イオン化エネルギー

固体物性研究の観点から関心がもたれると思われる有機化合物を中心として、実験によって決められた孤立分子とその固体のイオン化エネルギーの値を集めた。

データの収集にあたっては、最近までの報告値をなるべく多く検討し、その結果として分子と固体についてそれぞれ次のような値の収録を行った。ただし、既に以前に報告値が収束しているような化合物も少なくなく、そのような場合には古い値をそのまま掲載したものもある。なお、たとえば次の文献を参照されたい。

K. Seki, "Ionization energies of free molecules and molecular solids," *Mol. Cryst. Liq. Cryst.* 171 (1989) 255.

(1) 孤立分子については、典型的な電子供与体と電子受容体を含む多くの芳香族化合物を対象として、気相の第一イオン化エネルギー（I_g）を集めた。同一化合物に対し複数の値が報告されている場合には、紫外光電子分光法（UPS）により決定された最も信頼性が高いと思われる値を一つだけ示すことを原則とした。

分子とその正イオンとの間に起こる電子の脱離／付加過程を考えると、分子のイオン化エネルギーの値には断熱値（adiabatic ionization energy, I^a）、垂直脱離値（vertical detachment ionization energy, I_d^v）、垂直付加値（vertical attachment ionization energy, I_a^v）の三種類がある。そして、しばしばこれらの間には $I_d^v > I^a > I_a^v$ の関係が認められる。今回収集したデータは UPS による決定値であり、この方法では多くの場合スペクトルの第一ピークの値から I_d^v が求まる。しかし、そのピーク形状から I^a が見積れる場合もあるため、原報に測定スペクトルが示されている場合にはそれも検討した。このようにして I^a が求められた化合物もあり、そのような値についてはそれと分かるようにした。

(2) 固体のイオン化エネルギー（I_s）としては、高分子のデータを別にしてイオン化閾値が報告されている物質のほぼ総てについて、その値を集めた。なお、それらの値には、UPS で決められたものと、光電子放出の量子収量の励起光エネルギー依存性（PQY）やその他の方法で決められたものとがある。

孤立分子と固体のイオン化エネルギーの双方が報告されている物質については、分子の気相から固相への凝集に基づく緩和エネルギーも示した。この緩和エネルギーは、両相のイオン化エネルギーの差 $\Delta = I_g - I_s$ として定義される量である。この量がもつ意味などについては、たとえば次の文献を参照されたい。

N. Sato, "Molecular electronic relaxation in organic solids," *Electrical and related properties of organic solids*, R. W. Munn, A. Miniewicz and B Kuchta (eds.), (Kluwer Academic Publishers, Dordrecht, 1997), pp. 157 - 166.

【化合物別の収録順序（イオン化エネルギー）】

Compound	I_g/eV	Ref.	I_s/eV UPS	PQY etc.	Ref.	Δ/eV
RARE GASES AND SIMPLE INORGANIC COMPOUNDS						
Neon	21.56	SKJ85	20.3		SKJ85	1.3
Argon	15.76	SKJ85	13.9		SKJ85	1.9
Krypton	14.00	SKJ85	11.9		SKJ85	2.1
Xenon	12.13	SKJ85	9.7		SKJ85	2.4
Nitrogen	15.57	TBBB70	14.0		HSK75	1.5
			14.2		LFK82	
Oxygen	12.07	TBBB70	10.5		HSK75	1.6
Iodine	9.26*	KKAYI81	6.3_4		YSI87	2.92
H_2O	12.61	TBBB70	9.9		YMS75	2.7
			9.85		Su	
CO_2	13.78	TBBB70	12.3		HSK75	1.5
			11.9		FLK84	
NH_3	10.16	TBBB70	8.3†		YMS75	1.9?
SF_6	15.5	KMJBS76	14.3		FK85	1.2
SIMPLE ORGANIC COMPOUNDS						
Methane	12.70	TBBB70	11.2		HSK75	1.2
Neopentane	10.2*	JSGC72/3	8.7		SI83	1.5
Hexane	10.2_5*	Hp	8.5_5		SI83	1.7
3-Methylpentane	10.2*	Hp	8.8_5		SI83	1.4
2,2-Dimethylbutane	10.2*	Hp	8.8		SI83	1.4
Cyclohexane	9.88	BHHM77	8.2		SI83	1.7
Methylcyclohexane	9.5	BHHM77	8.3		SI83	1.2
Ethylene	10.51	B79a	9.1		?	1.4
1-Hexene	9.37	AB78	7.6		SI78	1.8
Acetylene	11.40	TBBB70	9.7		FK84	1.7
Methanol	10.8*	KKKAYI81	8.7		YMS75	2.1
Ethanol	10.3*	KKKAYI81	8.3		YMS75	2.0
Formaldehyde	10.9*	TBBB70	8.4		YMS75	2.5
CH_2Cl_2	11.2*	KKAIY81	9.4		YSIu	1.8
$CHCl_3$	11.3*	KKAIY81	9.3		YSIu	2.0
CCl_4	11.4*	KKAIY81	9.4		YSIu	2.0
			9.4		FK85	
CBr_4	10.2	GGJOT70	7.3		SI87	2.9
CI_4	9.00	JDS82	5.50		SI87	3.50
C_2Br_4	9.105	PNL83	6.17		SI87	2.9
C_2I_4	8.57	JVMDS82	5.04		SI87	3.5
Tetramethylsilane	9.79	JSGS72/3	8.2		SI83	1.6

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
POLYCYCLIC AROMATIC HYDROCARBONS						
Benzene	9.17	CBH72	7.3		YMS75	2.1
			7.1		Su	
				7.58	AS75	
Naphthalene	8.12*	CBH72	6.4		SSI81	1.7
	8.15	BMS72		6.84	LM62	
				6.76*f*	LM60	
Anthracene	7.36*	CBH72	5.6_7*f*		SSI83a	1.7
	7.47	BCS74	5.75		KSSI82	
			5.70		SSI81	
			5.88		NES74	
			5.7	5.75	HHI77	
				5.65	VS72	
				5.65*f*	LM60	
				5.85	HVK68	
			5.65	5.68	KHHI70	
				5.5	V13	
				5.6-6.2	H12	
				(4.9-5.6)	VZG63	
				5.85	MK70	
				5.95*f*	MK70	
				5.75	FHI72	
Naphthacene	6.89*	CBH72	5.10		SSI81	1.8
	7.04	BCS74	5.25		VZG63	
			5.40	5.43	KHHI70	
				5.26*f*	LM60	
				5.38†	KC61	
				5.3	HVK68	
				5.24	HI66	
				5.31	BL68	
				5.2	ZV71	
				5.3	SHKI76	
				5.4®	APH79	
Pentacene	6.58*	CBH72	4.85		Ht	1.7
	6.74	BMS72	5.1		VZG63	
			5.06	5.04	KHHI70	
				5.08†	KC61	
				4.95	SHKI76	
				5.07	HI66	
Hexacene	6.43	BCS74				
Phenanthrene	7.86	BMS72	6.0_8*f*		SISK85	1.8
			6.1_3		SISK85	
				6.45*f*	LM60	
Chrysene	7.51	BMS72	5.8		SSI81	1.7
				5.73*f*	LM60	
Benz[*a*]anthracene	7.38	BMS72	5.64		Ht	1.7
	7.41	BCS74		5.68*f*	LM60	
			5.76		ZV71	
Benzo[*c*]phenanthrene	7.6	BH72	6.2		SSI81	1.4
	7.60	S77				

