

ドナー、アクセプターの酸化還元電位、電荷移動吸収帯

各ドナー (D)、アクセプター (A) について、主に同一条件でのサイクリックボルタメトリ (CV) によるデータを記載する。以下は参照電極を飽和カロメル電極 (SCE) としたデータである (主に斎藤研究室で 1998 年までに測定したデータ)。同一条件でない測定値の比較は、大きな誤差を生じるので注意が必要。左側の欄に CH<sub>3</sub>CN での第一酸化還元電位 E<sup>1/2</sup><sub>1/2</sub> (V)、第二酸化還元電位 E<sup>2/2</sup><sub>1/2</sub> (V)、それらの差 ΔE (V)、中央の欄に他の条件 (溶媒、参照電極) での値、最後の欄にドナー、アクセプターの強さの目安として、ドナーの場合はその sym-トリニトロベンゼン錯体の CT 帯 (CHCl<sub>3</sub> 溶媒)、アクセプターの場合はそのピレン錯体の CT 帯 (CHCl<sub>3</sub> 溶媒) (hν<sub>CT</sub>/10<sup>3</sup> cm<sup>-1</sup>) を記す。

各記号の説明

E<sup>1/2</sup><sub>1/2</sub>=1/2[E<sup>p<sub>red</sub></sup>(A<sup>0</sup>→A<sup>-1</sup>)+E<sup>p<sub>ox</sub></sup>(A<sup>-1</sup>→A<sup>0</sup>)], E<sup>2/2</sup><sub>1/2</sub>=1/2[E<sup>p<sub>red</sub></sup>(A<sup>-1</sup>→A<sup>-2</sup>)+E<sup>p<sub>ox</sub></sup>(A<sup>-2</sup>→A<sup>-1</sup>)] アクセプター (A),  
E<sup>1/2</sup><sub>1/2</sub>=1/2[E<sup>p<sub>ox</sub></sup>(D<sup>0</sup>→D<sup>+1</sup>)+E<sup>p<sub>red</sub></sup>(D<sup>+1</sup>→D<sup>0</sup>)], E<sup>2/2</sup><sub>1/2</sub>=1/2[E<sup>p<sub>ox</sub></sup>(D<sup>+1</sup>→D<sup>+2</sup>)+E<sup>p<sub>red</sub></sup>(D<sup>+2</sup>→D<sup>+1</sup>)] ドナー (D),  
E<sup>p<sub>red</sub></sup>, E<sup>p<sub>ox</sub></sup>は酸化波、還元波のピーク電位、ΔE=(E<sup>1/2</sup><sub>1/2</sub>-E<sup>2/2</sup><sub>1/2</sub>), 信頼性は小数点以下 2 桁 \*: (E<sup>p<sub>ox</sub></sup>-E<sup>p<sub>red</sub></sup>)>100mV,  
{ } : scan speed mV/s 主に 10, 100mV/s, [ ] : 温度 °C, 支持電解質 0.1M TBA·BF<sub>4</sub>, 作用電極 Pt,  
溶媒: CH<sub>3</sub>CN (AN), CH<sub>2</sub>ClCH<sub>2</sub>Cl (DCE), ベンゾニトリル (BN), 参照電極 Ag: Ag/AgCl

## 1. Electron Donor

electron donor	in CH <sub>3</sub> CN			in CH <sub>2</sub> ClCH <sub>2</sub> Cl (DCE) or other			hν <sub>CT</sub>	
	E <sup>1/2</sup> <sub>1/2</sub>	E <sup>2/2</sup> <sub>1/2</sub>	ΔE	E <sup>1/2</sup> <sub>1/2</sub>	E <sup>2/2</sup> <sub>1/2</sub>	ΔE		
TTF	0.350 {100} 0.353 {20} 0.373 {10} 0.377 {100}	0.720 [15] 0.730 [15] 0.756 [19] 0.758 [19]	0.370 0.377 0.383 0.381	0.414 {100} 0.281 {100}	0.736 [20] 0.661 [19]	0.322 0.381	DCE, SCE AN, Ag	15.3 <sub>o</sub>
TMTTF	0.285 {100} 0.279 {100} 0.294 {50}	0.652 [22] 0.648 0.635 [22]	0.367 0.369 0.341	0.383 {100} 0.090 {100}	0.863 [16] 0.460 [ ]	0.480 0.370	DCE, SCE AN, Ag	13.9 <sub>o</sub>
OMTTF	0.292 {20} 0.292 {100}	0.676 [22] 0.685 [22]	0.384 0.393	0.390 {100}	0.875 [20]	0.485	DCE, SCE	13.8 <sub>o</sub>
HMTTF	0.292 {10}	0.634 [22]	0.342	0.423 {100} 0.235 {10}	0.870 [20] 0.570 [22]	0.447 0.335	DCE, SCE AN, Ag	13.7 <sub>o</sub>
DBTTF	0.625 {100}	0.950 [15]	0.325	0.744 {100} 0.541 {100}	1.160 [16] 0.867 [16]	0.416 0.326	DCE, SCE AN, Ag	17.3 <sub>o</sub>
TTF (CO <sub>2</sub> Me) <sub>4</sub>				0.970 {100}	1.268 [24]	0.297	DCE, SCE	
BEDO-TTF	0.430 {100} 0.431 {10} 0.425 {100}	0.690 [19] 0.689 [19] 0.683	0.260 0.258 0.258	0.765 {10} ? 0.776 {100} ? 0.344 {10}	0.461 [19] ? 0.434 [19] ? 0.604 [19]	0.304 0.342 0.260	DCE, SCE DCE, SCE AN, Ag	14.9 <sub>7</sub>
BEDO-DBTTF	0.505 {10}	0.800 [22]	0.295	0.446 {10}	0.730 [22]	0.284	AN, Ag	15.8 <sub>o</sub>
TTC <sub>1</sub> -TTF	0.520 {100}	0.752 [21]	0.232	0.640 {100}	0.930 [20]	0.290	DCE, SCE	16.1 <sub>o</sub>
TSeC <sub>1</sub> -TTF	0.473 {100}	0.745 [21]	0.272	0.583 {100}	0.914	0.331	DCE, SCE	15.8 <sub>o</sub>
TTeC <sub>1</sub> -TTF	不可			0.519 {100}	0.900 [17]	0.381	DCE, SCE	15.0
C <sub>1</sub> TET-TTF								16.0
C <sub>7</sub> TET-TTF	0.535 {100}	0.783 [22]	0.248	0.635 {200}	0.975 [24]	0.340	DCE, SCE	16.1
EOET-TTF	0.465 {10}	0.734 [22]	0.269	0.389 {10}	0.655 [22]	0.266	AN, Ag	15.5 <sub>o</sub>
BEDT-TTF	0.530 {10} 0.532 {100} 0.520 {100} 0.535 {100}	0.775 [19] 0.776 [19] 0.765 0.776 [23]	0.245 0.244 0.235 0.241	0.635 {100} 0.615 {100} 0.448 {10}	0.970 [16] 0.915 [23] 0.698 [18]	0.335 0.300 0.250	DCE, SCE BN, SCE AN, Ag	16.0 <sub>s</sub>
BMDT-TTF				?0.640 {100}	[16]		DCE, SCE	

