COMMENTS: This abstract illustrates a characteristic difficulty in extracting synthetic organic text: the indispensability of the graphic material of the paper. For example, the reader cannot deduce the structure of compound no. 3 of Table V. In spite of this, the reader should receive an accurate impression of the paper and be able to decide whether or not he wants to read it.

STATISTICS: Full original document = 884 words.
ADAM abstract = 143 words.
CA abstract = 76 words.

Effects of Vasoactive Agents and Diuretics on Isolated Superfused Interlobar Renal Arteries. J. W. Strandhoy, R. Cronnelly, J. P. Long and H. E. Williamson. CA-77-25-160038M.

Little information is available concerning the actions of diuretics and other drugs on renal vascular smooth muscle, uncomplicated by reflex, hormonal or other extraneous influences. The purpose of this study therefore was to isolate a segment of the renal vascular tree for evaluation in vitro of direct actions of diuretics and other vasoactive agents. Two diuretics were evaluated for activity on the interlobar artery. No relaxant effects were obsd. with either agent. No change in base line tension was obsd. The isolated intralobar artery was found to contract in response to KCl and symmpathetic nerve stimulation. No evidence was found to indicate that tension of larger renal arteries is decreased in response to furosemide. Superfusion of the tissue with hydrochlorothiazide was found to attenuate the contractile responses of norepinephrine. The highest doses of norepinephrine used were not antagonized sufficiently suggesting a competitive depression of reactivity. Hydrochlorothiazide was found to produce dose-related contractions of the interlobar strips. High doses were necessary. The interlobar arteries contribute to the renal vasoconstriction produce by norepinephrine and dopamine, but do not contribute to the renal vasodilation produced by furosemide or small doses of dopamine.

COMMENTS: Too much background, negative, and trivial information is given but the abstract still contains enough information for an indicative abstract.

STATISTICS: Full original document = 1502 words.
ADAM abstract = 199 words.
Boldface abstract = 165 words.
CA abstract = 83 words.

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Computer Programs for Editing and Validation of Chemical Names†

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Chemical Abstracts Service (CAS) has developed computer procedures for editing chemical names, including both CA Index Names and names from the original literature. These editing programs include steps which will automatically correct errors in punctuation, format, capitalization, and italicization where possible, as well as error detection steps which generate diagnostic messages. Nomenclature translation processes have been incorporated into these editing programs in order to detect errors in names generated as CA index entries and to validate such names by comparing them to their structural records.

Chemical Abstracts Service (CAS) has long paid considerable attention to careful editing of material which is going into its publications, and has attempted to correct errors before they are published and thus avoid scattering or loss of information. As the computer-based publication system of CAS has developed during the last several years and as the volume of material being processed has grown rapidly, considerable emphasis has been placed on using computer programs to reduce the amount of human effort spent in editing data that enter the system. Some of these edits have previously been described.[1-3] The development of these edits has emphasized that data which are correct should be verified as early as possible in the system, so that data which have been keyboarded and edited can be placed on file in a correct form and brought out only as needed for inclusion in particular products. Our goal has been to develop error detecting edits which are sufficiently effective so that items which pass these edits do not require human review; only the questioned data (i.e., those items which do not pass the edits) need to be reviewed.

† Presented to the 168th National Meeting of the American Chemical Society, Atlantic City, N.J., Sept 11, 1974.

CHEMICAL SUBSTANCE PROCESSING

The steps involved in chemical substance processing in the CAS publication system have recently been described.[4,5] In the CAS system (see Figure 1), there are basically two places where chemical names are recorded in computer-readable form. First, if a substance selected as a Chemical Substance Index entry has a name provided in the source document, Name Match can be attempted; that is, the name given in the document can be matched against substance names already on file. If a match occurs, the CAS Registry Number and CA Index Name are retrieved. Names input for Name Match represent a relatively uncontrolled vocabulary. They are not formulated according to the rigid rules used for CA Index Names and therefore cannot be subjected to as rigorous editing, but some computer edits are applied to them.

