

enantiotopic after being built in 17.

It is worthwhile to mention morphic and topic relationships. The two ligands [L1(A) and L1(B)] in 17 are homomorphic and enantiotopic; L1(A) and L1(C) in 17 are homomorphic but diastereotopic.

CONCLUSION

The design of highly symmetric molecules is discussed in terms of subductive and inductive derivations. In a subductive derivation, global orbits are generated by desymmetrization of parent orbits, which is described by the subduction of coset representations. In an inductive derivation, infraorbits in a ligand (as a fragment) are restricted to local orbits (of the corresponding segment) and then incorporated into a molecule to afford global orbits. This process is described in terms of the induction of coset representations. The relationship between the two derivations is discussed.

REFERENCES AND NOTES

- (1) van't Hoff, J. H. *Arch. Néerl. Sci. Exactes Nat.* **1874**, 9, 445.
- (2) (a) Prelog, V. *Science* **1976**, 193, 17. (b) Nakazaki, M. *Top. Stereochem.* **1984**, 15, 199. (c) Nakazaki, M.; Naemura, K. *Yuki Gosei Kagaku Kyokaiishi* **1977**, 35, 883. (d) Eaton, P. E. *Tetrahedron* **1979**, 35, 2189. (e) Naemura, K. *Yuki Gosei Kagaku Kyokaiishi* **1987**, 45, 48. (f) Paquette, L. A. *Chem. Rev.* **1989**, 89, 1051. (g) Prelog, V.; Thix, J. *Helv. Chim. Acta* **1982**, 65, 2622.
- (3) Farina, M.; Morandi, C. *Tetrahedron* **1974**, 30, 1819.
- (4) Fujita, S. *Tetrahedron* **1991**, 47, 31.
- (5) Fujita, S. *Bull. Chem. Soc. Jpn.* **1990**, 63, 315.
- (6) Fujita, S. *J. Am. Chem. Soc.* **1990**, 112, 3390.
- (7) The regular representation (RR) is a kind of coset representation that stems from a coset decomposition of G by an identity group (C_1).
- (8) For this type of D_2 molecules, see Skell, P. S.; Wescott, L. D.; Golstein, J. J. P.; Engel, R. R. *J. Am. Chem. Soc.* **1965**, 87, 2829.
- (9) For the subduction table of T_d group, see ref 6.
- (10) Fujita, S. *Theor. Chim. Acta* **1990**, 78, 45.
- (11) Such a segment (ligand) has both chemical and mathematical meanings. The concept of "block" described in ref. 10 has a mathematical meaning only where it is concerned with a set of equivalent objects. The segment can be now restated as being a set of blocks so as to have a chemical meaning in addition.
- (12) (a) Fujita, S. *Theor. Chim. Acta* **1989**, 76, 247. (b) Fujita, S. *Bull. Chem. Soc. Jpn.* **1989**, 62, 3771. (c) Fujita, S. *Bull. Chem. Soc. Jpn.* **1990**, 63, 203. (d) Fujita, S. *Tetrahedron* **1990**, 46, 365. (e) Fujita, S. *J. Math. Chem.* **1990**, 5, 99. (f) Fujita, S. *J. Math. Chem.* **1990**, 5, 121. (g) Fujita, S. *Bull. Chem. Soc. Jpn.* **1990**, 63, 1876. (h) Fujita, S. *Bull. Chem. Soc. Jpn.* **1990**, 63, 2033.
- (13) Hirschmann, H.; Hanson, K. R. *Tetrahedron* **1974**, 30, 3649.
- (14) Hirschmann, H.; Hanson, K. R. *Top. Stereochem.* **1983**, 14, 183.
- (15) Yale, P. B. *Geometry and Symmetry*; Dover: New York, 1988.
- (16) Strictly speaking, an atom in isolation has a spherical symmetry. However, it can be treated as a $C_{\infty v}$ object for simplicity of discussion.
- (17) It may be subtle which term (diastereomorphic or heteromorphic) should be adopted in this case. We use the term "diastereomorphic" for denoting ligands having a 3D structure.
- (18) Strictly speaking, the skeleton in isolation belongs to $D_{\infty d}$; and the two $C^{(b)}$ joints construct a $D_{\infty d}/C_{\infty v}$ orbit. However, we can start from such an appropriate symmetry as this [D_{2d}/C_{2v}] for simplifying our discussion.
- (19) The name "methyl acetate" stems from the viewpoint that regards the methyl group as a substituent.