BPDT-TTF				0.650 {100}	0.986 [20]	0.336	DCE, SCE	
BVDT-TTF								
EDT-TTF	0.440 {10} 0.437 {100}	0.745 [22] 0.746 [22]	0.305 0.309					15.7 <sub>o</sub>
EDO-TTF	0.385 {10}	0.706 [22]	0.321	0.311 {10}	0.623 [22]	0.312	AN, Ag	15.2 <sub>s</sub>
TH-TTF	0.295 {20}	0.635 [ ]	0.340	0.107 {100}	0.455 [ ]	0.348		
BHEDT-TTF	0.415 {100} 0.411 {20}	0.714 [ ] 0.708 [ ]	0.299 0.297	0.226 {100}	0.529 [ ]	0.310	AN, Ag	
BHMDT-TTF	0.405 {100}	0.675 [ ]	0.270	0.220 {100}	0.490 [ ]	0.270	AN, Ag	
BHEDO-TTF	0.361 {10}	0.666 [20]	0.308	0.292 {10}	0.600 [20]	0.308	AN, Ag	14.8 <sub>e</sub>
BHPDT-TTF	0.416 {100}	0.743 [ ]	0.327	0.233 {100}	0.558 [ ]	0.325		
BHVDT-TTF	0.482 {100}	0.770 [ ]	0.288	0.290 {50}	0.575 [ ]	0.285	AN, Ag	
MHEDO-TTF	0.377 {10}	0.693 [22]	0.316	0.315 {10}	0.628 [22]	0.313	AN, Ag	14.9 <sub>s</sub>

## TSF Derivatives

TSF	0.509 {100}	0.803 [26]	0.294					16.8
TMTSF	0.450 {10} 0.445 {100}	0.730 [23] 0.732 [23]	0.280 0.287	0.573 {100} 0.388 {10}	0.964 [20] 0.680 [23]	0.391 0.292	DCE, SCE AN, Ag	15.0 <sub>e</sub>
HMTSF				0.582 {100}	0.955 [20]	0.373	DCE, SCE	15.3
TSF (CO <sub>2</sub> Me) <sub>4</sub>				1.087 {100}	1.274 [16]	0.187	DCE, SCE	

## TTeF Derivatives

HMTTeF				0.573 {100}	0.865 [20]	0.289	DCE, SCE	15.8 <sub>o</sub>
--------	--	--	--	-------------	------------	-------	----------	-------------------

Azine System (E<sup>1,1/2</sup>のみ CH<sub>3</sub>CN, SCE)

phenothiazine	0.639 {10}	[17]	19.0
N-methyl-phenothiazine	0.717 {10}	[25]	19.6
benzo[c]-phenothiazine	0.549 {10}	[17]	17.9
dibenzo[c, h]phenothiazine	0.494 {10}	[16]	17.4
dibenzo[c, h]phenoselenazine			17.2
N, N-dimethyl-phenanazine	0.191 {20}	[16]	14.2

Aromatic Amine System (CH<sub>3</sub>CN, SCE)

p-phenylene-diamine	0.280 { }	[ ]		20.3
TMPD: N, N, N', N' -	0.147 {100}	0.724 [16]	0.577	15.7

tetramethyl-p-phenylenediamine	0.151{10}			
diaminodurene	0.172{100} 0.173{10}	0.678[16]	0.506	17.1

benzidine				20.2
o-dianisidine	0.47{ }	0.65[ ]	0.18	19.3
o-tolidine	0.49{ }	0.71[ ]	0.22	19.2
dichloro-o-tolidine				21.3
dibromo-o-tolidine				20.4
3,5-TMB:3,3',5,5'-tetramethyl benzidine	0.480{100} 0.485{10}	0.689[16]	0.209	18.0
N,N,N',N'-TMB	0.461{100} 0.474{10}	0.633[16]	0.172	17.0
1,6-DAP	0.27{10}	0.56[23]	0.29	16.1

TDAP	0.021(2e){10} 0.018(2e){100}	0.088(2e)[20] 0.083[20]	-0.055(2e){100}	0.007(2e)[21]	AN, Ag	13.2
------	---------------------------------	----------------------------	-----------------	---------------	--------	------

1,4-diamino-anthraquinone	0.750{100} 0.749{100} 0.748{100} 後の2つは	[20] 1.189[20] 1.181[20] 微分ハリス法	CV 0.44 0.433	
---------------------------	---	--	---------------------	--

## Polycyclic Condensed Aromatic Hydrocarbon and Related System

HMB:hexamethyl benzene	1.820{100}:peak				
triphenylene					27.5
naphthalene					27.4
phenanthrene					27.0
chrysene					24.0
pyrene	1.570{200}:peak				22.2
anthracene			1.580{100}[23] peak	BN, SCE	22.1
perylene	1.070{100}:peak 1.050{100}:peak 1.038{100} 1.078{100}	1.535:peak[18]	1.145{100}[23]	BN, SCE	20.8
naphthacene (tetracene)	1.025{500}:peak		1.10{100} 1.155{100}:peak	DCE, SCE DCE, SCE	19.2
decacyclene					