If a substance cannot be identified by Name Match, a

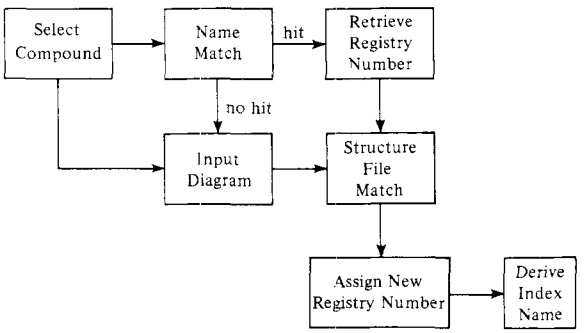


Figure 1. Chemical substance processing.

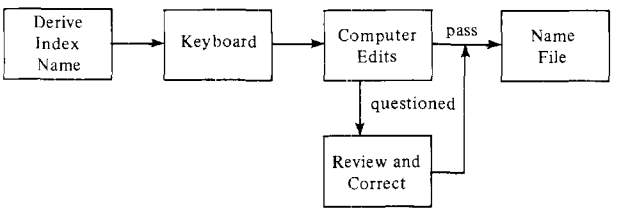


Figure 2. Index Name processing.

structure diagram is prepared, and the corresponding atom-bond connection table[5] is matched against the Registry structure files. If the structure is not on file, a new Registry Number is assigned, and the structure is forwarded to a nomenclature specialist who prepares its name by applying the CA Index Name selection rules.[6,7] (During one year more than 300,000 new CA Index Names are prepared.) The name is dictated and keyboarded, and computer edits are applied to it (see Figure 2). These editing procedures for CA Index Names are sufficiently rigorous so that names which pass the full range of edits need not be reviewed by nomenclature specialists, but can be added directly to the data base without human review. Names that are questioned by the edits are sent to the nomenclature specialist along with appropriate diagnostic messages. The specialist reviews a name and either verifies that it is correct or institutes a correction. Beginning in 1975, review and correction will take place at a terminal with on-line correction capability; the editor will then be able to see the corrected name before it enters the nomenclature file, and the chance that a new error will occur during the correction process will be reduced.

ERRORS IN NOMENCLATURE

In computer processing of CA Index Names, one can take advantage of the fact that these names are separated on CAS files into several segments, or data elements, which can be separately addressed. These data elements have been defined to meet the requirements of the programs which sort and format names during production of CA Indexes. For example, the name shown in Table I is divided into four segments. The Heading Parent segment "2-Naphthalenecarboxylic acid" describes the principal functional group present and the molecular skeletal fragment to which it is attached. The Substituent segment "decahydro-6-hydroxy-" cites structural units attached to the parent molecular skeleton or changes in its degree of unsaturation. The Name Modification segment "methyl ester" describes modifications to the principal functional group. Finally the Stereochemistry segment adds stereochemical detail.

These nomenclature segments provide a means for classifying the errors which occur in chemical names and for discussing the computer programs that have been developed to detect them. These errors represent a variety of human errors in preparing substance names and entering them into the system. While the accuracy rate is actually

Table I. Segments of a CA Index Name

Heading parent	2-Naphthalenecarboxylic acid
Substituent	decahydro-6-hydroxy-
Name modification	methyl ester
Stereochemistry	(2α,4aα,6β,8aβ)-

Table II. Correctable Errors in a Single Segment (Examples)

Incorrect	Correct
1H-Indene	1*H*-Indene
2,3- dimethyl	2,3-dimethyl
D-Glucose	D-Glucose

Table III. Noncorrectable Errors in a Single Segment (Examples)

2,4-trichloro-
bicyclo[4.2.1]octane
2-[dichloromethyl)amino]-

quite high, all work must be checked in order to find and correct those errors that do occur. Formerly this checking had to be done by highly skilled chemists; now much of it can be done by computer procedures.

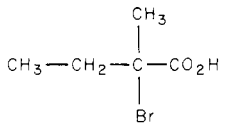
We can distinguish several types of errors in substance names. Some errors can be detected by examining a single segment of a name and can be corrected with no ambiguity. Most errors in capitalization and italicization are in this group, as are many errors in punctuation. We see some examples of such errors in Table II. These include the failure to italicize the letter "H" in "1*H*-Indene", the extra space in "2,3-dimethyl", and the use of an italic "D" in "D-Glucose" when a small capital is required.

