^{-4}Scm^{-1}$)	Dimer	149
θ-$(ET)_2I_3$	T_{SC}=3.6K	θ-type	62
κ-$(ET)_2I_3$	T_{SC}=3.6K	κ-type	99
λ-$(ET)_2I_3I_5$	I	ε-like	150
β'-$(ET)_2ICl_2$	I($0.03Scm^{-1}$)	β'-type	19
β''-$(ET)_2ICl_2$	M	β''_{211}	28
α-$(ET)_2I_2Br$	T_{MI}=265K	α-type	72
β-$(ET)_2I_2Br$	M	β_{21}	4
α'-$(ET)_2IBr_2$	I($1Scm^{-1}$)	α-type	70
β-$(ET)_2IBr_2$	T_{SC}=2.5K	β_{21}	5
$(ET)_2IBr_2(TCE)_{0.5}$	I($10^{-3}Scm^{-1}$)	ε-I_3like	151
α'-$(ET)_2ICl$Br	I	α-type	69
β'-$(ET)_2ICl$Br	I	β'-type	20
$(ET)IO_4(THF)_{0.5}$	I($10^{-5}Scm^{-1}$)	Dimer	152

$(ET)_3(IO_4)_2$	I	β"321?	40
$(ET)_3(HSO_4)_2$		β"311	33
$(ET)_3(FSO_3)_2$		β"311	33
$(ET)_2CF_3SO_3$	I	δ-type	116
κ-$(ET)_2CF_3SO_3$	I	κ-type	103
$(ET)_2SF_5CH_2CF_2SO_3$	T_{SC}=5.2K	β"211x2	31
$(ET)_2[N(SO_2CF_3)_2]$		β"210	27
$(ET)_2Cl_2SeCN$	T_{MI}=200K	β"211	30
$(ET)_2Br_2SeCN$	T_{MI}=200K	β"211	30
$(ET)4TeCl_6(BN)$	I	$=PtCl_6$	153
α-$(ET)_3(NO_3)_2$	T_{MI}=20K	β"312	38
α-$(ET)_2PF_6$	I(1Scm^{-1})	β_{21}	7
β-$(ET)_2PF_6$	T_{MI}=297K	δ-type	114
γ-$(ET)_2PF_6$	I(1Scm^{-1})		154
$(ET)PF_6$	I(10-3"Scm^{-1})		155
$(ET)_2PF_6(THF)$		α'-type	134
δ-$(ET)PF_6$		Dimer	181
ε-$(ET)PF_6$			182
$(ET)PF6(C_2H_2Cl_2)_{0.5}$		Dimer	183
$(ET)_2AsF_6$	T_{MI}=264K	δ-type	117
$(ET)_2SbF_6$	T_{MI}=273K	δ-type	117
$(ET)BiI_4$		Dimer	156
$(ET)_4SnCl_6(BN)$	I	$=PtCl_6$	153
$(ET)_6Pb_3Br_9PhCl(Acetone)$	T_{MI}=160K	β"-like	185
$(ET)(BF_4)_2$	I		186
$(ET)_2BF_4(TCE)_{0.5}$	M	β"412	157
$(ET)_2BF_4(CH_3CN)$			158
$(ET)_3(BF_4)_2$	T_{MI}=150K	β"311	34
$(ET)_2GaCl_4$	I(0.1Scm^{-1})	δ'-type	128
$(ET)_2GaI_4$	I(10-5Scm^{-1})	δ'-type	12
$(ET)_2InBr_4$	I	β_{42}	11
$(ET)_2InI_4$		δ'-type	12
$(ET)_2I_3TlI_4$	I(0.01Scm^{-1})	Mixed	132
$(ET)_4ZnCl_4(BN)$	T_{MI}=120K		159
$(ET)_3(ZnCl_4)_2$	I(0.4Scm^{-1})	$=MnCl_4$	160
$(ET)Zn(SCN)_3$	I(0.006Scm^{-1})	Mixed	55
$(ET)_2TlZn(SCN)_4$	T_{MI}=250K	θ-type	56
$(ET)_2CsZn(SCN)_4$	T_{MI}=20K	θ-type	55
$(ET)_2RbZn(SCN)_4$	T_{MI}=190K	θ-type	55
$(ET)Cd_{0.66}(SCN)_2$	I(4Scm^{-1})	θ-type	55
$(ET)_4Cd_2I_6$		β"412	44