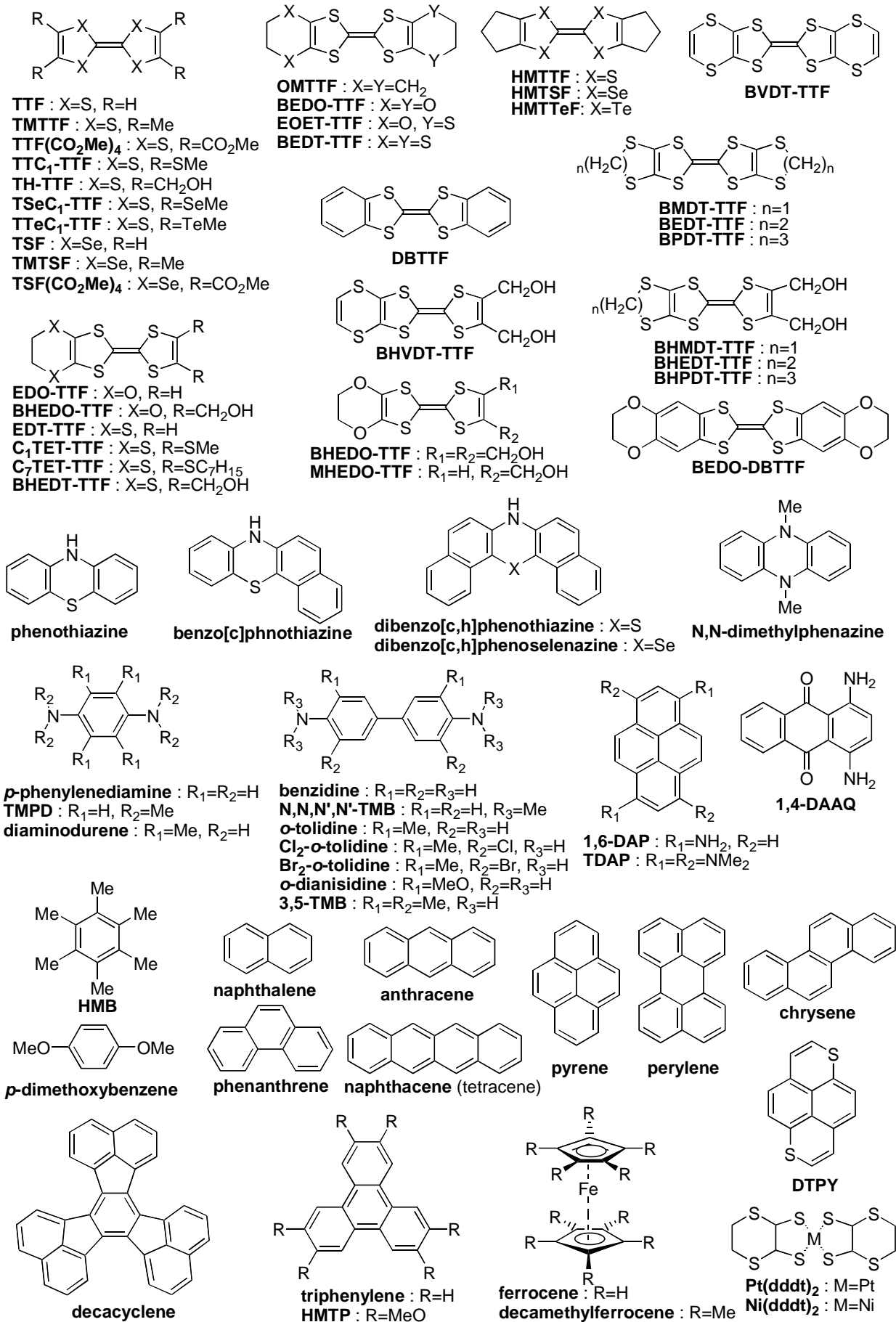
HMTp	0.474 {10} [23]				21.0
DTPY	0.396 {100} 0.394 {20}	0.795 [ ] 0.793 [ ]	0.399 0.399		15.0

## ferrocene

フェロセン	0.383 {100} 0.427 {50} [26]		0.574 {100} [26] 0.577 {50} [26] 0.574 {10} [26]	DCE, SCE DCE, SCE DCE, SCE	16.0 (sh)
デカメチルフェロセン	-0.89 {10}	-0.09 [23]	0.80		13.8

## dddt system

Pt (dddt)2		1.035 {200} [23] 1.050 {100} [23]	BN, SCE BN, SCE
Ni (dddt)2		1.005 {100} peak 1.105 [23]	BN, SCE



