「第 7 章 Chemical Abstracts」練習問題
(1973 年以降の資料を使うことが望ましい)

回答は次のようなかたちで記載することが望ましい.

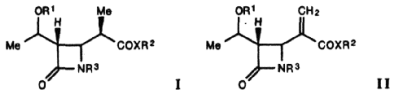
① Index Guide: 1986 年
Nitrilotriacetic acid
See Glycine, N,N-bis(carboxymethyl)- [139-13-9] (Index Guide の記載を写す)
② Chemical Substance Index 132 巻: (該当する索引を調べ, その見出しを記載する)
Glycine
N,N-bis(carboxymethyl)- (nitrilotriacetic acid) [139-13-9]
Trisodium salt [5064-31-3]
composite tablet for deliming or disinfection of water in cooking or hygienic applications, P141612g (適当な文献項目を一件選んで記載する)
③ CA 132, P141612g, Tablet composition for deliming or disinfection of water reservoirs in cooking or hygienic applications. Waeschenbach, Guido; Wiedemann, Ralf; Carbonell, Enric; Endlein, Edgar; Gibis, Karl-Ludwig (Benckiser N.V., Neth.). Ger. Offen. DE 19834172 A1 20000203, 22 pp. (German). (前記文献の抄録を調べ, 書誌事項を記載する)

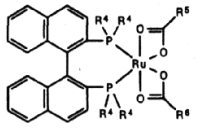
化学物質の問題については, Index Guide, Formula Index, Chemical Substance Index に記載されている CAS 登録番号を転記することが望ましい.

問題 1
自分の師事した先生または先輩の論文を一件調べなさい.
(Author Index → 本誌)

ここでは「野依良治」先生を例に取る. 名前は姓が先に書かれる. Author Index (例では 110 巻) で Noyori, Ryoji を見ると, 始めに See Hayakawa, Yoshihiro;… などと記載されているが, これらはここに示された著者が第一著者となっている文献なので, その著者の項目を見よという意味である. その後に, 長いダッシュで始まっているのが Noyori, Ryoji 先生が第一著者となっている文献である.

110: 231338x **Preparation of β-lactams by asymmetric hydrogenation in the presence of ruthenium catalysts.** Noyori, Ryoji; Kitamura, Masahito (Sankyo Co., Ltd.) **Jpn. Kokai Tokkyo Koho JP 63,290,862 [88,290,862]** (Cl. C07D205/08), 28 Nov 1988, Appl. 87/122,619, 21 May 1987; 8 pp. Title compds. **I** (R^1, R^2, R^3 = H,





protecting group; X = O, S) are prepd. by asym. redn. of β-lactams **II** in the presence of asym. ruthenium compds. **III** [R^4, R^5, R^6 = (substituted) aryl, alkyl, C_{3-7} cycloalkyl]. A mixt. of (3*S*,4*S*)-3-[(1=*R*)-1-*tert*-butyldimethylsilyloxyethyl]-4-(1-carboxyethylene)-azetidin-2-one and **III** (R^4 = Ph; R^5 = R^6 = Me) was autoclaved at 100 atm H and 26° to give 100% α,β-mixt. of the 4-(1-carboxyethyl)azetidin-2-one analog in ratio of 13.3:86.7, resp.

問題 2

Indomethacin (抗炎症剤) の毒性 (toxicity, adverse effect など) に関する文献を一件調べなさい.

(Index Guide → Chemical Substance Index → 本誌)

1. Index Guide で Indomethacin を見ると次のように記述されている.

Indolyl Red
See *1(3H)-Isobenzofuranone, 3,3-bis(1-ethyl-=2-methyl-1H-indol-3-yl)- [22091-92-5]*
Indomethacin
See *1H-Indole-3-acetic acid, 1-(4-chlorobenzo=yl)-5-methoxy-2-methyl- [53-86-1]*
Indomethacin farnesil
See *1H-Indole-3-acetic acid, 1-(4-chlorobenzo=yl)-5-methoxy-2-methyl-, 3,7,11-trimeth=yl-2,6,10-dodecatrienyl ester [85801-02-1]*

2. Chemical Substance Index (例では 113 巻) で 1H-Indole-3-acetic acid の項を見ると, 次のページのようになっている. ここで, 1H-Indole-3-acetic acid, anhydrides, 1H-Indole-3-acetic acid, compounds などの項は親の酸の誘導体である. 下の方に ----, 1-acetyl-α-[acetyl… とあるところからが, 基本骨格の誘導体になる. ここを見ていくと, 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- [53-86-1] の項が見つかった. この場合はカッコ内に (indomethacin) と記載されている.