Triphenylene	7.81	BS72	6.2		H2t	1.6
	7.89	BCS74				
Napth[2,1-*a*]anthracene	7.2	SSI81	5.45		H2t	1.8
	7.14	BCS74				
Dibenz[*a,h*]anthracene	7.35	SSI81	5.55		H2t	1.8
	7.38	BCS74		5.69*f*	LM60	
Picene	7.5	BMS72	5.7		H2t	1.8
	7.54	BCS74				
Dibenzo[*g,p*]chrysene	6.97*	BCS74	5.8		SSI81	1.2
Pyrene	7.37	BS72	5.5_8*f*		SISK85	1.7
	7.41	BCS74	5.8_3		SISK85	
			5.8		Ht	
			5.84	5.85	HHI74	
				5.81*f*	LM60	
				5.78®	GR69	
Benzo[*a*]pyrene	7.12	BMS72		5.4	BL68	1.7
Dibenzo[*fg,op*]naphthacene	7.26*	SSI81	5.7		SSI81	1.6
	7.40	BCS74				
Perylene	6.90*	SSI81	5.1_2*f*		SSI83	1.8
	7.00	BCS74	5.2		SHKI76	
			5.40	5.33	KHHI70	
				5.40	BL68	
				5.39†	KC61	
				5.40	KHI67	
				5.2	SHKI76	
				5.26®	GR69	
				5.65	ABM76	
Benzo[*ghi*]perylene	7.12*	BMS72	5.2_6*f*		SISK85	1.9
	7.19	BCS74	5.4_4		SISK85	
			5.4		SSI81	
Coronene	7.25*	BS72	5.52		Ht	1.7
	7.36	BCS74	5.59	5.58	HKAIH69	
			5.3		SHKI76	
				5.15	BL68	
Pyranthrene			5.05	5.04	HKAIH69	
Violanthrene A	6.42	SSI81	4.8_6		SSI81	1.6
			5.20	5.06	HKAIH69	
				4.96	HI66	
				5.20†	KC61	
				5.0	ABS74	
Isoviolanthrene A	6.36	SISAI82	4.9_2		SISAI82	1.4
				?5.20†	HKAIH69	
				5.0	ABS74	
Violanthrene B	6.36	SISAI82	4.8_2		SISAI82	1.5
			5.13		HKAIH69	
Isoviolanthrene B	6.54	SISAI82	4.9_6		SISAI82	1.6
Tetrabenzo[*a,cd,j,lm*]perylene	6.58	SISAI82	5.34		SISAI82	1.2
Tetrabenzo[*de,hi,op,st*]pentacene	6.13	SISAI82	4.98		SISAI82	1.2
Quaterrylene	6.11	CS78		4.76	HI66	1.4
Ovalene	6.86	BMS72				
Hexabenzo[*a,d,g,j,m,p*]coronene	6.87	SC78				
Graphite				4.7	WFF71	

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
Biphenyl	8.2	E72				
p-Terphenyl	7.9	HSI75	6.1†	5.8	HSI75	1.8
	7.8	SKEKS84	6.2		SHKI76	
Sexiphenyl	7.2	SKEKS84	5.9		SKEKS84	1.3
Bibenzyl	8.75*	PMRL71	7.2		Su	1.6
Acenaphthene	7.82	BCS74				
Acenaphtylene	8.22	BCS74				
Biphenylene	7.53	E72				
Fluoranthene	7.95	BCS74				
Decacyclene				5.40†	KC61	
				4.74	IKH67	
Azulene	7.43	BCS74				
Benz[*a*]indeno[1,2,3-*cd*]azulene	6.84	SSI81	5.0		SSI81	1.9

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
METHYL- AND PHENYL-SUBSTITUTED AROMATIC HYDROCARBONS						
Toluene	8.67	DR72/3	7.28		AS75	1.4
o-Xylene	8.4*	K72				
m-Xylene	8.5*	K72				
p-Xylene	8.3*	K72				
Hexamethylbenzene	7.85^	VT57				
1-Methylnaphthalene	7.95v	HHPT72				
2-Methylnaphthalene	7.93v	HHPT72				
9-Methylanthracene	7.23	HI74	5.7_5	5.6_8	HHI77	1.5
				5.56	VS72	
2,3-Dimethylanthracene			$5.4_1 f$		SISK85	
9,10-Dimethylanthracene				5.43	VS72	
9-Phenylanthracene	9.0*	SSBV72		6.10	MK70	2.9?
9,10-Diphenylanthracene	7.05	BCS74	5.85		SSI81	1.2
				6.25*f*	MK70	
				6.05	MK70	
				5.85	FHI73	
9,9'-Bianthryl	7.2	HHI77	5.9	5.96	HHI77	1.3
Rubrene	6.41	THSSIF79	5.3		THSSIF79	1.1
				5.10	BL68	

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
OTHER SUBSTITUTED AROMATIC HYDROCARBONS						
Phenol	8.48	E69				
Fluorobenzene	8.9*	BMT68				
Chlorobenzene	8.9*	BMT68				
Bromobenzene	9.0*	BMT68				
Iodobenzene	8.4*	BMT68				
Methoxybenzene	8.0*	BMT68				
Benzonitrile	9.2*	BMT68				
Nitrobenzene	9.6*	BMT68				
p-Dinitrobenzene	10.3	EGR75				
Hexachlorobenzene	8.98	SSI81a	7.3		SSI81a	1.7
Hexabromobenzene	8.80	SSSI81a	7.1		SSSI81a	1.7
Hexaiodobenzene	7.90	SSSI81a	5.9		SSSI81a	2.0
9-Bromoanthracene				6.10	MK70	
9,10-Dichloroanthracene	7.5*	SW74	5.8	5.7_5	HHI77	1.7
				6.10	MK70	
9,10-Dibromoanthracene	7.5*	SW74		6.08	MK70	1.4
1,6-Dicyanopyrene			6.33	6.23	HHI74	
1,3,6,8-Tetrachloropyrene			(6.26)		HHI74	
1,3,6,8-Tetrabromopyrene			5.97		HHI74	
1,3,6,8-Tetracyanopyrene			6.21	6.35	HHI74	
1,3,6,8-Tetranitropyrene			6.56	6.52	HHI74	
HETEROCYCLICS						
Thiophene	8.87	E69				
Pyrrole	8.209	DAEL71				
Pyridine	9.26	TBBB70	7.3†		YMS75	2.0
			(8.0)		FSK84	1.3
Pyrazine	9.28	E69				
Indole	7.75*	E69				
Quinoline	8.5*	VV72				
Isoquinoline	8.4*	VV72				
Carbazole	7.53	HCH75	5.87		KSSI82	1.5
	7.60	RKKG78	6.66		NES74	
Acridine	7.88	HCH75		ca.6.2	MK70	1.7?
	8.13	MMKY75				
Phenazine	8.4	MMKY75		ca.7.1	MK70	1.3?
Phenothiazine	6.82	HH75	$5.1_5 f$		SISK85	1.5
	6.72	DMH77	5.1_8		SISK58	
			5.18		KSSI82	
				4.99	KC61†	
				ca.4.8	Mt	
Dibenzophenothiazine			5.21	5.36	HKAIH69?	
Benzo[*b*]naphtho[2,3-*d*]furan (Brazan)			$5.7_7 f$		SISK85	
			5.8_1			