## 2) Electron Acceptor

electron acceptor	in CH <sub>3</sub> CN			in CH <sub>2</sub> Cl CH <sub>2</sub> Cl (DCE) or other			h ν <sub>CT</sub>	
	E <sup>1</sup> <sub>1/2</sub>	E <sup>2</sup> <sub>1/2</sub>	ΔE	E <sup>1</sup> <sub>1/2</sub>	E <sup>2</sup> <sub>1/2</sub>	ΔE		
DDQ	0.561*{100} 0.562{10}	-0.295*[19] -0.295*[19]	0.856 0.857	0.685{100} 0.586*{100} 0.493{10} 0.490*{100}	-0.195[15] -0.341*[15] -0.370*[20] -0.375*[20]	0.880 0.927 0.863 0.865	DCE, SCE DCE, Ag AN, Ag AN, Ag	11.7 <sub>6</sub>
CDDQ								
DBDQ	0.531*{100} 0.537{10}	-0.293*[23] -0.279[23]	0.824 0.816	0.675{100} 0.568*{100} 0.474{10} 0.474*{100}	-0.220[15] -0.328*[15] -0.339[23] -0.350*[23]	0.895 0.896 0.813 0.824	DCE, SCE DCE, Ag AN, Ag AN, Ag	11.6 <sub>6</sub>
DIDQ	0.514{10} 0.510{100}	-0.280[21] -0.280[21]	0.794 0.790	0.452{10}	-0.346[ ]	0.798	AN, Ag	11.8 <sub>3</sub>
2,3-Q(CN) <sub>2</sub>	0.345*{100} 0.348{10} 0.338{5}	-0.492*[21] -0.408*[22] -0.395*[22]	0.837 0.756 0.733					13.6 <sub>1</sub>
p-QF <sub>4</sub>	0.042*{100} 0.041{10}	第2波? [20]		0.032*{50} -0.021{10}[20]	-0.802*[20] 2波目?	0.834	DCE, Ag AN, Ag	17.0 <sub>4</sub>
p-QCl <sub>4</sub>	0.048*{100} 0.050{10} 0.071{100} 0.060{20}	-0.770*[19] -0.768*[19] -0.686*[15] -0.690[15]	0.818 0.818 0.757 0.750	0.141{100} 0.039{100} -0.013{10} -0.011{100}	-0.642[20] -0.751*[20] -0.840[19] -0.840*[19]	0.783 0.790 0.827 0.829	DCE, SCE DCE, Ag AN, Ag AN, Ag	15.9 <sub>7</sub>
p-QBr <sub>4</sub>	0.044{100} 0.044{10}	-0.746*[19] -0.746[19]	0.790 0.790	0.034{50} -0.025{10} -0.025{100}	-0.734[20] -0.815*[19] -0.825*[19]	0.768 0.790 0.800	DCE, Ag AN, Ag AN, Ag	15.8 <sub>2</sub>
p-QI <sub>4</sub>	-0.019{10} -0.003{100}	-0.690[22] -0.692*[22]	0.671 0.689	-0.070{10}	[ ]		AN, Ag	16.1 <sub>3</sub>
2,6-QCl <sub>2</sub>	-0.152{10} -0.149{100}	-0.913[24] -0.913[24]	0.761 0.764	-0.194{10}	-0.773[ ]	0.579	AN, Ag	18.1 <sub>5</sub>
2,5-QCl <sub>2</sub>	-0.169{50} -0.170{10} -0.147{10} -0.158{100}	第2波? -0.785[23] -0.786[23]	0.638 0.628	-0.197{10}	-0.740[ ]	0.543	AN, Ag	18.0 <sub>5</sub>
QCl <sub>2</sub> (OH) <sub>2</sub>	-0.160{100}[19] -0.130{10}	peak peak		-0.235{100}[19] -0.200{10}[ ]	peak peak		AN, Ag	18.6 <sub>6</sub>
QBr <sub>2</sub> (OH) <sub>2</sub>	-0.158{100}[24] -0.121{10}	peak peak		-0.235{100}[24] -0.202{10}[ ]	peak peak		AN, Ag AN, Ag	
Q(OH) <sub>2</sub>	-0.420{100}[18] -0.375{10}	peak peak		-0.462{10}[18]	peak		AN, Ag	
C <sub>18</sub> QMe	-0.64{20}							
QBr <sub>2</sub> Me <sub>2</sub>	-0.320{100} -0.318{20}	-1.039[20]	0.719					
Q	-0.460*{100} -0.456{20} -0.482{10} -0.475{100}	[21] [21] [24] [24]		-0.507{10}			AN, Ag	21.7 <sub>9</sub>

## Naphthoquinone System

DCNNQ	0.383 {10} 0.384*{100}	-0.409[21] -0.412*[21]	0.792 0.796	0.303 {10}	-0.483 [ ]	0.786	AN, Ag	13.1 <sub>s</sub>
DCNQ	0.210*{100} 0.214 {10}	-0.626*[20] -0.612[20]	0.836 0.826	0.147 {10} 0.147 {100}	-0.683*[20] -0.695*[20]	0.830 0.842	AN, Ag AN, Ag	14.6 <sub>o</sub>
Cl <sub>2</sub> NNQ	-0.203 {100}	-1.060 peak		-0.255 {10}	-1.042 peak		AN, Ag	17.7 <sub>s</sub>
Cl <sub>2</sub> NQ	-0.379 {100} -0.376 {20} -0.391*{10} -0.398*{100}	-0.967*[20] -0.961[20] -1.077[24] -1.031*[24]	0.588 0.585 0.686 0.633	-0.449*{10}	-1.077 [ ]	0.628	AN, Ag	19.6 <sub>s</sub>
Br <sub>2</sub> NQ	-0.412 {100} -0.415 {50}	-1.250 peak						
NQ	-0.679 {10} -0.674 {5} -0.675 {10} -0.674*{100}	[24] [24]		-0.713*{10}			AN, Ag	22.1 <sub>z</sub>

## DCNQI System

Me <sub>4</sub> DCNQI	-0.033 {100} -0.036 {10}	? [18] -0.549*[18]		-0.114 {10}	-0.633[18]	0.519	AN, Ag	
C <sub>18</sub> MeDCNQI	約0.095 {200} 0.090 {500}	?						