topical liq. pharmaceutical contg. soly. enhancer and, P 237854w
topical pharmaceuticals contg. penetration enhancers and, P 103404r
toxicity of
  gastroduodenal, in humans, 145040z
  to stomach, healing process evaluation by thymidine incorporation in, 72876q
transdermal controlled delivery of, polymer adhesive matrixes for, 158525m
transdermal delivery system for, P 138500w
transdermal or topical pharmaceutical compn. contg. amine oxide and, P 29278j
transport of, into skin stratum corneum, alkanols and urea effect on, 90892w
ulcer healing delay by, omeprazole prevention of, inhibition of stomach acid secretion in, 165241u
ulcerogenicity of, PGE_2 formation in relation to, 273t
urinary tract infection therapy with, 91112d
vasotocin-induced oviposition in hen inhibition by,

3. 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- [53-86-1] の項には多くの文献が記載されている (次ページ). 毒性について調べるので, toxic の文献がないかと見ていくと, toxicity of の項に 2 件の文献が見つかった.

4. この文献の抄録が見つかった.

113: 145040z **The effects of indomethacin on gastroduodenal morphology and mucosal pH gradient in the healthy human stomach.** Shorrock, Christopher J.; Prescott, Richard J.; Rees, Wynne D. W. (Dep. Gastroenterol., Hope Hosp., Salford, UK M6 8HD). *Gastroenterology* 1990, 99(2), 334-9 (Eng). To define further the injury and the mechanisms of mucosal injury induced by indomethacin, the effect of 28-day continuous administration of oral indomethacin on gastroduodenal morphol., gastric histol., and the protective mucus-bicarbonate barrier overlying gastroduodenal mucosa in humans was studied. In the studies, indomethacin caused acute gastroduodenal damage in 100% cases, with maximal damage at 24 h of administration. With continued intake this damage resolves, although a minority (two study subjects) progressed to discrete ulceration. Biopsy specimens taken during the studies showed no significant changes in inflammatory or regenerative features, and thus failed to shed any light on this process of adaptation to damage. Mucosal pH gradient studies showed a significant increase in juxtamucosal pH at the time of maximal damage (24 h); this is thought to represent passive diffusion of alkali from damaged mucosa. In conclusion, mucosal adaptation to acute damage by indomethacin occurs in humans. The mechanisms through which the mucosa adapts in this intriguing way remain unknown.

Consult 1990 Index Guide for Cross-references and Indexing Policies

問題 3

SbF_5 が触媒 (catalysis, catalytic など) として作用することに関する文献を一件調べなさい.
(Formula Index → Chemical Substance Index → 本誌)

1. SbF5 は Hill 方式で書くと F5Sb なので Formula Index (例では 113 巻) でその項を調べると Antimomy fluoride (SbF5) *[7783-70-2]* See *Chemical Substance Index* と記載されている. このように Formula Index では文献数の多い化合物については索引が省略されている. この場合は Formula Index はこの化合物の正式な CAS 索引名を調べるツールとして役だった.

2. Chemical Substance Index の Antimony fluoride (SbF5) *[7783-70-2]* を見る. 触媒に関する文献なので catalyst の小見出しを見るといくつか文献が見つかった.

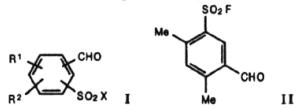
F_5S

F_5S
Sulfate(1−), pentafluoro− *[31140-82-6]*, 141464t
Sulfur(1+), pentafluoro− *[19167-14-7]*, 87577s, 138942s, 141464t, 222735j
Sulfur fluoride (SF_5) *[10546-01-7]*, 43467b
F_5Sb
Antimonate(2−), pentafluoro−diammonium, (*SP*-5-11)− *[38640-84-5]*, 33454f
Antimony fluoride (SbF_5) *[7783-70-2]*. See *Chemical Substance Index*
F_5Si
Silicate(1−), pentafluoro−(*TB*-5-11)− *[52610-90-9]*, 138868x