Compound	I_g/eV	Ref.	I_s/eV UPS	PQY etc.	Ref.	Δ/eV
Promazine				ca.5.1	Mt	
Promazine hydrochloride				ca.5.4	Mt	
Chloropromazine				ca.4.7	Mt	
Chloropromazine hydrochloride				ca.5.2	Mt	
Adenine	8.0*	PPL76	7.0		PI76	1.0
				6.4	SBRPS73	
Guanine	7.85	DYVAM78				
Cytosine	8.45	DYVAM78	7.5		PI76	1.0
Tymine	8.95	DWMM76	7.7		PI76	1.3
Uracil	9.34	DWMM76	7.8		PI76	1.5
Tryptophan	7.3	SI79	6.1		Su	1.2
Reserpine				5.2	Mt	
Tetraphenyl[3,4-*c*]thienothiophene	6.1	MSCL76				
6*a*-Thiathiophthene	8.11	GHLHL71	5.8_8		SKu	2.1
2,5-Dimethyl-6*a*-thiathiophthene	7.59	GHLHL71?	5.7_3		SKu	1.9
2,5-Dimethyl-6*a*-thia-1-azapentalene	7.00	GHLHL71?	5.6_1		SKu	1.4
NMe,NMe,H,H?			(5.2_5)		SKu	
1,2,5,6-Tetramethyl-6*a*-thia-1,6-diazapentalene	6.3*	GGR75	4.93		SKu	1.4
1,8-Dithianaphthalene	7.0*	SCNEH78	5.75		SCNEH78	1.3
Tetrathianaphthacene (TTN)	6.07	SIS81	4.4		SIS81	1.7
			4.55	4.42	KHHI70	
				4.56	HI66	
				4.53	KHI67	
				4.56	IKH67	
			4.75	4.75	BA71	
Tetraselenanaphthacene			4.45		SKIH76	
Tetrathiafulvalene (TTF)	6.4	GSCF73	5.0		NES74	1.4
	6.4	BCW74				
DimethylTTF (DMTTF)	6.00	SIS81	5.1		SIS81	0.9
TetramethylTTF (TMTTF)	6.03	SIS81	4.9		SIS81	1.1
HexamethyleneTTF (HMTTF)	6.06	SSI83	4.6_3		SSI83	1.4
TetrathiomethoxyTTF (TTMTTF)	6.29	SSI83	5.0_0		SSI83	1.3
Bis(ethylenedithiolo)TTF (BEDT-TTF)	6.21	SSI83	4.7_8		SSI83	1.4
DibenzoTTF (DBTTF)	6.68	SIS81	4.4		SIS81	2.3
Tetraselenafulvalene (TSF)	6.68	STE77	4.9_9		SSI83	1.7
TetramethylTSF (TMTSF)	6.27	GKSFBBC79	4.8_4		SSI83	1.4
HexamethyleneTSF (HMTSF)	6.12	SSI83	4.7_5		SSI83	1.4
Hexamethylenetetratellurafulvalene (HMTTeF)	6.81	SSIp	4.87		SSIp	2.9

Compound	I_g/eV	Ref.	I_s/eV UPS	PQY etc.	Ref.	Δ/eV
AMINES						
Methylamine	8.95	TWI85				
Ethylamine	8.78	TWI85				
n-Butylamine	8.59	TWI85				
Dimethylamine	8.18	TWI85				
Diethylamine	7.99	TWI85				
Trimethylamine	7.79	TWI85				
Triethylamine	7.37	TWI85				
Tri(*n*-propyl)amine	7.18	TWI85				
Tetrakis(dimethylamino)ethylene (TDAE)	5.36	CKKLP71				
Aniline	7.71	E69				
N-Methylaniline	7.4*	TBBB70	5.9		Su	1.5
N,*N'*-Dimethylaniline	7.1	EGR75				
o-Phenylenediamine	7.2	TST73				
m-Phenylenediamine	7.44	TST73				
p-Phenylenediamine (PD)	6.84	TST73		5.2	HVK68	1.7
N,*N*,*N'*,*N'*-Tetramethyl-*p*-phenylenediamine (TMPD)	6.2	EGR75	5.0		Su	1.2
				4.63	BL68	
				4.7	HVK68	
1-Naphthylamine	7.1*	M74				
2-Naphthylamine	7.5*	M74				
1,5-Naphthalenediamine	6.74	M74				
1,8-Naphthalenediamine	6.65	M74				
1,6-Pyrenediamine				4.71	BL68	
Diphenylamine	7.18	DR74				
Triphenylamine	6.82	SY92	5.4_2		SY92	1.4
	6.75	DR74				
Diphenyl-*p*-tolylamine	6.78	SY92	5.5_9		SY92	1.2
Phenyldi(*p*-tolyl)amine	6.52	SY92	5.5_2		SY92	1.0
Tri(*p*-tolyl)amine	6.48	SY92	5.4_2		SY92	1.1
Benzidine (BD)				5.10	BL68	
N,*N*,*N'*,*N'*-TetramethylBD				5.26	BL68	
N,*N*-Diethyl-*N'*-(2,4-dinitrobenzo)-*p*-phenylenediamine (AK-4)			5.5		ZV71	
			5.55	5.55	ABB70	

Compound	I_g/eV	Ref.	I_s/eV UPS	PQY etc.	Ref.	Δ/eV
QUINONES						
p-Benzoquinone	9.95	DW69				
p-Chloranil (CA)	9.74	SSI81a	8.1		SSI81a	1.6
				5.0?	HVK68	
p-Bromanil (BA)	9.59	SSI81a	7.4		SSI81a	2.2
				5.0?	HVK81a	
p-Iodanil (IA)	8.58	SSI81a	5.6		SSI81a	3.0
Dichlorodicyano-*p*-benzoquinone (DDQ)			5.68	5.64	HKAIH69	
Anthraquinone	9.05	LSS75	7.6		NSAFI88	1.5
Pyranthrone			5.83	5.71	HKAIH69	
Violanthrone			5.10		KHHI70	
				5.32	KLu	
Indanthrone				5.10	KHI67	
				5.17	KHHI70	
				5.26	KLu	
ELECTRON ACCEPTORS						
Pyromellitic dianhydride (PMDA)	10.9*	GCD79	8.0†		ISSSI76	2.9
Tetracyanoethylene (TCNE)	11.7	ISFIOK74				
Tetracyano-*p*-quinodimethane (TCNQ)	9.5	ISFIOK74	7.4		St	2.1
			7.88		NES74	
Tetracyanonaphthoquinodimethane (TNAP)	8.5	ISSKKI SSITH79	6.0		ISSKKI AAITH79	2.5