There are also many errors which can be detected by examination of a single name segment, but for which we have not found it possible to write unambiguous correction rules; these must be reviewed by the human editor. Such errors include many errors in punctuation, spelling errors in general, and some cases of omitted data. The examples in Table III include a case where a locant has been omitted from the series preceding "trichloro"; one cannot determine what that locant should be without knowing the structure. In the second name in Table III, the numerals "4.2.1" require nine atoms and are therefore inconsistent with "octane", but one must know the structure to determine whether the numbers or the term is incorrect. In the third case, we can recognize that one enclosing mark is missing, but we do not know where it should go.

Another class of error is that in which the individual segments do not contain detectable errors, but the segments cannot be validly combined. In the name "2-Hexanol, 7,7-dichloro-", for example, the "7,7-dichloro-" term uses locants which refer to a position that does not exist on the "hexanol" structure. A similar type of error occurs in "Benzoic acid, 1,1-dimethyl-" where the locants "1,1" refer to an atom which does exist but is not available for substitution.

More difficult to detect are those errors in which the name is a perfectly valid name but, unfortunately, not for the substance which is being indexed. Such an error can be detected only by comparison against the structure or, in some cases, the molecular formula of the substance. Figure 3 illustrates some examples of incorrect names for the structure which is shown along with its correct name "Butanoic acid, 2-bromo-2-methyl-". In the first incorrect name, the term "2-methyl-" has been accidentally omitted; in the second, we see the fairly common confusion of "methyl" and "ethyl". The third example in Figure 3 is a more difficult case in which the use of an incorrect locant causes the name to describe an isomer of the intended structure. A related type of error is one in which the name describes a stereoisomer of the intended structure. Table IV, for example, shows an error in the Stereochemistry segment, with "4aβ" used in place of "4aα".

Perhaps the most difficult type of error to detect is one



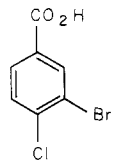
Correct:

Butanoic acid, 2-bromo-2-methyl-

Incorrect:

Butanoic acid, 2-bromo-
Butanoic acid, 2-bromo-2-ethyl-
Butanoic acid, 2-bromo-3-methyl-

Figure 3. Errors detected by checking against structure record.



Correct: Benzoic acid, 3-bromo-4-chloro-

Incorrect: Benzoic acid, 4-chloro-3-bromo-
Benzene, 1-bromo-5-carboxy-2-chloro-

Figure 4. Incorrect choice of preferred Index Name.

Table IV. Incorrect Name Describing Stereoisomer of Intended Structure

Incorrect	Correct
2-Naphthalenecarboxylic acid, decahydro-6-hydroxy-, (2α,4aβ,6β,8aβ)-	2-Naphthalenecarboxylic acid, decahydro-6-hydroxy-, (2α,4aα,6β,8aβ)-

in which the name correctly describes the substance being indexed but is not the preferred name according to the CA Index Name selection rules. Figure 4 shows two incorrect names along with the correct name "Benzoic acid, 3-bromo-4-chloro-". The first incorrect name is a simple case of two radical names, "bromo" and "chloro", being out of alphabetic order. In the second example, the name does not include the carboxy principal functional group as part of the parent compound. These names are not errors in the sense that they are misleading descriptions, but they are unacceptable for use as CA Index headings even though they might serve quite well for some other purpose.

AUTOMATIC ERROR DETECTION AND CORRECTION

CAS has developed nomenclature editing procedures that can be divided into three groups: automatic error detection and correction, automatic error detection with manual correction, and nomenclature translation. The first is a series of steps that automatically correct errors that can be corrected unambiguously. These correction steps include some that are designed to handle specific errors that occur frequently and other steps that the nomenclature specialists have requested to combat some bothersome errors. If these procedures are applied to a name and a correction is made, that error is not called to the attention of an editor. In general, these steps are applied not only to new CA Index Names but also to author-supplied nomenclature being input for Name Match. Many of these steps correct common errors in punctuation. Table V shows some examples in which extraneous blanks are removed, missing blanks are added, or erroneous characters are corrected. Note that some of these steps are applied to the characters associated with fairly specific types of character strings, such as a ratio or a charge.

Automatic correction also includes steps which ensure the correct capitalization and italicization of certain characters or character strings under specified conditions.