## TCNQ System

TCNQ	0.218 {100} 0.222 {10} 0.232 {200} 0.200 {100} 0.245 {100}	-0.333*[18] -0.335[18] -0.313[21] -0.346[16] -0.302*[14]	0.551 0.557 0.545 0.546 0.547	0.320 {100} 0.228*{100} 0.113 {100} 0.169 {100} 0.153 {10} 0.154 {100}	-0.275[15] -0.365*[15] -0.423[16] -0.381[21] -0.402[18] -0.396*[18]	0.595 0.593 0.536 0.550 0.555 0.550	DCE, SCE DCE, Ag AN, Ag, TEA AN, Ag AN, Ag AN, Ag	12.8 <sub>z</sub>
F <sub>4</sub> TCNQ	0.601 {100} 0.600 {10} 0.600 {100} 0.615 {50}	0.054*[19] 0.052[19] 0.070[15] 0.073*[14]	0.547 0.548 0.530 0.542	0.743 {100} 0.638*{100} 0.528 {20} 0.528 {100}	0.078 [15] -0.024*[15] -0.015[19] -0.015*[19]	0.665 0.662 0.543 0.543	DCE, SCE DCE, Ag AN, Ag AN, Ag	12.0 <sub>s</sub>
CF <sub>3</sub> TCNQ	0.435 {10} 0.438 {10} 0.435 {100}	-0.140 [ ] -0.136[21] -0.137[21]	0.575 0.574 0.572	0.359 {10}	-0.205[22]	0.564	AN, Ag	11.6 <sub>o</sub>
F <sub>2</sub> TCNQ	0.412 {100} 0.408 {10}	-0.137[22] -0.132[22]	0.549 0.540	0.345 {10} 0.343 {100}	-0.211[22] -0.207[22]	0.556 0.550	AN, Ag AN, Ag	11.5 <sub>s</sub>
FTCNQ	0.325 {100} 0.321 {10} 0.340 {100}	-0.232[23] -0.235[23] -0.212*[14]	0.557 0.556 0.552	0.431 {100} 0.331*{100} 0.258 {10} 0.256 {100}	-0.185[15] -0.290*[15] -0.304[23] -0.298[23]	0.616 0.621 0.562 0.554	DCE, SCE DCE, Ag AN, Ag AN, Ag	12.2 <sub>z</sub>
TNAP	0.260 {10} 0.259 {100}	-0.110[23] -0.109[23]	0.370 0.368	0.179 {10} 0.174 {100}	-0.194[23] -0.198[23]	0.373 0.372	AN, Ag AN, Ag	
C <sub>10</sub> TCNQ	0.203 {100} 0.205 {10}	-0.328[20] -0.323[20]	0.531 0.528	0.127 {10} 0.128 {100}	-0.398[20] -0.396[20]	0.525 0.524	AN, Ag AN, Ag	13.6 <sub>1</sub>
C <sub>14</sub> TCNQ	0.208 {100} 0.210 {10}	-0.317[21] -0.318[21]	0.525 0.528	0.124 {10} 0.123 {100}	-0.406[20] -0.403[20]	0.530 0.526	AN, Ag AN, Ag	14.0 <sub>1</sub>
C <sub>18</sub> TCNQ	0.170 {100} 0.180 {50}	-0.365 [ ] -0.370 [ ]	0.535 0.550					

C <sub>22</sub> TCNQ	0.180 {200}	-0.370 [ ]	0.550					
DHBTCNQ	0.185 {100} 0.184 {10}	-0.308* [19] -0.313 [19]	0.493 0.497	0.117 {10} 0.155 {100}	-0.373 [19] -0.374 [19]	0.490 0.489	AN, Ag AN, Ag	13.3 <sub>7</sub>
THBTCNQ	0.160 {100} 0.160 {10}	-0.330* [19] -0.327 [19]	0.490 0.487	0.094 {10} 0.093 {100}	-0.391 [19] -0.395 [19]	0.485 0.488	AN, Ag AN, Ag	13.6 <sub>2</sub>
Et <sub>2</sub> TCNQ	0.155 {100} 0.151 {10}	-0.338 [23] -0.337 [23]	0.493 0.488	0.095 {10} 0.100 {100}	-0.399 [23] -0.393 [23]	0.494 0.493	AN, Ag AN, Ag	13.9 <sub>1</sub>
Me <sub>2</sub> TCNQ	0.147 {100} 0.147 {10} 0.168 {100}	-0.339* [19] -0.338 [19] -0.301* [14]	0.486 0.485 0.469	0.245 {100} 0.135* {100} 0.079 {10} 0.078 {100}	-0.303 [15] -0.404* [15] -0.410 [19] -0.415 [19]	0.548 0.539 0.489 0.493	DCE, SCE DCE, Ag AN, Ag AN, Ag	13.7 <sub>4</sub>
TCNNQ	0.061 {100} 0.070 {10}	-0.309 [22] -0.313 [22]	0.37 0.383	-0.006 {10} -0.004 {100}	-0.387 -0.378 [22]	0.393 0.374	AN, Ag AN, Ag	14.6 <sub>4</sub>
(MeO) <sub>2</sub> TCNQ	0.054 {100} 0.053 {10} 0.058 {100}	-0.434* [19] -0.435 [19] -0.418* [14]	0.488 0.488 0.476	0.095 {100} -0.005 {100}	-0.383 [15] -0.528 [15] -0.520* [19]	0.478 0.523 0.493	DCE, SCE DCE, Ag AN, Ag	14.7 <sub>1</sub>
BTDA-TCNQ	0.034 {100} 0.032 {10}	-0.449* [18] -0.444 [18]	0.483 0.476	0.152 {100} 0.055 {100} -0.044 {10} -0.043 {100}	-0.388 [20] 0.483 [20], -0.512 [18] -0.525* [18]	0.540 -1.208 (3波目) 0.468 0.482	DCE, SCE DCE, Ag AN, Ag AN, Ag	14.4 <sub>1</sub>
(EtO) <sub>2</sub> TCNQ	0.008 {10} 0.01 {100}	-0.462 [23] -0.46 [23]	0.470 0.47	-0.043 {10}	-0.516 [22]	0.473	AN, Ag	15.2 <sub>9</sub>
Me <sub>4</sub> TCNQ	-0.045 {100} -0.048 {10} -0.045 {5}	一波のみ " "		-0.108 {10} -0.110 {100}	1波のみ "		AN, Ag AN, Ag	19.3 <sub>1</sub> (sh)
TCAQ	-0.322 (2e) {10} [20] -0.329 (2e) {100} [20]							
TCNDQ2-	0.17 {100} 0.15 {10}	0.015 [23] 0.019 [23]	0.155 0.131					

## TNF System

DTENF	0.229 {100} 0.234 {10}	-0.359 [19] -0.357 [19]	0.588 0.591	0.152 {10} 0.152 {100}	-0.436 [19] -0.441* [19]	0.588 0.593	AN, Ag AN, Ag	14.0 <sub>1</sub>
DTNF	0.017 {100} 0.019 {10}	-0.605* [20] -0.607 [20]	0.622 0.626	-0.056 {10} -0.059 {100}	-0.687 [20] -0.692 [20]	0.631 0.633	AN, Ag AN, Ag	15.6 <sub>2</sub>
TENF	-0.140 {100} -0.138 {10}	-0.407 [19] -0.406 [19]	0.267 0.268	-0.217 {10} -0.221 {100}	-0.487 [19] -0.490* [19]	0.270 0.269	AN, Ag AN, Ag	16.5 <sub>4</sub>
TNF	-0.425 {100} -0.425 {10}	-0.667 [20] -0.668 [20]	0.242 0.243	-0.496 {10} -0.495 {100}	-0.730 [20] -0.732* [20]	0.234 0.237	AN, Ag AN, Ag	18.7 <sub>3</sub>