Compound	I_g/eV	Ref.		I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
PHTHALOCYANINES AND PORPHYRINS							
Metal-free-phthalocyanine(PC)	6.1*	B79		5.15		VZG63	0.95
					5.12	BL68	
					5.15†	KC61	
					5.20®	P62	
					5.05-5.22	KLu	
				§6.0(error)!		VT60	
				5.0		St1	
Al-PC				5.0		VZG63	
Ca-PC				5.00		KLu	
Cu-PC	6.1*	B79	(α-form)	4.8_8		CSISQ83	1.2
			(β-form)	4.6_2		CSISQ83	1.5
				5.0		VZG63	
					5.0®	P62	
Chlorinated Cu-PC				6.0		St1	
Fe-PC	6.1*	B79		4.85		VZG63	1.25
					4.95†	KC61	
					5.00®	P62	
Pb-PC	6.1*	B79			5.00	KLu	1.1
Mg-PC	6.1*	B79		4.75		VZG63	1.35
					4.96®	P62	
					4.85®	P62a	
					4.70	BBFA72	
					4.80	BBFA72	
Ni-PC	6.2*	B79		4.8		St1	1.4
					4.95†	KC61	
Na-PC				5.1		St1	
					4.94	KLu	
Zn-PC	6.1*	B79		6.0(error)!		VT60	
				5.2		St1	0.9?
Co-PC	6.1*	B79					
Protoporphyrin				4.9		St1	1.2?
Tetraphenylporphyrine (TPP)	6.39v	KR75					
Zn-TPP	6.2	KR75		5.0		SKIY80	1.2
Mg-TPP	6.3	KR75					
				4.85		BA71a	1.5?
Ethioporphyrin					5.29†	KC61	
Hemin				5.3		SKIY80	
Chlorophyll *a*				(4.8)		VZG63	
Chlorophyll *b*				5.25		NFI79	
Cytochrome *c*			(oxidized)	6.1		KSHYI78	
			(reduced)	5.8		KSHIY78	
Cytochrome c_3			(oxidized)	5.4		KSHYI78	
			(reduced)	4.6		SKIY80	

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
METALLOCENES						
Ferrocene	6.72	RWBKHS72	5.4		RNM77	1.3
				5.75	MK70	
Ruthenocene				6.15	MK70	
Nickellocene	6.2	RWBKHS72				
Decamethylferrocene	5.7	CGKPTRS80	4.7		RNM77	1.0
Decamethylnickellocene	4.4	CGKPTRS80				
LONG ALKYL COMPOUNDS						
Hexatriacontane			9.1		SHSH11K77	
Stearic acid (on In_2O_3: crystalline)			7.8		MTSSI85	
(on Cu)			8.1		MTSSI85	
(on Au: amorphous)			8.4		MTSSI85	
Perfluoroundecanoic acid			8.5		MSI88	
1,4-Bis-stearylaminoanthraquinone			6.0		NFSAI87	
Tetrakis(ethylthia)TTF			5.15		STMWSI86	
			5.00		YSIS87	
Tetrakis(propylthia)TTF			4.9_4		Yu	
Tetrakis(butylthia)TTF			4.8_3		Yu	
Tetrakis(pentylthia)TTF			4.8_6		Yu	
Tetrakis(hexylthia)TTF			4.8_3		Yu	
Tetrakis(hepthylthia)TTF			4.8_9		Yu	
Tetrakis(octylthia)TTF			4.8_0		STMWSI86	
Tetrakis(nonylthia)TTF			4.6_5		STMWSI86	
Tetrakis(decylthia)TTF			4.70		STMWSI86	
			4.6_5		Yu	
			4.6_0		YSIS87	
Tetrakis(undecylthia)TTF			4.6_4		Yu	
Tetrakis(dodecylthia)TTF			4.6_7		Yu	
Tetrakis(tridecylthia)TTF			4.6_3		Yu	
Tetrakis(tetradecylthia)TTF			4.7		STMWSI86	
Tetrakis(pentadecylthia)TTF			4.7_1		Yu	
Tetrakis(hexadecylthia)TTF			4.7_4		Yu	
Tetrakis(heptadecylthia)TTF			4.6_9		Yu	
Tetrakis(octadecylthia)TTF			4.8_5		STMWSI86	
DIACETYLENE COMPOUNDS						
2,4-Hexadiyne-1,6-bis(*p*-toluene sulfonate)				6.9®	A82	
				7.1	MSB82	
Tricosa-10,12-diynoic acid			6.7		NFSAI87	

DYES AND PIGMENTS

#: Compound cannot be identified definitely.
#1: Probably.
#2: Probably 3-allyl-3'-ethyl-5',6'-dimethyl-4-keto-5-[2-(4(1*H*)-dihydroauinolinylidene)-ethylidene]-thiazolinooxacyanine bromide.
#3: The figure in the original paper corresponds to 3-amino-2-*p*-methoxyphenylindene-1-one.
#4: Probably 1-oxo-3-oxido-2-pyridinioindene is a better structure reflecting the properties of this.
#5: The structural formula in the original paper corresponds to 3-phenylamino-2-phenylindenone-1.
#6: Probably victoria pure blue BO.

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
Alizaline Dyes						
Alizarin blue	7.35	V60	5.4		KV61	1.9
Azine Dyes						
Phenosafranine			5.4		KV61	
Azo Dyes						
Bismarck brown				5.5	Mt	
Carotenoids						
β-Carotene	6.5	DYVAM78	5.5§		VT60	1.0
Cyanines						
Cyanine#				5.28	F30	
Kryptocyanine				5.0	ABVT67	
				4.2-3	N61	
Pinacyanol	7.25Δ		4.9		VT60a	2.35
Pinacyanol (chloride)				4.6	N61	
Pinakryptol yellow			5.4		KAB71	
Quinoline blue#1 (ethylcyanine)	7.35	V60	4.5		KV61	2.85
3,3'-Diethylthiacyanine						
bromide			5.5		TYIISOTu	
perchlorate			5.4		TYIISOTu	
tosylate (*p*-toluene sulfonate)			5.65		TYIISOTu	
3,3'-Diethylthiacarbocyanine				5.0	N61	
bromide			5.15		TYIISOTu	
perchlorate			5.05		TYIISOTu	
tosylate			5.27		TYIISOTu	
3,3'-Diethylthiadicarbocyanine						
bromide			4.9		TYIISOTu	
perchlorate			4.9		TYIISOTu	
tosylate			5.1		TYIISOTu	