Table V. Correction of Punctuation Errors

methyl ester → methyl ester 1,2- dihydro- → 1,2-dihydro- ion (1-) → ion(1-)	Extraneous blank spaces removed
acetate(salt) → acetate (salt) compd. with acetaldehyde(1:1) → compd. with acetaldehyde (1:1)	Missing blank spaces added
furo[3,4,c]furan → furo[3,4-c]furan (Comma changed to hyphen in fused ring system) 3,4--dichloro- → 3,4-dichloro- (One of two successive hyphens removed)	Erroneous characters corrected

Table VI. Automatic Italicization

1H-Indole → 1*H*-Indole
(E)- → (*E*)-
pyrrolo[3,2-b]azepine → pyrrolo[3,2-*b*]azepine
D-arabino-Hexopyranose → D-*arabino*-Hexopyranose

Table VII. Correction of Element Symbols and Associated Data

N-oxide → *N*-oxide
se,se-dimethyl- → *Se*,*Se*-dimethyl-
Cyclohexane-1,2-d_2 → Cyclohexane-*1,2-*d_2
L-Cystine-35S2 → L-Cystine-$^{35}S_2$

Table VIII. Correction of "D" and "L"

L-Leucine → L-Leucine
D-Glucose → D-Glucose
D-Homocysteine → D-Homocysteine
D-Homopregnane → *D*-Homopregnane
A:D-Neoursane → *A*:*D*-Neoursane

Table VI gives several examples of italicization: the "H" which places a hydrogen atom on a ring in "1*H*-Indole", the stereochemical term "E", an alphabetic in a fused ring name, and the stereochemical prefix "arabino" ("arabino" is one of about fifty terms which are automatically italicized when bounded by punctuation).

Several correction steps concern element symbols and associated data. These include, as shown in Table VII, italicization of element symbols under specified conditions (first two examples), capitalization where that can be done unambiguously (second example), italicization of locants for labeled atoms (third name), and superscripting and subscripting of numeric data used in describing labeled compounds (last example). Another set of steps deals with the characters "D" and "L", which usually describe stereochemistry and are printed as small capitals, as in "L-Leucine" and "D-Glucose" (see Table VIII). The rules applied by these steps are somewhat more complex, however, since "D" sometimes refers to a ring within a ring system; it is then printed as a capital italic, as in "*D*-Homopregnane" and "*A*:*D*-Neoursane".

AUTOMATIC ERROR DETECTION WITH MANUAL CORRECTION

Error detection in CA Index Names is for the most part handled by the nomenclature translation procedures which are discussed in a later section of this paper. There are, however, some other steps which detect common errors and which are run prior to nomenclature translation. Names which are questioned by any of these steps are put out, with appropriate diagnostic messages, for review by the nomenclature specialists. Table IX shows several examples of error detection steps. If the left- and right-hand enclosing marks in a name segment are not properly balanced, as in the first name, a possible error is indicated. An incorrect atomic mass in a description of a labeled compound will be detected at this stage, as in the case of mercury (Table IX), where one digit has been omitted from the mass 197. The incorrect ring name "bicyclo[4.2.1]octane" (from Table III)

Table IX. Detection of Common Errors

Name	Diagnostic Message
2,4-bis[(2-chloroethyl) amino-	BRACKETS UNEQUAL
Mecury-^{97}Hg	INVALID MASS
Bicyclo[4.2.1]octane	INCONSISTENT RING NAME
2-chloro-hydroxy-	PUNCTUATION
3,a-methyl-	PUNCTUATION

Table X. Spelling and Punctuation Errors Detected by Translation Program

Incorrect name	Correct name
Alinene	Alanine
2(1*H*)-Primidinone	2(1*H*)-Pyrimidinone
1-Piperidine carbothioic acid	1-Piperidinecarbothioic acid
2,6-(1*H*,3*H*)-Pyridinedione	2,6(1*H*,3*H*)-Pyridinedione

Table XI. Errors in Omission of Data From Name Segment

Incorrect segment	Should have been
Butenamide	2-Butenamide
4-Pentanamide	4-Pentenamide
(2-hydroxy-3-methoxy)-	(2-hydroxy-3-methoxypropyl)-

would be detected at this point by a step in which the number of atoms required by the bridge lengths given is calculated and compared to the value indicated by the term which follows the bridge lengths. In this case the bridges require nine atoms, while "octane" implies eight.