## Nitro Compounds

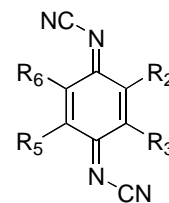
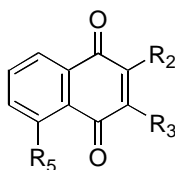
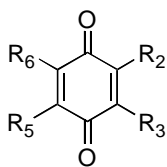
TNBP テトラニトロヒフェニール	-0.595 {100} [19] -0.560 {10} [19] 共にpeak			-0.640 {10} [19] peak -0.690 {100} [19] peak			AN, Ag AN, Ag	22.1 <sub>2</sub> (sh)
H-PICt <sup>-</sup> クリン酸	-0.24 [20] [ ] peak ?							
TBA (PIC)	peak無し [20]							
DNBP ジニトロヒフェニール	-0.979* {100} [20] -0.976 {10} [20]			-1.057 {10} [20] -1.059 {100} [20]			AN, Ag AN, Ag	



## Percyano System

TCNE	0.286 {100} 0.270 {100}	-0.916* [20] -0.775* [14]	1.202 1.045	0.195 {10} 0.201 {100}	-1.051* [20] -0.836* [14]	1.246 1.037	AN, Ag AN, Ag	13.5s
HCBD	0.727 {100} 0.719 {10} 0.629 {100}	0.056* [19] 0.048 [19] 0.038 [13]	0.671 0.671 0.591	0.76* {100} 0.626 {10} 0.624 {100}	-0.04* [14] -0.045 [20] -0.050* [20]	0.80 0.671 0.674	DCE, Ag AN, Ag AN, Ag	9.8s
KC(CN) <sub>3</sub>	1.34 {100} [19]	peak (-1→0)						
TBA (PCA)	peak (-1→0)	[20]		peak (-1→0)無し peak 1.25 {20} [19]	[24]		DCE, SCE AN, Ag	
TBA <sub>2</sub> (HCP)	-2→-1 1.210 {100} 1.208 {10}	-1→0 0.419 [19] 0.420 [19]	0.791 0.788	1.130 {10} 1.130 {100}	0.343 [18] 0.339 [18]	0.787 0.791	AN, Ag AN, Ag	
TBA <sub>2</sub> (HCTMM)	-2→-1 peak 1.20 {100} 1.16 {10}	-1→0 peak 0.99 [20] 0.96 [20]	0.21 0.20	-2→-1 peak 1.290 {200} 1.139 {200} 1.02 {200} 1.08 {20}	-1→0 peak 1.095 [24] 0.946 [24] 0.845 [rt] 0.89 [20]	0.195 0.193 0.175 0.19	DCE, SCE DCE, Ag BN, Ag AN, Ag	

I <sub>2</sub>	0.657 {10} 0.654 {100}	0.221* [20] 0.195* [20]	0.436 0.459				
TBA·I	0.233 {10} 0.200* {100}	[19] [19]					
TBA·I <sub>3</sub>	0.642 {10} 0.645 {100}	0.243 [20] 0.214* [20]	0.399 0.431	0.55* {200} [rt]	1波のみ		DCE, Ag
TBA·I <sub>5</sub>				0.658 {10} 0.660 {100}	[20] [20]		



**DDQ** :  $R_2=R_3=Cl, R_5=R_6=CN$

**DBDQ** :  $R_2=R_3=Br, R_5=R_6=CN$

**CDDQ** :  $R_2=R_5=Cl, R_3=R_6=CN$

**p-QF<sub>4</sub>** (*p*-Fluoranil) :  $R_2=R_3=R_5=R_6=F$

**p-QCl<sub>4</sub>** (*p*-Chloranil) :  $R_2=R_3=R_5=R_6=Cl$

**p-QBr<sub>4</sub>** (*p*-Bromanil) :  $R_2=R_3=R_5=R_6=Br$

**p-QI<sub>4</sub>** (*p*-Iodanil) :  $R_2=R_3=R_5=R_6=I$

**2,3-Q(CN)<sub>2</sub>** :  $R_2=R_3=CN, R_5=R_6=H$

**2,6-QCl<sub>2</sub>** :  $R_2=R_6=Cl, R_3=R_5=H$

**2,5-QCl<sub>2</sub>** :  $R_2=R_5=Cl, R_3=R_6=H$

**QCl<sub>2</sub>(OH)<sub>2</sub>** (Choloranillic Acid) :  $R_2=R_5=Cl, R_3=R_6=OH$

**QBr<sub>2</sub>(OH)<sub>2</sub>** (Bromanillic Acid) :  $R_2=R_5=Br, R_3=R_6=OH$

**Q(OH)<sub>2</sub>** :  $R_2=R_5=OH, R_3=R_6=H$

**C<sub>18</sub>QMe** :  $R_2=Me, R_5=C_{18}H_{37}, R_3=R_6=H$

**QBr<sub>2</sub>Me<sub>2</sub>** :  $R_2=R_5=Br, R_3=R_6=Me$

**Q** :  $R_2=R_3=R_5=R_6=H$

**DCNNQ** :  $R_2=R_3=CN, R_5=NO_2$

**DCNQ** :  $R_2=R_3=CN, R_5=H$

**Cl<sub>2</sub>NNQ** :  $R_2=R_3=Cl, R_5=NO_2$

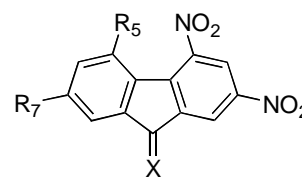
**Cl<sub>2</sub>NQ** :  $R_2=R_3=Cl, R_5=H$