$(ET)_2Cd_3I_6$		θ-type?	44
$(ET)_4Hg_{2.78}Cl_8$	T_{SC}=1.8K(12kbar)	κ-type	107
$(ET)_4Hg_2Cl_6$(CB)	M	β"41?x2	54
$(ET)_3(HgCl_3)_2$	I(10^{-2}Scm^{-1})	δ-like	142
$(ET)_4Hg_{2.89}Br_8$	T_{SC}=4.3K	κ-type	106
$(ET)_4Hg_2Br_6$(CB)	T_{MI}=90K	β"41?x2	54
$(ET)_4Hg_2Br_6$(TCE)		δ'-type	129
$(ET)_3(HgBr_3)_2$	I	$\beta"_{321}$	56
$(ET)_2HgBr_4$(TCE)	I		161
$(ET)_5Hg_3Br_{11}$	T_{MI}=120K	β_{75}	14
$(ET)HgBr_3$	I(10^{-4}Scm)	Dimer	14
$(ET)_4Hg_3I_8$	I(3Scm^{-1})		40
$(ET)_2HgI_3$	I		40
$(ET)_2Hg_2I_5$	I(1.6Scm^{-1})		40
$(ET).Hg_{0.766}(SCN)_2$	I		161
$(ET)_3Li_{0.5}Hg(SCN)_4(H_2O)_2$	T_{MI}=170K	$\beta_{12,6}$	17
$(ET)_2KHg(SCN)_4$	M	α-type	67
$(ET)_2RbHg(SCN)4$	M	α-type	74
$(ET)_2NH_4Hg(SCN)_4$	T_{SC}=0.8K	α-type	67
$(ET)_2TlHg(SCN)_4$	M	α-type	73
$(ET)_2TlHg(SeCN)_4$	M	α-type	73
$(ET)_2KHg(SeCN)_4$	M	α-type	75
$(ET)_2CsHg(SCN)_4$	T_{MI}=210K	α"-type	89
$(ET)_2Hg(SCN)_2Cl$	T_{MI}=50K	κ-type	101
$(ET)_2Hg(SCN)Cl_2$	T_{MI}=35K	κ-type	101
$(ET)_2Hg(SCN)_2Br$	T_{MI}=140K	κ-type	104
$(ET)_2Hg(SCN)_2I$	T_{MI}=50K	κ-type	102
$(ET)_4Hg_2I_{14}$		Mixed	187
α'-$(ET)_2CuCl_2$	I($4x10^{-2}$Scm^{-1})	α'-type	136
$(ET)_3CuCl_4H_2O$	M		162
$(ET)CuCl_2$		β_{11}	1
$(ET)_2CuCl_2$	I(10-4Scm^{-1})	α'-type	136
$(ET)_3CuBr_4$	I(0.6Scm^{-1})	θ_{31}	79
$(ET)_3CuCl_2Br_2$	I(0.7Scm^{-1})	$=CuBr_4$	163
$(ET)_2Cu_5I_6$	M	α"-type	87
α-$(ET)_2Cu(SCN)_2$	T_{MI}=200K	α	71
κ-$(ET)_2Cu(NCS)_2$	T_{SC}=10.4K	κ-type	95
$(ET)Cu_2(SCN)_3$	I(2x10-5Scm^{-1})	Dimer	60
κ-$(ET)_2$Cu[N(CN)2]Cl	T_{SC}=12.5K(0.3kbar)	κ-type	91
κ-$(ET)_2$Cu[N(CN)2]Br	T_{SC}=11.6K	κ-type	98
κ-$(ET)_2Cu[N(CN)_2]I$	M	κ-type	92