Application of Standard Robotic Methods to Water Analysis

J. R. LEE and T. L. ISENHOUR*

Department of Chemistry, Kansas State University, Manhattan, Kansas 66506

J. C. MARSHALL

Department of Chemistry, Saint Olaf College, Northfield, Minnesota 55507

Received May 15, 1991

The use of standard methods in water and wastewater analysis^{1,2} does not ensure the complete standardization of analytical procedures because of variability in implementation. Mechanical systems are reproducible; thus, a robotic system can be used to guarantee an almost perfectly reproducible execution of an analytical procedure. The purpose of this research is to establish the Standard Robotic Method (SRM) paradigm. This paper describes in detail how to convert a standard analytical method for water hardness and calcium to an SRM.^{2,3}

INTRODUCTION

To date, the majority of robot applications involve programming the robot to perform a specific, invariant task.⁴ Once the instructions for a given task have been developed and stored, the almost perfect reproducibility of the robot allows the task to be repeated without variation any number of times. Significantly, such a procedure could be activated at any time and by anyone with the same results.

There are standard methods of analysis in many fields. These methods specify, in detail, exactly how an analysis is to be performed. It is not uncommon for such methods to specify the exact details of sample preparation, reagent preparation and purity, specific laboratory apparatus, how the measurements should be made, and how the data should be analyzed. Such standard methods, once stored as instructions in a robot's environment, are reproducible by anyone using the system. The robotic environment containing instructions for standard method(s) of analysis could be moved to or reproduced in any other laboratory. The exportability of reproducible methods for chemical analysis by robotics, in the

form of a Standard Robotic Method (SRM), is the subject of this paper.

This paper will describe a system that can transform a classical standard method of analysis into an SRM. A frame-structured production system is used to build the SRM.^{5,6} The general procedure can be described in three steps:

- (1) Obtain the standard method for the problem.
- (2) Convert the method to an SRM by parsing and mapping.
- (3) Test, optimize, and save the procedure.

The conversion of a standard analytical method for the determination of hardness and calcium in water to an SRM will be used to demonstrate the system.

THEORY

For the purposes of this paper, a standard method or procedure is one that has been subjected to a thorough evaluation, has demonstrated its applicability for a specific purpose on the basis of extensive use, and has been successful, collaboratively tested, and then approved by some recognized agency

such as APHA (the American Public Health Association), AWWA (the American Water Works Association), WPCF (the Water Pollution Control Federation) or EPA (the Environmental Protection Agency). In a standard method nearly every step is specified in detail to minimize the variability of interlaboratory results. Such rigid procedure specifications are consistent with the capabilities of a laboratory robot. The reproducibility of a robotic procedure can ensure that when a standard method has been converted to an SRM it will not be subject to operator variation.

Standard methods for water and wastewater analysis are used in this paper as typical standard methods of analysis.³ The SRMs are derived using AI techniques to convert standard laboratory directions to robot commands. The components of the procedure are placed into a small number of general categories or generalized procedure steps. These are as follows: (a) sample preparation, (b) reagent preparation, (c) apparatus assembly, (d) analytical procedure parsing, and (e) interpretation of results.

In general, the components of an SRM are constructed as a sequence of unit operations that are already part of the robot's procedure library. The design and content of this library is critical to the success of the SRM project. Furthermore, for an SRM to be transferred among robotic systems, there must be agreement on a comprehensive set of robot unit operations supported by each installation. It is important to realize that SRM's require a high-level language whose detailed implementation will depend on each local robotic environment. All function definitions will cite only the purpose and arguments required, not the detail of every robot movement.

A useful analogy is found in the function set of a high-level computer language like PASCAL or C where the source code describing the functions is exportable to a wide variety of machines while the executable code derived from the source code is machine specific. How this library is applied in the construction of an SRM is illustrated in the following discussion.

Frequently, the first step in sample preparation is to measure the volumes or weights of the samples, and then to treat them according to the sample type. For example, to weigh the sample, the command could be a combination of library commands called WEIGHT. The component library routines of WEIGHT could include gettube.sub, weightube.sub, puttube.sub, etc., where it is assumed that the names convey at least the general function of the routines. These library commands are themselves composed of more fundamental routines defined in detail to be consistent with the hardware of each target system.