**Br<sub>2</sub>NQ** :  $R_2=R_3=Br, R_5=H$

**NQ** :  $R_2=R_3=R_5=H$

**Me<sub>4</sub>DCNQI** :  $R_2=R_3=R_5=R_6=Me$

**C<sub>18</sub>MeDCNQI** :  $R_2=Me, R_5=C_{18}H_{37}, R_3=R_6=H$

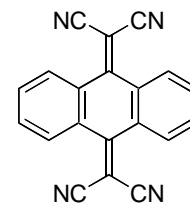
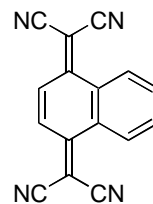
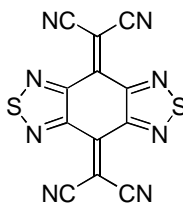
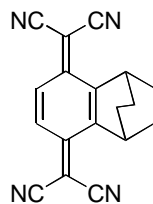
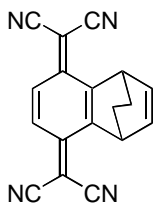
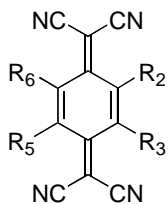


**DTENF** :  $X=C(CN)_2, R_5=R_7=NO_2$

**DTNF** :  $X=C(CN)_2, R_5=H, R_7=NO_2$

**TENF** :  $X=O, R_5=R_7=NO_2$

**TNF** :  $X=O, R_5=H, R_7=NO_2$



**TCNQ** :  $R_2=R_3=R_5=R_6=H$

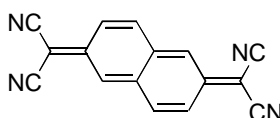
**CF<sub>3</sub>TCNQ** :  $R_2=CF_3$

$R_3=R_5=R_6=H$

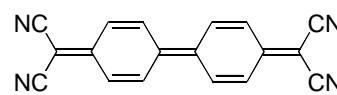
**C<sub>n</sub>TCNQ** :  $R_2=C_nH_{2n+1}$

$R_3=R_5=R_6=H$

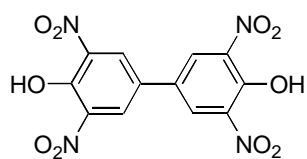
2 置換体は 2,5-置換体



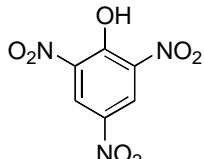
**TNAP**



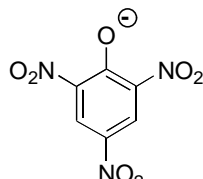
**TCNDQ**



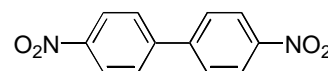
**TNBP**



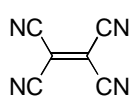
**H-PIC (Picric Acid)**



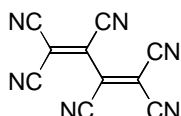
**PIC<sup>-</sup>**



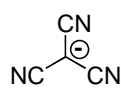
**DNBP**



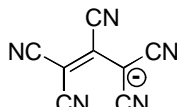
**TCNE**



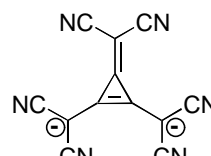
**HCBD**



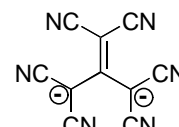
**C(CN)<sub>3</sub><sup>-</sup> (CF<sup>-</sup>)**



**PCA<sup>-</sup>**



**HCP<sup>2-</sup>**



**HCTMM<sup>2-</sup>**

以下に、相関が見られる

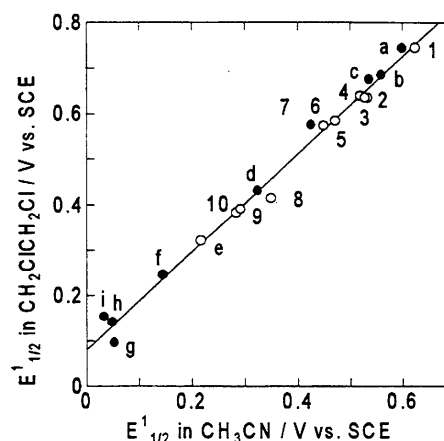
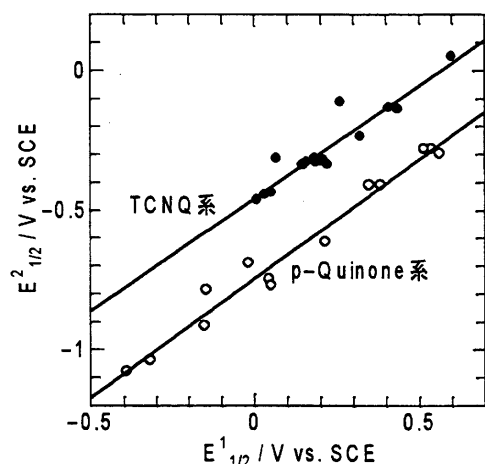
1) 酸化還元電位  $E^{2}_{1/2}$  と  $E^{1}_{1/2}$  の関係

例 p-キノン系  $E^{2}_{1/2} = (0.85 \pm 0.05) E^{1}_{1/2} - (0.75 \pm 0.03)$   
 TCNQ系  $E^{2}_{1/2} = (0.81 \pm 0.05) E^{1}_{1/2} - (0.46 \pm 0.03)$

2) 溶媒  $\text{CH}_3\text{CN}$  と  $\text{CH}_2\text{ClCH}_2\text{Cl}$  の酸化還元電位  $E^{1}_{1/2}$  に対する効果

$E^{1}_{1/2}$  (ジクロロエタン) =  $1.09 E^{1}_{1/2}$  (アセトニトリル) + 0.072

1. DBTTF, 2. C-TET-TTF, 3. TTC<sub>1</sub>-TTF, 4. BEDT-TTF, 5. TSC<sub>1</sub>-TTF, 6. TMTSF, 7. フェロセン, 8. TTF, 9. TMTTF, 10. OMTTF  
 a. F<sub>4</sub>TCNQ, b. DDO, c. DBDQ, d. FTCNQ, e. TCNQ, f. Me<sub>2</sub>TCNQ, g. (MeO)<sub>2</sub>TCNQ, h. p-クロロニル, i. BTDA-TCNQ