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
3,3'-Diethylthiatricarbocyanine						
bromide			4.7		TYIISOTu	
perchlorate			4.73		TYIISOTu	
tosylate			5.0		TYIISOTu	
3,3'-Diethylenthiapentacarbocyanine iodide				5.1	ABVT67	
3-Allyl-3'-ethyl-5,6'-dimethyl-4-keto-5-(1-dihydro-quinolidene-4-ethylidene)thiazalinooxacyanine bromide#2			4.8		KV61	
3,3'-Dimethyl-9,11,15,17-bis(*b,b'*-dimethyltri-methylene)thiapentacarbocyanine iodide				5.2	ABVT67	
1,1'-Dimethyl-10-phenyl-2,2'-carbocyanine bromide				4.6	N61	
Furanquinone Pigments						
8,13-dioxodinaphto[2,1-*b*:2',3'-*d*]furan-		(on Al)	6.45		PN72	
6-(2-pyridyl)carboxamide		(on ox. Al)	6.3		PN72	
Indene Derivatives						
3-Amino-2-methoxyphenylindone-1#3			5.25		BA69	
				5.50	GST73	
2-Pyridino-1,3-indanedione (betaine)#4				5.75	NSS77	
3-Phenylamino-2-phenylindone-1#5			5.35		BA69	
				5.50	GST73	
1-Phenylamino-2-phenylindene-*i*-thione-3				5.25	BA69	
				5.25	GST73	
trans-Bis-bindodiene#			4.80		BA69	
			4.85	4.85	ABB71	
Merocyanines						
Merocyanine#	7.35	V60	5.6		KV61	1.75
3-Ethyl-5-(3-ethylbenzothiazolin-2-ylidene)rhodanine			5.55		TSIT86	
3-Ethyl-5-[2-(3-ethylbenzothiazolin2-ylidene)-ethylidene]rhodanine			5.10		TSIT86	
3-Ethyl-5-[4-(3-ethylbenzothiazolin2-ylidene)-2-butenylidene]rhodanine			4.85		TSIT86	
3-Ethyl-5-[6-(3-ethylbenzothiazolin2-ylidene)-2,4-hexadienylidene]rhodanine			4.75		TSIT86	
3-Ethyl-5-{4-[3-(3-sulfopropyl)benzothiazolin-2-ylidene]-2-butenylidene}rhodanine			4.80		TSIT86	
3-Ethyl-5-[2-(3-ethylthiazolidin-2-ylidene)ethyl-indene]rhodanine			5.20		TSIT86	
3-Carboxymethyl-5-[2-(3-ethylthiazolidin-2-ylidene)ylideneethylidene]rhodanine			5.20		TSIT86	
5-[2-(1,3-Diethyl-5-chlorobenzimidazolin-2-ethylidene]-3-hexylrhodanine			5.15		TSIT86	
5-[2-(1,3-Diethyl-5-nitrobenzimidazolin-2-ylidene)ethylidene]-3-hexylrhodanine			5.20		TSIT86	

Compound		I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
Oxazine Dyes							
Nile blue A					5.17	Mt	
Triphenodioxazine (TPDO)				4.94		SSNFKI86	
DichloroTPDO				5.75		SSNFKI86	
Thiazine Dyes							
Methylene blue				5.4		KV61	
					5.2	Mt	
Triphenodithiazine(TPDT)				5.12		SSNFKI86	
DichloroTPDT				5.61		SSNFKI86	
TetrachloroTPDT					5.2	Mt	
Triphenylmethane Dyes							
Aurin				5.4§		VZG63	
Crystal Violet				5.0		KV61	
					3.45	Mt	
					5.00	KLu	
	(Br-)				5.0	N61	
	(Cl-)				5.1	N61	
	(acetate)				5.2	N61	
Malachite green				5.2		KV61	
	(Cl-)				5.2	N61	
	(oxalate)				ca.5.2	N61	
Night blue					4.7	Mt	
Victoria pure blue 30#6					5.00	Mt	
Fuchsin					4.15	F30	
Basic fuchsin (Cl)					5.6%	N61	
Viologen Dyes							
Methyl viologen	(reduced)				3.6	MKI76	
	(oxidized)				4.8	4.8-9 MKI76	
Xanthene Dyes							
Erythrosine					5.5	VT60	
Erythrosine (Na)					5.5%	N61	
Rhodamin B					5.10®	GR69	
				5.1		KV61	
Rhodamin 6G		7.26	V60	5.7		VT60	1.6
Others							
Indigo red#		7.32	V60		5.0	KV61	1.3
Indigo blue		7.17	V60		5.4	KV61	1.7
Golden-orange indanthrene#					(5.3-5.8)	VZG63	
Pinakryptol#				5.2§		VT60a	
Yellow indanthrene#					(5.2-5.6)	VZG63	

MOLECULAR COMPLEXES

DDQ: Dichlorodicyano-*p*-benzoquinone PMDA: Pyromellitic dianhydride
TCNQ:Tetracyanoquinodimethane TMPD: *N*,*N*,*N'*,*N'*-Tetramethyl-*p*-phenylenediamine
TNB: 1,3,5-Trinitrobenzene

Compound	I_g/eV	Ref.	I_s/eV UPS	I_s/eV PQY etc.	Ref.	Δ/eV
Organic-Organic Complexes						
(Anthracene)(TNB)				(5.88)	BL68	
(Anthracene)(TCNQ)			6.17		NES74	
				5.03	BL68	
(Anthracene)(PMDA)			6.00		KSSI82	
			6.0		ISSSI76	
				5.26	BL68	
(Pyrene)(TNB)				5.60	BL68	
(Pyrene)(TCNQ)				5.70	BL68	
(1,2-Benzanthracene)(TCNQ)				5.00	BL68	
(Chrysene)(TNB)				(5.50)	BL68	
(Coronene)(Trinitrobenzene)				5.62	HKAIH69	
(Perylene)(TNB)				(5.54)	BL68	
(Perylene)(Dicyanomethylenetrinitrofluorene)				5.23	BL68	
(Perylene)(*p*-Chloranil)				5.40	BL68	
(Perylene)(*o*-Chloranil)				5.35	BL68	
(Perylene)(TCNQ)				(5.50)	BL68	
(Perylene)(PMDA)				5.16	BL68	
(Violanthrene)(*o*-Chloranil)				5.32†	KC61	
(Carbazole)(TCNQ)			6.76		NES74	
(Carbazole)(PMDA)			6.22		KSSI82	
(Acridine)(PMDA)			6.3		KSSI82	
(Phenothiazine)(*o*-Chloranil)				5.38†	KC61	
(Phenothiazine)(PMDA)			5.41		KSSI82	
(*N*-Methylphenazinium)(TCNQ)			6.0		NES74	
(Bibenzophenothiazine)(DDQ)				4.99	HKAIH69	
(Bibenzophenothiazine)$_2$(DDQ)				4.75	HKAIH69	
(Tetrathianaphthacene)(TCNQ)$_2$			4.75		AAB77	
(Tetrathiafulvalene)(TCNQ)			(5.07)¿		NES74	
			(5.6)¿		GPEMS74	
(*p*-Phenylenediamine)(Chloranil)				5.4	HVK68	
(*p*-Phenylenediamine)(Bromanil)				5.4	HVK68	
(TMPD)(*p*-Chloranil)				5.0	HVK68	
				4.88	BL68	
(TMPD)(*p*-Bromanil)				4.85	HVK68	
				4.87	BL68	
(TMPD)(TCNQ) (from *p*-xylene)				4.86	BL68	
(from glacial acetic acid)				4.72	BL68	
(1,6-Diaminopyrene)(*o*-Chloranil)				4.88	BL68	
(1,6-Diaminopyrene)(*p*-Chloranil)				4.39	BL68	
(1,6-Diaminopyrene)(*p*-Bromanil)				(4.65)	BL68	
(1,6-Diaminopyrene)(TCNQ)				4.58	BL68	
(Benzidine)(TCNQ)				5.03	BL68	
(*N*,*N*,*N'*,*N'*-Tetramethylbenzidine)(TNB)				4.72	BL68	

(H_2-Phthalocyanine)(*o*-Chloranil)		5.29†	KC61
(Fe-Phthalocyanine)(*o*-Chloranil)		5.32†	KC61
(Decamethylferrocene)(TCNQ)2	4.7		RNM77
(Quinolinium)($TCNQ)_2$	5.35		NES74
	4.85		HKAIH69

Inorganic-Organic Complexes

Li(TCNQ)	5.6		NES74
Na(Anthracene)		3	MKu
Na(*o*-Chloranil)		5.50	Mt
Na(TCNQ)	5.6		NES74
K(*o*-Chloranil)		5.35	Mt
K(TCNQ)	5.8		GPEMS74
Rb(Benzonitrile)		5.01	KTI70
		5.05	KI72
Rb(Benzonitrile) (+H_2)		4.90	KTI70
Cs(Pyrene)		1.5	OIIH65
Cs(Perylene)	2.2		YSIu
Cs(Triphenylene)		2.40	KI72
Cs_2(Triphenylene)		2.43	KI72
Cs(Violanthrene)		1.54	IH63
		2.95	ABS74
Cs(Tetranitropyrene)		1.8	OIIH65
Cs(Tetrachloropyrene)		1.8	OIIH65
Cs(Tetrabromopyrene)		1.8	OIIH65
Cs(Tetracyanopyrene)		1.3	OIIH65
$Cs_2(TCNQ)_3$		3.0	LSS75a
NH_4(TCNQ)	4.9		SKSI75

NOTES

Gas phase

*: Value read from the reported spectrum.
v: Vertical ionization energy.
^: Value determined from photoionization experiment.