Antimony europium sulfide ($Sb_4Eu_3S_9$) *[78402-67-2]*
classification of, in homologous series, based on archetypal structures, 26928k
Antimony fluoride (SbF_5) *[7783-70-2]*
132255y
aprotic solvent complexes, for soln. processing of ladder and rigid-chain polymers, P 213248a
benzoquinone−tetramethylenecyclooctane copolymer doped with, elec. conductors from, P 182918n
bis(chloromethylphenylsilyl)furan homopolymer doped with, elec. cond. of, 172864c
carbocation formation in cryogenic matrix of, 171250n
catalyst
for formylation and sulfonylation of dialkylbenzenes, P 58688y
for rearrangement of perfluoro(ethylindan), 97149t
supported on non−zeolitic inorg. oxides, catalytic distn. with, for alkylation and oligomerization processes, P 194705d
catalyst contg., for fluorination of perchloroethylene, P 190733p

3. 抄録が見つかった.

113: **58688y Preparation of formyldialkylbenzenesulfonyl halides as intermediates for drugs, agrochemicals, and resins.** Soma, Yoshiye; Iyoda, Atsushi; Sano, Hiroshi (Agency of Industrial Sciences and Technology) **Jpn. Kokai Tokkyo Koho JP 02 78,654 [90 78,654]** (Cl. C07C309/86), 19 Mar 1990, Appl. 88/230,388, 13 Sep 1988; 5 pp. The title compds. **I** (R^1, R^2 = C_{1-5} alkyl; X = halo;



CHO and sulfonyl halide are para to alkyl) were prepd. by reaction of dialkylbenzenes with XSO_3H (X = halo) and CO in the presence of antimony halide. A mixt. of *m*-xylene FSO_3H, SbF_5, and CF_3CO_2H under CO was stirred at 25° for 6 h to give 83% benzenesulfonyl fluoride **II**.

問題 4

Alinamin に関する文献を一件調べなさい.
(Index Guide → Chemical Substance Index → 本誌)

1. Index Guide で Alinamin を調べると, See *Formamide, N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-[4-hydroxy-1-methyl-2-(propyldithio)-1-butenyl]- [59-58-5]* と記載されている.

2. そこで Chemical Substance Index (例では 113 巻) の Formamide の項を見る. Formamide そのものの文献が示された後, 置換基誘導体がアルファベット順に並べられている. 置換基の前の長いダッシュは Formamide が省略されていることを示している.

Alimezine
See *10H-Phenothiazine-10-propanamine, N,N,β-trimethyl- [84-96-8]*
Alinamin
See *Formamide, N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-[4-hydroxy-1-methyl-2-(propyldithio)-1-butenyl]- [59-58-5]*
Alinamin F
See *Formamide, N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-[4-hydroxy-1-methyl-2-[[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]- [804-30-8]*

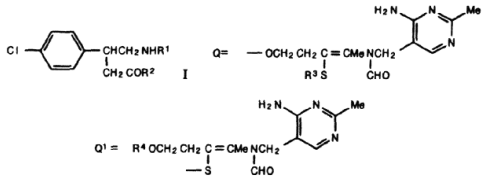
Formamide, compounds

copper complex *[128138-63-6]*, prepn. and IR spectrum of, 164308j
iron complex *[129033-86-9]*, formation and charge-transfer spectrum of, 125303j
manganese complex *[129062-46-0]*, prepn. and crystal structure and magnetic susceptibility and heat of fusion of, 108031b
nickel complex *[36026-35-4]*, ligand-field splitting energies of nickel solvate in, coordination power of solvent in relation to, 47514n
propanoate *[129137-37-7]*, templates, oxygen permeability of polysulfone fibers spun from, increased free vol. in relation to, 99265b
Formamide *[75-12-7]*, **derivatives (general)**
N-alkyl derivs., metab. of, by liver microsomes, 36034e
derivs., soldering flux contg., for clean joints, P 216520u
Formamide
——, ***N*-[5-acetyl-3-cyano-4-(2-furanyl)-6-methyl-4*H*-pyran-2-yl]-** *[128998-33-4]*, 114997n

3. ずっと見ていくと, 該当項目が見つかった. CAS 登録番号 *[59-58-5]* が一致することを確認する.