κ-$(ET)_2Cu(CN)[N(CN)_2]$	T_{SC}=10.7K	κ-type	94
κ-$(ET)_2Cu_2(CN)_3$	T_{SC}=3.8K	κ-type	94
κ-$(ET)_2Cu(CF_3)_4(TCE)$	T_{SC}=9.2K	κ-type	96
$(ET)_2Cu(CN)[N(CN)_2]$		θ-type	63
$(ET)_4[C(CN)_2CONH_2]CuCl_2$		θ-type	63
$(ET)_4[C(CN)_2CONH_2]CuBr_2$		θ-type	63
$(ET)_5[CuHg(SCN)_4]_2$	T_{MI}=180K	$\beta_{10,?}$	15
$(ET)Cu_3I_4$			188
$(ET)Ag_{2.4}Br_3$		θ-type	58
$(ET)_3Ag_{6.4}I_8$	T_{MI}=60K	θ^{21}-type	90
α'-$(ET)_2Ag(CN)_2$	I	α'-type	137
κ-$(ET)_2Ag(CN)_2H_2O$	T_{SC}=5K	κ-type	100
θ-$(ET)_2Ag(CN)_2$(orth.)	M	θ-type	61
α-$(ET)_2Ag(CN)_2$(monocli.)	?	θ-type	61
$(ET)Ag_4(CN)_5$	T_{MI}=100K		164
$(ET)Ag_{1.6}(SCN)_2$	I(0.013Scm^{-1})	θ-type	60
κ-$(ET)_2Ag(CF_3)_4(TCE)$	T_{SC}=11.1K	κ-type	96
β'-$(ET)_2AuCl_2$	I(0.1Scm^{-1})	β'	18
$(ET)AuCl_2$	I(0.01Scm^{-1})	Mixed	18
$(ET)AuCl_2AuCl_4$	I(0.25Scm^{-1})	Mixed	165
β-$(ET)_2AuCl_4$		$\beta\,\bar{2}1$	6
α'-$(ET)_2AuBr_2$	I	α'-type	137
β''-$(ET)_2AuBr_2$	M	β''_{211}	26
δ-$(ET)_2AuBr_2$	I	δ-type	125
$(ET)_2AuBr_2AuBr_4$	I		166
$(ET)AuBr_2Cl_2$	I		167
β-$(ET)_2AuI_2$	T_{SC}=3.8K	β_{21}	3
γ'-$(ET)_2AuI_2$	I	δ-like	141
δ-$(ET)_2AuI_2$	I	δ	125
α'-$(ET)_2Au(CN)_2$	I	α'-type	137
η-$(ET)_2Au(CN)_2$		α-like	168
$(ET)_2Au(CN)_2Cl_2$	T_{MI}=250K	δ-type	115
α'-$(ET)_2AuBrI$	I(1.5x$10^{-4}Scm^{-1}$)	α-type	169
β''-$(ET)_2AuBrI$	M	β''_{211}	29
κ-$(ET)_2Au(CF_3)_4(TCE)$	T_{SC}=10.5K	κ-type	97
$(ET)_3NiCl_4H_2O$	M	β"3?x2	52
$(ET)_4Ni(CN)_4$	T_{MI}=230K	β''_{411}	45,46
$(ET)_4Ni(CN)_4$	I	θ_{42+40}	84
$(ET)_2Ni(CN)_4(H_2O)_4$	T_{MI}=180K	δ-type	121
$(ET)[Ni(mnt)_2]$	I($10^{-6}Scm^{-1}$)	Mixed	170
$(ET)[Ni(dmit)_2]$	I(0.002Scm^{-1})	Mixed(β'')	171

$(ET)_2Pd(CN)_4$	T_{MI}=250K	β"411	47
$(ET)_2Pd(CN)_4H_2O$	T_{SC}=1.2K(7kbar)	β"421	47
$(ET)[Pd(mnt)_2]_x$	I(10^{-3}Scm^{-1})		170
$(ET)_4PtCl_6(BN)$	I(10Scm^{-1})	κ-like	153
$(ET)_4PtBr_6(BN)$	I(1Scm^{-1})	=$PtCl_6$	153
$(ET)_4Pt(CN)_4$	T_{MI}=250K	β"411	45,51
$(ET)_4Pt(CN)_4$	I(5Scm^{-1})	θ_{42+40}	84
$(ET)_2Pt(CN)_4H_2O$	T_{SC}=2K(6.5kbar)	β"421	49
$(ET)_2Pt(CN)_4(H_2O)_4$	T_{MI}=150K	δ-type	121
$(ET)_4Pt(CN)_4(TCE)$	I		160
$(ET)[Pt(mnt)_2]_x$	I(10^{-6}Scm^{-1})		170
$(ET)_4[Pt(C_2O_4)_2]$	T_{MI}=60K		172
$(ET)_2K_{1.4}Co(SCN)_4$	T_{MI}=130K	α"-type	56
$(ET)_2TlCo(SCN)_4$	T_{MI}=250K	θ-type	57
$(ET)_2RbCo(SCN)_4$	T_{MI}=190K	θ-type	56
$(ET)_2CsCo(SCN)_4$	T_{MI}=20K	θ-type	55
$(ET)_4Et_4NCo(CN)_6(H_2O)_3$	I(10Scm^{-1})	κ-like	93
$(ET)_2FeCl_4$	I(10^{-2}Scm^{-1})	δ'-type	130
$(ET)_2FeBr_4$	I(10^{-6}Scm^{-1})	dimer	130
$(ET)_4NH_4[Fe(C_2O_4)_3]PhCN$	I(10^{-1}Scm^{-1})	θ+κ	53
$(ET)_4H_2O[Fe(C_2O_4)_3]PhCN$	T_{SC}=8.5K	β"31?x3	53
$(ET)_4K[Fe(C_2O_4)_3]PhCN$	I(10^{-1}Scm^{-1})	θ+κ	53
$(ET)_2[Fe(C_{12}H_{26}B_{18}S_2)]$	I(0.5Scm^{-1})	β_{42x2}	13
$(ET)_4Et_4NFe(CN)_6(H_2O)_3$	I(0.2Scm^{-1})	κ-like	93
$(ET)_3(MnCl_4)_2$	I(0.04Scm^{-1})	β'-type	23
$(ET)_2ReO_4$	T_{MI}=81K T_{SC}=2K(4kbar)	β_{21x2}	8
α-$(ET)_3(ReO_4)_2$	T_{MI}=88K	β"3??	41
β-$(ET)_3(ReO_4)_2$	T_{MI}=100K		41
γ-$(ET)_3(ReO_4)_2$	I	β"321?	41
$(ET)_2ReO_4(THF)_{0.5}$	I(1Scm^{-1})		41
$(ET)ReO_4(THF)_{0.5}$	I(10-5Scm^{-1})	=IO_4	152
$(ET)_4Re_6S_5Cl_9$	M		173
$(ET)_4Re_6Se_5Cl_9$	T_{MI}=20K		173
$(ET)_4Re_6Se_5Cl_9(DMF)_2$	I(4x10-6Scm^{-1})		174
$(ET)_3Re_2(NCS)10CH_2Cl_2$	I(0.01Scm^{-1})	Mixed	189
$(ET)_2Cr(NCS)_4(NH_3)2$	I(30Scm^{-1})	β"-like	190
$(ET)_2[Cr(C_4H_{22}B_{18})]$	I(0.002Scm^{-1})	β'-type	13
$(ET)_4Et_4NCr(CN)_6(H_2O)_3$	I(10Scm^{-1})	κ-like	194
$(ET)_4(Mo_6Cl_8)Cl_6(THF)$	I	β"-like	168