A number of common punctuation errors are also detected by specific error detection steps; these are situations which are definitely in error but cannot be corrected unambiguously. For example (see Table IX), a hyphen between two alphabetic strings is definitely incorrect and may indicate that a locant was omitted. A comma between a numeric and a nonitalic alphabetic also indicates an error; perhaps in this case (last example) "3a" was intended, or maybe the "a" should have been an "α". Also checked at this stage is the agreement between the number of locants in a series and the following multiplying term; thus "2,4-trichloro-" would be questioned as incorrect. Allowance is made, however, for the cases where the term following the locants is a hydrocarbon word root rather than a multiplier, as in "2,4-pentanedionato" and "1,6-hexanediyl".

NOMENCLATURE TRANSLATION

The steps just described detect certain common errors and highlight them for review by the nomenclature specialist. They do not by any means provide a full validation of a name; these checks are not rigorous enough to ensure that the name is a fully accurate description of the intended structure. Such a rigorous validation is provided by the nomenclature translation process (see Figure 5). Nomenclature translation is a program which converts a systematic chemical name to an atom-bond connection table, which can then be compared with the structural record already on file to determine if the structure represented by the name corresponds to that on file. If the name is not translated or if the two structural records do not correspond, the name must be reviewed and the name or the structural record may have to be corrected. If the name is translated and the two structural records are identical, then the name is considered to be a fully accurate description.

Since the logic followed by the nomenclature translation program has been previously described,[8,9] this discussion concentrates on the program's use as an editing tool. The translation progam itself detects many errors because it recognizes as correct only certain spellings and patterns of punctuation allowed by the nomenclature rules. Unrecognized spellings or punctuations cause rejections. In this way most of the errors which can be detected upon examination of a single segment will be found. These include

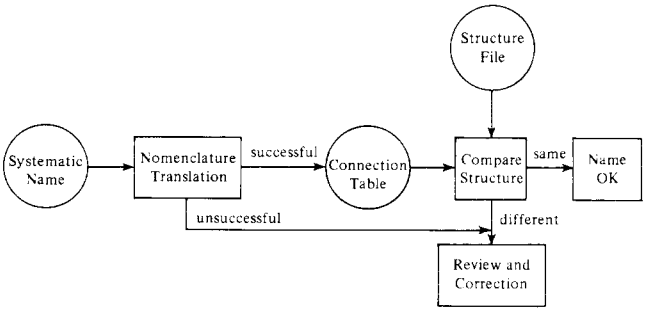


Figure 5. Nomenclature translation.

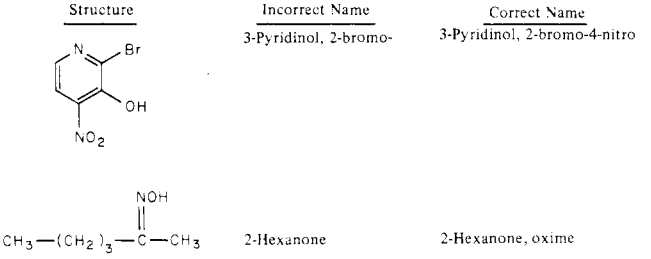


Figure 6. Errors detected by name–structure comparison—omission of data.

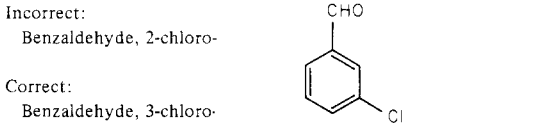


Figure 7. Errors detected by name–structure comparison—positional isomerism.

spelling errors, as in the first two names shown in Table X, and punctuation errors as seen in the latter examples. Similarly, some errors will be detected because a segment does not contain sufficient information to allow it to be processed. In the first case shown in Table XI, the program is unable to set up a structure corresponding to the parent name "butenamide" because a locant specifying placement of the double bond is missing. In the second case, the misspelling of "pentenamide" is perceived by the program as the presence of an extraneous locant. The omission of the "propyl" term in the third example creates internal inconsistencies which the program cannot resolve.

The translation program will also reject a name if the segments of that name are mutually inconsistent, even though they may be individually correct. For example, the program would be unable to assemble a total connection table for "1-Propanol, 8-chloro-" because the locant "8" refers to a nonexistent atom. Similarly, given the name "Cyclohexene, 4-fluoro-1,1-dimethyl-", the program recognizes that the attachment of two methyl groups to atom 1 of cyclohexene creates a pentavalent carbon atom; this is an unacceptable situation which the program cannot resolve.