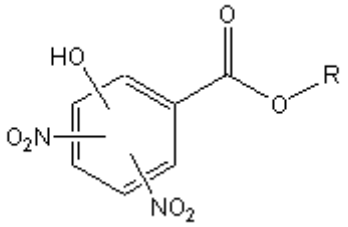
cobalt complex *[130637-89-7]*, prepn. and antigastritis activity of, P 224579k
——, ***N*-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-*N*-[4-hydroxy-1-methyl-2-(propyldithio)-1-butenyl]-** (*prosultiamine*) *[59-58-5]*
condensation of, with baclofen deriv., P 6365w
reaction of, with inorg. acid, solvents in, P 6040m
hydrochloride *[127545-52-2]*, P 6040m
——, ***N*-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-*N*-[4-hydroxy-1-methyl-2-[[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]-** (*fursultiamine*) *[804-30-8]*
mercury of human mustache response to, 110597j
prepn. of, by reaction of thiol-form thiamin salt with sulfurating agent prepd. from tetrahydrofurfuryl mesylate and sodium thiosulfate, P 131892s
reaction of, with inorg. acid, solvents in, P 6040m
hydrochloride *[10238-39-8]*, granular formulation of, P 197975c
monohydrochloride *[2105-43-3]*, P 6040m

113: **6365w Preparation of baclofen conjugate with thiamin derivatives.** Mazaki, Mitsuo; Kondo, Seiji; Takeda, Hiromitsu (Nippon Chemiphar Co., Ltd.) **Jpn. Kokai Tokkyo Koho JP 01,319,466 [89,319,466]** (Cl. C07D239/42), 25 Dec 1989, Appl. 88/151,534, 20 Jun 1988; 8 pp. The title compds. (**I**; R^1 = H, COR;



R = Q, Q^1; R^2 = OH, R; R^3 = C_{2-7} alkylcarbonyl, C_{7-10} arylcarbonyl, C_{1-6} alkylthio; R^4 = H, C_{2-7} alkylcarbonyl, C_{7-10} arylcarbonyl; provided that at least one of R^1 and R^2 contains R), which readily crosses the blood brain barrier and efficiently transports baclofen (muscle relaxant) into brain and have potent and prolonged physiol. activity, are prepd. Thus, acylation of baclofen with *tert*-Bu *S*-(4,6-dimethylpyrimidin-2-yl)thiolcarbonate in aq. Et_3N gave 91% *N*-(*tert*-butoxycarbonyl)baclofen which was treated with $ClCO_2Et$ in THF contg. Et_3N at ≤-10° followed by an ice-cooled aq. NaOH soln. of *O*-acetylthiamine-HCl to give, after standing 30 min at room temp., 26% *O*-acetyl-*S*-[4-(*N*-*tert*-butoxycarbonylamino)-3-(4-chlorophenyl)butanoyl]thiamine. Deprotection of the latter with 3N HCl in EtOAc gave 88% **I**.2HCl (R^1 = H, R^2 = Q^1, R^4 = Ac) (**II**). When **II** was administered at 138.8 mg/kg in rats through a femoral vein, amts. of **II** transported into the brains were 84.6-203 μg/g vs. 2.22-3.76 μg/g for **I**.Na (R^1 = COQ, R^2 = OH, R^3 = iso-PrS).

問題 5
次の化合物に関する文献を一件調べなさい.



（OH と NO_2 はどこについていてもよい. R は水素ではない）
(Chemical Substance Index → 本誌)

1. この化合物は Benzoic acid に NO2 が 2 個と OH が置換した酸のエステルである. したがって Benzoic acid に dinitro と hydroxy がついたものを Chemical Substance Index で探せばよい. CAS の命名法の規則では, 置換基は数を表す接頭辞 (di-, tri- など) を無視してアルファベット順に並べることになっているので, Benzoic acid, hydroxy-dinitro- を探す. 置換基はこのように, いつも基本骨格の後にカンマで区切られて示されている.

2. Chemical Substance Index (例では 107 巻) を見ると, まず Benzoic acid そのものの文献が並び, そのあとに置換基のついた化合物が並べられている. 順々に見ていくと 2-hydroxy-3,5-dinitro- *[609-99-4]* が見つかった. 置換基の前の長いダッシュは Benzoic acid が省略されていることを示している. エステルなどは親の酸の文献の終わった後に記載されている. ここでは methyl ester *[22633-33-6]* があった.