Solid state

†: Raw value determined from photoemission quantum yield measurements.
(Those authors also reported values corrected for estimated surface/bulk difference effects).
( ): Values claimed to be dubious by the authors.
?: Dubious values.
f: Value for a single crystal.
®: Millikan method.
!: Stated to be erroneous in VZG63.
Δ: Cast doubt on the possibility of decomposition by Nelson [N67].
§: Photoelectron spectrum is rather featureless.
%: Resolution is reduced to 0.4 eV due to low light intensity.
¿: Cast doubt on the possibility of different surface composition from the bulk [LSS75, NSE75].

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電子親和力

固体物性研究の観点から関心がもたれると思われる有機化合物を中心として、実験によって決められた孤立分子の電子親和力の値を集めた。

データの収集にあたっては、十年ほど前に相次いで総説（たとえば、後に掲げる文献のうち DMB84, KC87, JB87, LBLHLM88, CW89 など）が出版されて以来、この方面の研究がクラスターを含むイオンやラジカルなどに向かったため、実質的にはあまりデータが増えていないことを踏まえて、それらの総説中に取り上げられた物質とその値を主に選んだ。

ただし、近年、アメリカの National Institute of Standards and Technology (NIST) が種々のデータベースを構築している中に S. G. Lias らが編集している電子親和力のデータベースも存在するので、その最新（1998 年 11 月）版の内容もチェックしたうえで必要に応じてデータを NIST98 からの引用として加えた。

いうまでもなく、電子親和力の実験的な決定方法は次頁に示すように一通りではない。そのため、方法の違いによって得られる値には偏差が認められる場合がある。また、同じ方法を用いたとしても測定装置に依存する誤差要素が異なりうる。これらの結果として、同一物質に対する報告値が広い範囲にわたってばらつく場合も少なくない。そこで、今回収集したデータにはなるべくその決定方法や誤差を記すこととし、また、複数の値が報告されている場合には、一応の評価を行って selected value を示すことにした。ただし、このような作業は実は膨大な労力を要するものであるため、決して十分に行えたとはいえない状況にある。なお、上述の NIST のデータベースについては、収録されている値の出典が明示されていないため、その評価は必ずしも容易ではないことを付記しておく。

分子とその負イオンとの間に起こる電子の付着／脱着過程を考えると、分子の電子親和力の値には断熱値（adiabatic electron affinity, A^{a}）、垂直脱着値（vertical detachment electron affinity, A_{d}^{v}）、垂直付着値（vertical attachment electron affinity, A_{a}^{v}）の三種類がある。そして、しばしばこれらの間には $A_{d}^{v} > A^{a} > A_{a}^{v}$ の関係が認められる。今回収集したデータがこれらのどれに当たるかを本来は明確に示すべきだが、それには値のそれぞれについて少なくとも原報を調べる必要があり、そこまでは手が回らなかった。ただし、どの電子親和力に当たるのか示したものが一部にはあり、また測定方法の判明している値については、次頁に記す方法の特徴から求まる値の素性が分かるものもある。

【電子親和力の測定方法】

略号	方法名 → 主に求まる値 （英語名称）	《参考文献》
CD (or CI)	**衝突脱離（イオン化）法** → A_d^v （Collisional detachment; Collisional ionization technique）	《JB79》
CT (or ECT)	**（吸熱）電荷移動法** → A_d^v （Charge transfer; Endothermic charge-transfer）	《JB79》
CTS	**電荷移動吸収分光法［溶液法］** → A^v （Charge-transfer spectroscopic method in solution）	《CW75》
EC (or ECD)	**電子捕獲法** → A^a （Electron capture; Electron capture detector technique）	《CW89》
ET	**電子透過（分光）法** → A^a （Electron transmission）	《JB87》
ETE	**電子移動平衡法** → A^a （Electron transfer equilibrium）	《KC87》
HWRP	**半波還元電位［溶液法］** → A^a （Half-wave reduction potential method in solution）	《CW89》
LPES	**レーザー光電子分光法** → A_d^v （Laser photoelectron spectroscopy）	《HL85》
LPT (or LPD)	**レーザー光脱離閾値法** → A_d^v （Laser photodetachment threshold; Laser photodetachment technique）	《HL85》
MT (or M)	**マグネトロン法** → A^a （Magnetron method）	《CW89》
PT	**光脱離閾値法** → A_d^v （Photodetachment threshold）	《HL85》

【化合物別の収録順序（電子親和力）】

SIMPLE INORGANIC COMPOUNDS
- Diatomic molecules
- Triatomic molecules
- Polyatomic molecules

SIMPLE ORGANIC COMPOUNDS
- Methane derivatives
- Benzophenone derivatives
- Alkene derivatives
- Alkyne derivatives

AROMATIC HYDROCARBONS AND THEIR DERIVATIVES
- Benzene derivatives
- Naphthalene derivatives
- Anthracene derivatives
- Others

QUINONES AND THEIR DERIVATIVES
- Benzoquinone derivatives
- Naphthoquinone derivatives
- Anthraquinone derivatives

NONBENZENOID COMPOUNDS

HETEROCYCLIC COMPOUNDS

REFERENCES

Compound	A_g/eV	Method	Ref.	Comment
SIMPLE INORGANIC COMPOUNDS				
Diatomic molecules				
O_2	0.440(8)	LPES	DMB84	
S_2	1.670(15)	LPES	DMB84	
Se_2	1.96(5)	LPT	SCMFB89	
Te_2	1.92(7)	LPES	DMB84	
NO	0.024(10)	LPES	DMB84	
F_2	3.08(10)	CT	DMB84	
Cl_2	2.38(10)	CT	DMB84	
Br_2	2.55(10)	CT	DMB84	
I_2	2.55(5)	CT	DMB84	
IBr	2.55(10)	CT	DMB84	
Triatomic molecules				
CS_2	0.895(20)	LPES	OE	
NO_2	2.275(25)	LPT	DMB84	selected value
	2.30	ETE	KC87	
N_2O	≤1.465	CT	DMB84	
O_3	2.1028(25)	LPT	DMB84	
SO_2	1.097(36)	LPES	CBH74	
	1.107(8)	LPES	NE	selected value
S_2O	1.877(8)	LEPS	NE	
SeO_2	1.83(5)	LPES	SCMFB89	
Polyatomic molecules				
$Fe(CO)_2$	1.22(2)	LPES	DMB84	
$Fe(CO)_3$	1.8(2)	LPES	DMB84	
HNO_3	0.57(15)	CD	DMB84	
$Ni(CO)_2$	0.643(14)	LPES	DMB84	
$Ni(CO)_3$	1.077(13)	LPES	DMB84	
SF_6	0.5 - 0.8	CD	CW89	
	1.05(10)	ETE	GCK85	
	1.15(15)	EC	CW89	
	1.10(10)		CW89	selected value
	1.4(4)	MT	CW89	
PCl_3	0.82(10)	CD	DMB84	
PBr_3	1.59(15)	CD	DMB84	
SO_3	≥1.70(15)	CD	DMB84	
C_{60}	2.6-2.8		YPCCS87	
	2.650(50)	LPD	WCJS91	
C_{72}	3.300		NIST98	
C_{78}	3.010		NIST98	
C_{80}	3.700		NIST98	
C_{84}	3.050		NIST98	