If the translation program is successful in generating a connection table, that table is then compared to the structure already on file for the substance being named, i.e., the structure associated with the same CAS Registry Number. Two kinds of errors are caught by this comparison. One is the omission of a portion of a name, for example, the omission of the radical name "nitro" in the first case shown in Figure 6 or the omission, in the second case, of the Name Modification data element which would state that the compound is the oxime of 2-hexanone. The other class of error is that in which the name describes an isomer of the correct structure. In Figure 7 we see a case of positional isomerism caused by use of the wrong locant; this error is detected by comparison of the two structural records. This structure comparison also detects errors in which the name describes

Table XII. Errors Detected by Name–Structure Comparison. Stereochemical Discrepancy

Name: Cyclopentanone, 2,2,3-trimethyl-, (*S*)-(−)-
Text descriptor: S
Name: L-Proline, 1-(4-ethoxy-5-methoxy-2-nitrobenzoyl)-4-hydroxy-, (*R*)-
Text descriptor: S-TRANS

Table XIII. Errors in Ordering of Radicals

Incorrect error	Correct
1-chloro-3-bromo-	3-bromo-1-chloro-
6,7-dibromo-4-	4-[bis(2-chlomethyl)amino]-
[bis(2-chloroethyl)amino]-	6,7-dibromo-

a different stereoisomer from the one intended. In the CAS Chemical Registry System, stereochemistry is described by a linear Text Descriptor, which is constructed and formatted according to rigid rules. The nomenclature translation program generates a Text Descriptor from stereochemical information present in a name. The generated Text Descriptor and the descriptor in the Registry record should be identical; if they are not, the discrepancy is called to the attention of the editor. Table XII shows two examples of such discrepancy. In the first case, the name contains information not present in the descriptor, specifically, the minus sign denoting negative optical rotation. In the second example, the name and the descriptor disagree entirely, with one stating "R" and the other "S".

CURRENT STATUS OF NOMENCLATURE EDITING

The editing procedures described here, including nomenclature translation, provide a sufficiently rigorous validation to ensure that those names which pass the full set of edits need not be further examined by human editors; the residual error level is too low to justify the expense of having a professional nomenclature expert examine each validated name. Names that are not validated by the full range of edits must still be checked, however. CAS is therefore continuing to expand the capabilities of the translation program in order to increase the proportion of names for which full validation is possible. At the present time, the program successfully handles 40 to 50% of new CA Index Names; even this stage of development represents a twofold savings in human effort for editing names. The names now handled include the majority of systematic names of monomeric organic substances, as well as systematically constructed names of amino acids, carbohydrates, and steroids. In practice, a screening procedure run prior to nomenclature translation identifies many substances that belong to classes that cannot be handled and causes them to bypass the full translation process. We have recently defined and are currently implementing some modifications to the program which will improve its coverage of general organic nomenclature and will extend coverage to the large area of polymer nomenclature. The most important class of nomenclature that has not yet been handled is coordination compounds.

The errors not caught by the editing procedures described in this paper are primarily one of the types mentioned previously—a name which is a completely adequate description of a substance but is not the correct name according to the CA Index Name selection rules. We are incorporating into the nomenclature translation program a procedure for detecting one variety of such errors, that in which names of radicals are not in correct alphabetic order. Table XIII shows two such examples, one in which "chloro" and "bromo" are out of order and the more complex case of misordering "bis" and "bromo". Some other errors of this class present much more difficult computing problems, and it is questionable whether the complex procedures which would be required to validate, for example, that substituents on a symmetrical ring have the lowest possible locants, would be justifiable in terms of the actual infrequency of these errors.

FUTURE DEVELOPMENTS IN NOMENCLATURE PROCESSING

Future developments in nomenclature processing can be expected to reduce the occurrence of those errors which result from incorrect application of the CA Index Name selection rules. The introduction of interactive devices for review of names and later for input of names should aid in reducing error levels. We are also actively developing automatic nomenclature generation programs. These programs will analyze the Registry structural record for a new substance and generate from it a candidate CA Index Name for that substance. We anticipate that within two to three years we will develop the capability to prepare automatically much of the general organic nomenclature and coordination-compound nomenclature used in CA Indexes. The use of nomenclature generation programs to name a significant proportion of new substances will ensure that those substances are named consistently according to the rules and will allow the human specialist to concentrate on the more complex and intellectually challenging cases.

ACKNOWLEDGMENT

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