Benzoic acid, 4-hydroxy-,

with 2,2-dimethyl-1,3-propanediol, hexanedioic acid and 1,3-isobenzofuran⊃ndione *[108786-43-2]*, prepn. of crosslinkable liq.-cryst., as coating binders, 8949q
with formaldehyde *[28087-79-8]*, IR-sensitive photog. films contg., P 246637f
with formaldehyde and 1,3,5-triazine-2,4,⊃

107: **77224m Kinetics of hydrogen isotope exchange in molecule with strong intramolecular hydrogen bonds.** Bureiko, S. F Oktyabrskii, V. P. (Inst. Phys., State Univ., 198904 Leningrad USSR). *React. Kinet. Catal. Lett.* **1986,** 31(1), 245-8 (Eng) Rate consts. and activation energies of H exchange between methanol and mols. with intramol. H bonds were measured. The rate-detg. step is the dissocn. of the H bond.

——, 2-hydroxy-3,6-dimethyl-4-⊃(phenylmethoxy)-3-hydroxy-4-(methoxycarbonyl)-2,5-⊃dimethylphenyl ester *[111258-35-6]*, redn. of, 214846g
——, 2-hydroxy-3,5-dinitro- *[609-99-4]*
coordination of, with nickel(II), equil. and kinetics of, 121975h
in detn. of reducing sugars in molasses, limitations of, 9203d
electronic spectroscopic studies on intra- and intermol. hydrogen bonding in, 144069e
in ytterbium detn. by flame at. absorption spectrometry, signal enhancement in relation to, 51015u
zinc complexes, formation const. and thermodn. of coordination of, 224061m
compd.
with *N'*-[[4-(dimethylamino)phenyl]⊃methylene]-*N,N*-dimethyl-1,4-⊃benzenediamine (1:1) *[110467-02-2]*, IR spectrum of, 153817z
with *N,N*-dimethyl-4-[(phenylimino)⊃methyl]benzenamine (1:1) *[110467-00-0]*, IR spectrum of, 153817z
with *N,N*-dimethyl-*N'*-(phenylmethylen⊃e)-1,4-benzenediamine (1:1) *[110467-01-1]*, IR spectrum of, 153817z
with *N*-(phenylmethylene)benzenamine (1:1) *[87775-94-8]*, IR spectrum of, 153817z
methyl ester *[22633-33-6]*, hydrogen exchange between methanol and, kinetics of, 77224m
[(5-nitro-2-furanyl)methylene]hydrazide (*nifursol*) *[16915-70-1]*, hyperprolactinemia from, in newborn, maternal administration during lactation in relation to, 126890m

3. 文献の抄録が見つかった.

問題 6
鯨の肉に関する文献を一件調べなさい.
(Index Guide → General Subject Index → 本誌)

1. Index Guide で Whale を見ると meat-----see *Meat,* whale とあり, 肉については Meat の項を見ることがわかる.

2. General Subject Index (例では 113 巻) で Meat の項を見るとさまざまな文献が並んでいる. 小見出しの whale の項では 2 件の文献が見つかった.

113: **22302d Determination of total L-ascorbic acid and erythorbic acid in foods.** Ogata, Kuniaki; Kimura, Tomoko; Hosoya, Emiko; Sato, Takao (Yamagataken Eisei Kenkyusho, Yamagata, Japan). *Yamagata-ken Eisei Kenkyushoho* **1989,** 22, 27-31 (Japan). HPLC with a Finpak SIL-5 column was used to det. L-ascorbic acid (**I**) and erythorbic acid (**II**) in food products. **I** and **II** were reacted with hydrazine before HPLC anal. The detector wavelength was 495 nm. The mobile phase contained hexane-EtOAc-HOAc-propanol (4:4:0.1:0.1). The recovery rates of **I** and **II** were 95-103 and 97-102%, resp. The contents of **I** and **II** in whale meat, fruit juice (10%)-supplemented soda, sausage, ham, and wiener sausage are tabulated.

問題 7
廃水のオゾン処理についての文献を一件調べなさい.
(Index Guide → General Subject Index → 本誌)

1. Index Guide で Ozone, uses and miscellaneous の項を見ると, in water and wastewater treatment, see *Wastewater treatment* となっているので, 廃水処理については Wastewater treatment をみればよいことがわかる.