Compound	A_g/eV	Method	Ref.	Comment
SIMPLE ORGANIC COMPOUNDS				
Methane derivatives				
CH_3CN	–2.84		LBLHLM88	
CH_3I	0.2(1)	CT	DMB84	
CH_3NO_2	0.44(20)	CD	DMB84	
	0.45(10)	EC	CW89	selected value
	0.48(10)	ETE	KC87	
CH_2Cl_2	1.31(5)	MT	CW89	
$CHCl_3$	1.70(5)	MT	CW89	selected value
	1.76		LBLHLM88	
CCl_4	2.0(2)	CT	CW89	
	2.06(10)	MT	CW89	selected value
	2.08(20)	CT	CW89	
Benzophenone derivatives				
Benzophenone	0.64(5)	EC	CW89	selected value
	0.65(10)	CT	CW89	
4-Fluorobenzophenone	0.64(5)	EC	CW89	
	0.65(5)		CW89	selected value
	0.66(10)	CT	CW89	
4-Bromobenzophenone	0.90		CW89	
4-Chlorobenzophenone	0.8(1)	EC	CW89	
	0.84(10)	CT	CW89	selected value
4-Iodobenzophenone	1.00		CW89	
4-Methoxybenzophenone	0.64		CW89	
Perfluorobenzophenone	1.61		LBLHLM88	
Alkene derivatives				
Ethylene	–1.3		JB87	adiabatic value
	–1.74		JB87	vertical value
Trichloroethylene	0.400		NIST98	
1,1-Diphenylethylene	0.390		NIST98	
Maleic anhydride	1.4(2)	CD	DMB84	
	1.42(10)		CW89	selected value
	1.44(10)	CT	CW89	
trans-Dicyanoethylene	0.78(10)	MT	CW89	
	1.0(2)		CW89	
	1.24(10)	ETE	KC87	selected value
Tetracyanoethylene	2.3(3)	PT	DMB84	
	2.88(5)	MT	FP67	
	2.90(10)	CTS	CW89	selected value
	3.17(10)	ETE	CK86	
t*rans*-2-Butene	–2.10		LBLHLM88	
Butadiene	–0.62	ET	JB87	
Hexacyanobutadiene	3.24(7)	MT	CW89	
Cyclohexene	–2.13	ET	JB87	
Cyclooctatetraene	0.60		CW89	
1,3-Cyclopentadiene	–1.05		LBLHLM88	
Alkyne derivatives				
Acetylene	–2.6	ET	JB78	

Compound	A_g/eV	Method	Ref.	Comment
AROMATIC HYDROCARBONS AND THEIR DERIVATIVES				
Benzene derivatives				
Benzene	0.72	EC	CW89	adiabatic value
	–1.15	ET	CW89	vertical value
tert-Butylbenzene	–1.06		LBLHLM88	
Bromobenzene	–0.70		LBLHLM88	
Chlorobenzene	–0.75		LBLHLM88	
o-Dichlorobenzene	0.09		CW89	
p-Dichlorobenzene	0.18		CW89	
Pentachlorobenzene	0.729		NIST98	
Hexachlorobenzene	0.915		NIST98	
o-Dicyanobenzene	0.95(10)	CT	CW89	
	1.0(1)		CW89	selected value
	1.04(10)	MT	CW89	
p-Dicyanobenzene	1.10		CW89	
Fluorobenzene	–0.89		LBLHLM88	
1,2,3,5-Tetramethylbenzene	0.108		NIST98	
1,2,4,5-Tetramethylbenzene	0.048		NIST98	
Pentamethylbenzene	0.182		NIST98	
Hexamethylbenzene	0.121		NIST98	
Nitrobenzene	>0.7(2)	CT	DMB84	
	>0.8(2)	EC	CW83	
	1.01(10)	CT	CW89	selected value
o-Dinitrobenzene	1.65		CW89	
m-Dinitrobenzene	1.62		CW89	
p-Dinitrobenzene	1.96		CW89	
o-Bromonitrobenzene	1.17		CW89	
m-Bromonitrobenzene	1.32		CW89	
p-Bromonitrobenzene	1.29		CW89	
o-Chloronitrobenzene	1.12		CW89	
m-Chloronitrobenzene	1.28		CW89	
p-Chloronitrobenzene	1.26		CW89	
m-Cyanonitrobenzene	1.53		CW89	
p-Cyanonitrobenzene	1.72		CW89	
m-Fluoronitrobenzene	1.22		CW89	
p-Fluoronitrobenzene	1.11		CW89	
m-Methoxynitrobenzene	1.04		CW89	
p-Methoxynitrobenzene	0.91		CW89	
m-(Trifluoromethyl)nitrobenzene	1.41		CW89	
2,3-Dimethylnitrobenzene	0.81		CW89	
2,6-Dimethylnitrobenzene	0.71		CW89	
3,4-Dimethylnitrobenzene	0.89		CW89	
1,3,5-Trichlorobenzene	0.34		CW89	
1,2,4,5-Tetrachlorobenzene	0.45		CW89	
1,2,4,5-Tetracyanobenzene	2.15(22)	MT	CW89	
1,4-Dicyanotetrafluorobenzene	1.89		CW89	
Pentafluorobenzene	0.434		NIST98	
Hexacyanobenzene	2.48(13)	MT	CW89	
Hexafluorobenzene	0.52(10)	CT	CGHK86	
	0.86(3)	EC	CW89	selected value
	1.20(8)	MT	CW89	