3) 種々のアクセプター分子のピレン錯体の電荷移動吸収エネルギー  $h\nu_{CT}^N$  (クロロホルム溶液) と酸化還元電位  $E^{1}_{1/2}$  との関係。□: TCNQ系, ○: p-キノン系, ▲: ペルシアノ系, ●: フルオレン系。p-キノン系での直線は、p-フルオロニル、p-ベンゾキノンを除いた最小自乗法により求めた。

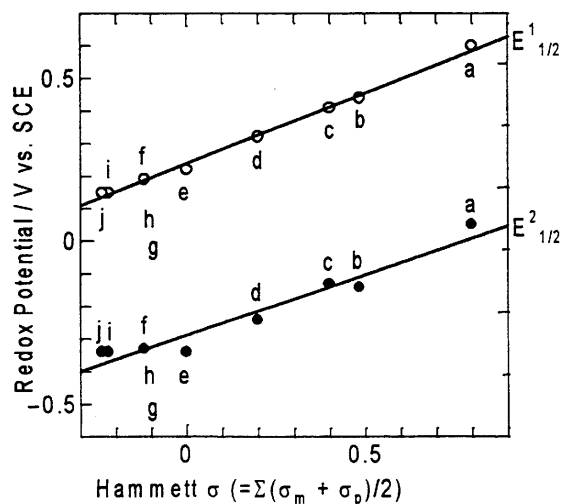
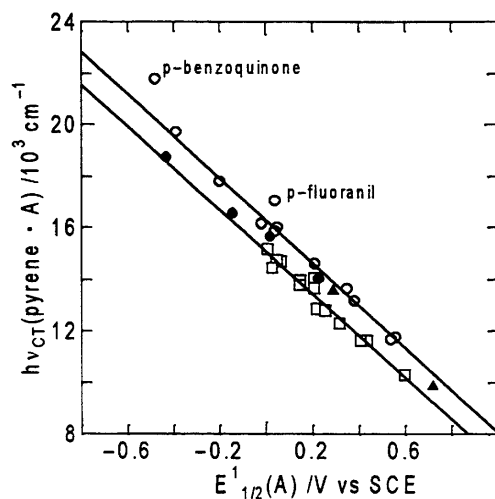
4) Hammett  $\sigma$  と 酸化還元電位  $E^{1}_{1/2}$  の関係

TCNQ系の第一、第二酸化還元電位  $E^{1}_{1/2}$ ,  $E^{2}_{1/2}$  と Hammett  $\sigma$  との関係。

$E^{1}_{1/2} = 0.437 (\sigma_m + \sigma_p) / 2 + 0.236$

$E^{2}_{1/2} = 0.385 (\sigma_m + \sigma_p) / 2 - 0.292$

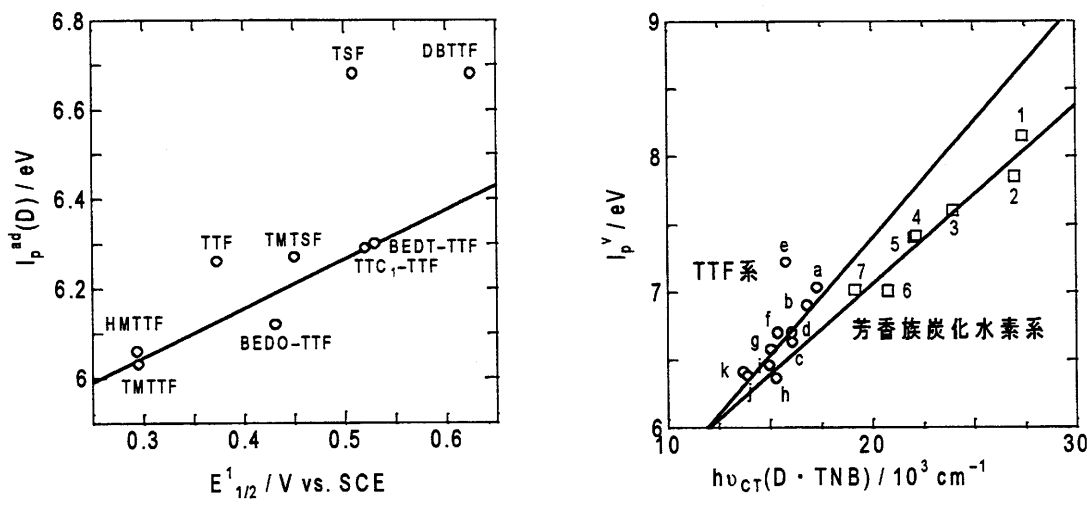
a. F<sub>4</sub>TCNQ, b. CF<sub>3</sub>TCNQ, c. F<sub>2</sub>TCNQ, d. FTCNQ, e. TCNQ, f. MeTCNQ, g. (EtO)<sub>2</sub>TCNQ, h. (MeO)<sub>2</sub>TCNQ, i. Et<sub>2</sub>TCNQ, j. Me<sub>2</sub>TCNQ



5) TTF系でのイオン化電位(断熱値)と酸化還元電位  $E^{1/2}$  の関係。 直線はDBTTF、TSF、TTFを除いた最小自乗直線  
 $I_p^{ad}(D) = 1.08 e E^{1/2}(D) + 5.73$

6) 芳香族炭化水素およびTTF系ドナーのイオン化電位(垂直値)と  $h\nu_{CT}(D \cdot TNB)$  の関係  
 1. ナフタレン、2. フェナントレン、3. クリセン、4. ピレン、5. アントラセン、6. ペリレン、7. ナフタセン、  
 a. DBTTF, b. TSF, c. TTC<sub>1</sub>-TTF, d. BEDT-TTF, e. HMTTeF, f. TTF, g. TMTSF, h. BEDO-TTF, i. TMTTF, j. HMTTF

図5, 6中のイオン化電位は主に佐藤直樹「紫外光電子分光法による芳香族固体の物性化学(分光研究、36,243(1987))より。



7) p-フェニレンジアミン系、ベンジジン系、アジン系、TTF系の電荷移動吸収エネルギーと  $E^{1/2}$  の関係