$(ET)_4(Mo_6Cl_8)I_6(THF)_2$		α-like	175
$(ET)_2Mo_6O_{19}$		Dimer	176
$(ET)_8[PMo_{12}O_{40}](CH_3CN)_2(H_2O)_2$	I(0.1Scm^{-1})	θ_{42+40}	81
$(ET)[MoOCl_4(H_2O)]$	I(0.5Scm^{-1})	Mixed	189,190
$(ET)_{11}[P_2W_{18}O_{62}](H_2O)_3$	T_{MI}=150K	$\beta_{11,5}$?	16
$(ET)_8SiW_{12}O_{40}$	I(2Scm^{-1})	θ-like	82
$(ET)_8[BW_{12}O_{40}](H_2O)_9$	I	θ_{42+40}	191
$(ET)_8[CoW_{12}O_{40}](H_2O)_{5.5}$	I	θ_{42+40}	83,191
$(ET)_8[FeW_{12}O_{40}](H_2O)_9$	I	θ_{42+40}	191
$(ET)_8[PMnW_{11}O_{39}](H_2O)_2$	I	θ_{42+40}	85
$(ET)_5[VW_5O_{19}](H_2O)_6$	I	θ_{42+40}	80
$(ET)_2W_6O_{19}$		Dimer	176
$(ET)_3[V(dmit)_3]_2$	I(3Scm-1)		177
$(ET)_3Ta_2F_{11}$			178
OrganicAnions			
$(ET)_2C_{60}$	I	Mixed	184
$(ET)_2N(CN)_2$		α'-type	138
$(ET)_2[C(CN)_3]$	T_{MI}=180K	δ-type	119
$(ET)_2[C_3(CN)_5]$	I(1Scm^{-1})		120
$(ET)_2[C_4(CN)_6](BN)$	I(0.4Scm^{-1})	α'-type	120
$(ET)_2[C_5(CN)_5](TCE)_x$	I(0.4Scm^{-1})	α'-type	178
$(ET)_2(C_7H_7SO_3)$	I	α'-type	116
$(ET)_2$(PrO-TCA)		β''_{421}	50
t-(ET)(TCNQ)	T_{MI}=330K	Segregated	21
m-(ET)(TCNQ)	I(10-6Scm^{-1})	Mixed	21
$(ET)(F_1TCNQ)$	M	β''_{10}	197
$(ET)(F_2TCNQ)$	I	Mixed(β")	198
$(ET)(F_4TCNQ)$	I	Mixed(β")	199
$(ET)(C_{12}H_2N_4S_2)$	I	Mixed(β")	200
(ET)	I	Dimer	179

TCE:1,1,2-trichloroethane, THF: tetrahydrofurane, BN: benzonitrile, CB: chlorobenzene, DMF: dimethylformamide, mnt: maleonitriledithiolate, dmit: isotrithionedithiolate.

$C_{12}H_2N_4S_2$