2. General Subject Index (例では 113 巻) を見ると, Wastewater treatment の項は大変文献の数が多い. そこで小見出しをたどっていくと ozonization が見つかった.

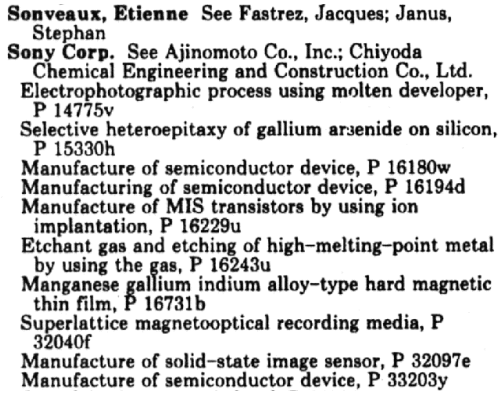
Wastewater treatment

3. 文献の抄録が見つかった.

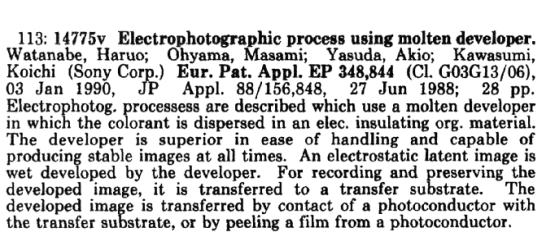
113: **28702f Dye removal from water by ozonation with adsorption on carbon.** Sid'ko, R. Ya.; Kerzhner, B. K.; Goncharuk, V. V. (Inst. Kolloidn. Khim. Khim. Vody, Kiev, USSR). *Khim. Tekhnol. Vody* **1989,** 11(10), 902-5 (Russ). Decolorization of anthraquinone- and 220 dye-contg. (1g/L) wastewaters by ozonization (23-27 mg O_3/L) followed by batch adsorption on granular activated C (0.25-0.5 mm) revealed the dependence of decolorization effectiveness on pH. The adsorption was ineffective in the removal of 220 dye ozonization products if the ozonization was done at alk. pH. Adsorption on activated C (~1 kg/m^3) gave an addnl. 40-60% redn. in COD if the ozonization was done at neutral or acidic pH levels.

問題 8
Sony Corp. 社の特許を一件調べなさい.
(Author Index → 本誌)

Author Index (ここでは 113 巻) を調べると Sony Corp. が出ている. 文献の番号に P がついているのが特許である.



Sonveaux, Etienne See Fastrez, Jacques; Janus, Stephan
Sony Corp. See Ajinomoto Co., Inc.; Chiyoda Chemical Engineering and Construction Co., Ltd.
Electrophotographic process using molten developer, P 14775v
Selective heteroepitaxy of gallium arsenide on silicon, P 15330h
Manufacture of semiconductor device, P 16180w
Manufacturing of semiconductor device, P 16194d
Manufacture of MIS transistors by using ion implantation, P 16229u
Etchant gas and etching of high-melting-point metal by using the gas, P 16243u
Manganese gallium indium alloy-type hard magnetic thin film, P 16731b
Superlattice magnetooptical recording media, P 32040f
Manufacture of solid-state image sensor, P 32097e
Manufacture of semiconductor device, P 33203y



113: 14775v **Electrophotographic process using molten developer.** Watanabe, Haruo; Ohyama, Masami; Yasuda, Akio; Kawasumi, Koichi (Sony Corp.) **Eur. Pat. Appl. EP 348,844** (Cl. G03G13/06), 03 Jan 1990, JP Appl. 88/156,848, 27 Jun 1988; 28 pp. Electrophotog. processess are described which use a molten developer in which the colorant is dispersed in an elec. insulating org. material. The developer is superior in ease of handling and capable of producing stable images at all times. An electrostatic latent image is wet developed by the developer. For recording and preserving the developed image, it is transferred to a transfer substrate. The developed image is transferred by contact of a photoconductor with the transfer substrate, or by peeling a film from a photoconductor.

会社名で調べる場合, 次の注意が必要である.

(1) 会社名は合併・吸収やその他の理由で時代とともに変化している. Chemical Abstracts には, 文献発表時の名前で収録されている.

(2) 人名から取った会社名に付いては, 過去においては姓を先にして索引することになっていた. しかし 1967 年以降は正式の会社名をそのままの形で索引するようになった.

例:
1966 年まで: DuPont, E. I., de Nemours and Co.
1967 年以降: E. I. DuPont de Nemours and Co.

(3) 日本の会社名に付いては, なるべく正式の英文社名を使用するようにしているが, 著者が違う記述法を使った場合, 必ずしも統一されていないことがある.

例:
Sumitomo Chemical Co.
Sumitomo Kagaku Kogyo K. K.