Compound	A_g/eV	Method	Ref.	Comment
(Trifluoromethyl)benzene	0.002		NIST98	
Acetophenone	0.34		CW89	
p-Cyanoacetophenone	1.13		LBLHLM88	
o-Nitroacetophenone	1.38		LBLHLM88	
m-Nitroacetophenone	1.31		LBLHLM88	
p-Nitroacetophenone	1.55		LBLHLM88	
Aniline	–1.13		LBLHLM88	
m-Nitroaniline	0.95		LBLHLM88	
N,*N*-Dimethyl-3-nitroaniline	0.95		CW89	
Anisole	–1.09		LBLHLM88	
Benzaldehyde	0.41		CW89	
m-Phthalaldehyde	0.971		NIST98	
m-Cyanobenzaldehyde	1.00		LBLHLM88	
p-Cyanobenzaldehyde	1.22		LBLHLM88	
o-Nitrobenzaldehyde	1.51		LBLHLM88	
m-Nitrobenzaldehyde	1.41		LBLHLM88	
p-Nitrobenzaldehyde	1.67		LBLHLM88	
Benzonitrile	0.24		CW89	
o-Nitrobenzonitrile	1.61		LBLHLM88	
m-Nitrobenzonitrile	1.56		LBLHLM88	
p-Nitrobenzonitrile	1.72		LBLHLM88	
2,6-Dinitrobenzonitrile	0.72		LBLHLM88	
3,5-Dinitrobenzonitrile	2.16		LBLHLM88	
Pentafluorobenzonitrile	0.94		LBLHLM88	
Toluene	–1.11		LBLHLM88	
o-Nitrotoluene	0.92		CW89	
m-Nitrotoluene	0.8(2)	EC	CW89	
	0.99(10)	CT	CW89	selected value
p-Nitrotoluene	0.95		CW89	
Octafluorotoluene	>1.7(3)	CT	DMB84	
Phenol	–1.01		LBLHLM88	
o-Xylene	–1.12		LBLHLM88	
m-Xylene	–1.06		LBLHLM88	
p-Xylene	–1.07		LBLHLM88	
Biphenyl	–0.3		LBLHLM88	
o-Nitrobiphenyl	1.07		CW89	
p-Nitrobiphenyl	1.20		CW89	
Perfluorobiphenyl	0.91		LBLHLM88	
Phthalic anhydride	1.21		CW89	

Compound	A_g/eV	Method	Ref.	Comment
Naphthalene derivatives				
Naphthalene	0.15		CW89	
1-Chloronaphthalene	0.28		CW89	
1-Ethylnaphthalene	0.147		NIST98	
2-Ethylnaphthalene	0.195		NIST98	
1-Methylnaphthalene	0.160		NIST98	
2-Methylnaphthalene	0.143		NIST98	
1-Naphthalenecarbonitrile	0.6765		NIST98	
1-Naphthalenecarboxaldehyde	0.681		NIST98	
2,3-Dimethylnaphthalene	0.173		NIST98	
2,6-Dimethylnaphthalene	0.160		NIST98	
1-Naphthaldehyde	0.68(3)	EC	CW89	
	0.69(3)		CW89	selected value
	0.70(10)	CT	CW89	
2-Naphthaldehyde	0.62(3)	EC	CW89	
	0.63(3)		CW89	selected value
	0.65(10)	CT	CW89	
1-Nitronaphthalene	1.23		CW89	
2-Nitronaphthalene	1.18		CW89	
1,3-Dinitronaphthalene	1.78		LBLHLM88	
1,5-Dinitronaphthalene	1.77		LBLHLM88	
Anthracene derivatives				
Anthracene	0.56(5)	EC	CW89	
	0.57(5)		CW89	selected value
	0.60(10)	CT	CW89	
1-Chloroanthracene	0.78		CW89	
2-Chloroanthracene	0.75		CW89	
9-Chloroanthracene	0.86		LBLHLM88	
9-Cyanoanthracene	1.27		LBLHLM88	
9-Nitroanthracene	1.43		LBLHLM88	

Compound	A_g/eV	Method	Ref.	Comment
Others				
Phenanthrene	0.31		CW89	
Naphthacene	0.88		CW89	
Chrysene	0.41		CW89	
Triphenylene	0.29		CW89	
Benz[*a*]anthracene	0.64		CW89	
Benzo[*c*]phenanthrene	0.54		CW89	
Pyrene	0.56		CW89	
Dibenz[*a,h*]anthracene	0.64		CW89	
Dibenz[*a,j*]anthracene	0.64		CW89	
Pentacene	1.392		NIST98	
Perylene	0.350		NIST98	
Benzo[*a*]pyrene	0.67		CW89	
Benzo[*e*]pyrene	0.534		NIST98	
Picene	0.542		NIST98	
Benzo[*ghi*]perylene	0.420		NIST98	
Coronene	0.540		NIST98	
Indene	0.173		NIST98	
Biphenylene	0.890		NIST98	
Fluorene	0.278		NIST98	
Acenaphthylene	0.403		NIST98	
Fluoranthene	0.63		CW89	
QUINONES AND THEIR DERIVATIVES				
Benzoquinone derivatives				
o-Benzoquinone	1.620		NIST98	
p-Benzoquinone	1.34(9)	MT	CW89	
	1.89(30)	CD	DMB84	
	1.91(10)	CT	CW89	selected value
	1.92(10)	CT	CW89	
Methyl-*p*-benzoquinone	1.85		CW89	
Phenyl-*p*-benzoquinone	2.04		CW89	
tert-Butyl-*p*-benzoquinone	1.88		CW89	
2,6-Di(tert-butyl)-*p*-benzoquinone	1.88		CW89	
2,5-Dichloro-*p*-benzoquinone	2.41		CW89	
2,6-Dichloro-*p*-benzoquinone	2.48		CW89	
2,5-Dimethyl-*p*-benzoquinone	1.77		CW89	
Trimethyl-*p*-benzoquinone	1.63		CW89	
Tetrafluoro-*p*-benzoquinone	2.27	MT	CW89	
	2.45(10)	CT	CW89	
	2.6(1)		CW89	selected value
	2.70(10)	CT	CW89	
	2.92(20)	CD	DMB84	
Tetrachloro-*o*-benzoquinone	2.440		NIST98	
Tetrachloro-*p*-benzoquinone	2.40(26)	MT	CW89	
	2.7(1)		CW89	selected value
	2.76(20)	CD	DMB84	
	2.77(10)	CT	CW89	
	2.78(10)	CT	CW89	
Tetrabromo-*p*-benzoquinone	2.44(20)	CD	DMB84	

Compound	A_g/eV	Method	Ref.	Comment
Tetracyano-*p*-quinodimethane	2.80(10)	MT	CW89	
	2.80(10)	CD	CW89	
	2.80(3)	CD	CW89	
	2.8(3)	CD	DMB84	
	2.82(10)		CW89	selected value
	2.83(18)	MT	CW89	
Tetrafluorotetracyano-*p*-quinodimethane	3.38(10)		CW89	
Naphthoquinone derivatives				
1,4-Naphthoquinone	1.81		CW89	
2,3-Naphthoquinone	2.19		LBLHLM88	
2-Methyl-1,4-naphthoquinone	1.74		CW89	
Anthraquinone derivatives				
9,10-Anthraquinone	1.15(10)	MT	CW89	
	1.59		CW89	selected value
2-*tert*-Butyl-9,10-anthraquinone	1.56	ETE	HCSK88	
2-Ethyl-9,10-anthraquinone	1.56	ETE	HCSK88	
NONBENZENOID COMPOUNDS				
Azulene	0.69(5)	EC	CW89	selected value
	0.69(10)	CT	CW89	
HETEROCYCLIC COMPOUNDS				
Pyrrole	–2.38		LBLHLM88	
Furan	–1.76		LBLHLM88	
Thiophene	–1.17		LBLHLM88	
Pyridine	–0.62		LBLHLM88	
2,3,5,6-Tetracyanopyridine	1.59(10)	CT	CW89	
	2.12(17)	MT	CW89	selected value
	2.17		CW89	
Pentafluoropyridine	0.681		NIST98	
Pyridazine	0.250		NIST98	
Pyrazine	0.400		NIST98	
1,3,5-Triazine	0.450		NIST98	
Acridine	0.906		NIST98	
Phenazine	1.305		NIST98	

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