To make the function commands compatible with other laboratories, many commands require installation-specific parameters from the user. During the process of building the SRM, the parsing/mapping process will allow users to implement their own installation-specific information. For example, in a command like WEIGHT, the user will have the opportunity to specify things such as which hand to attach, the source of the sample, the destination of the sample, etc. Defaults are supplied whenever possible.

The development of an SRM, consistent with the design parameters discussed above, is carried out in three steps:

- (1) Cross-reference procedure steps to library functions.
- (2) Establish appropriate knowledge frames from procedure steps.
- (3) Create production system.

Cross-Reference Steps. A standard method is converted to an SRM using a keyword mapping strategy. The simplified text of the target method is analyzed for keywords, and each

keyword is used to point to entries in a knowledge base that establish the correspondence of the keywords with the robot routines. This is an evolving process. Each new procedure may both require and provide additions to the knowledge base. A highly interactive program has been written to assist the user in this process.

Establish Knowledge Frames. The robot commands, parsed from the procedure description, are arranged for efficient execution using knowledge frames.⁶ Every procedure has logical groupings of procedure steps, which taken together represent some laboratory unit operation. These logical groupings or knowledge frames are used to encapsulate the appropriate robot commands of a unit laboratory operation. The "slots" within knowledge frames may contain information and/or executable code.

A useful idea of frame implementation is the "action slot". In this system, trigger procedures attached to action slots in the frame are used to decide what to do in the event that the frame is found to match the current situation. The trigger's part of this system can be described as a production system and will be discussed later.

The content of a frame-structured procedure can be given by a simple example, TITRATE, which has the following frame structure:

```
Titrate.sub:
    apparatus      :spectrophotometer
    reagent type   :A,B,C...
    where          :container,tube
    indicator types :D,E,F...
    where          :container,tube
    Absorbance range :from 344 nm to 820 nm
    specific wavelength :G
    pH values      :from 0 to 14
    process         :command1,command2,command3...
```

In the frame procedure for titrate.sub, several slots are available to receive information from the parsing step that is relevant to the specific titration to be performed. The process part of titration.sub can be treated as the trigger part. The process slot contains several commands that may be activated when the frame is completed and when it matches the desired action. Each command is a specific robot procedure. For the successful transfer of an SRM to another laboratory, that laboratory must have implemented a command set that spans the commands required for the procedure. While this command set must be standardized in terms of naming conventions and actions, the details of the movements used in each laboratory to accomplish a given action will depend on the exact nature of the robot installation. For example, in our Zymate system we define a procedure, "ATTGP.SUB", to attach the robot's general purpose hand. It is likely that nearly all Zymate installations would have such a procedure. However, it is possible that no two of these procedures would be exactly the same in detail.

Create Production System. The production system is a computer program consisting entirely of if-then statements called productions. Production systems have two databases, the working database and the production database. The working database contains a model of the current state of the problem, and the production database stores the production rules. Productions are so structured that if a set of conditions about the working data are true, some specified set of actions will be initiated.

The if-then rules of the system are extracted from books and journals and comprise an expert system that "knows" about the procedures and methods under consideration.^{1-3,7}

This knowledge is applied to make certain that the knowledge frames based on the parsed procedure, when ordered and linked, form a complete and correct procedure. A useful analogy is that the production system compiles and links knowledge frames into complete and correct procedures.

The hierarchy of operations leading to an SRM is as follows:

---->	GOAL	---->	SELECT THE ANALYTICAL DOMAIN
1	1		
1	1		
1	SRM CREATION	---->	1) CROSS REFERENCE
1	1		2) PARSING/CHECKING
1	1		3) FRAME STRUCTURED PROCEDURE
1	1		4) PRODUCTION SYSTEM
1	1		
1	EVALUATE		
1	1		
1	1		
----	IMPLEMENT	---->	ARCHIVE/EXPORT SRM

The hierarchy of SRM development includes four levels. The first level is the goal level in which the user selects the target method. The second level, SRM creation, requires the user to verify that the knowledge sources include expertise and methods that satisfy the requirements of the target method. Then the preliminary SRM may be created by using a parsing/checking utility to create a frame-structured procedure that can be implemented with the production system. The third level is to evaluate the SRM, by comparison with manual results using known samples. This step may require modifications to the SRM to improve its accuracy and efficiency. Finally, the fourth level is the implementation and archiving of the evaluated SRM.

IMPLEMENTATION

The determination of the hardness of water will be used to demonstrate how an SRM can be created. In the first stage of the implementation, the knowledge sources are established. For this determination a method is adapted from *Standard Methods for the Examination of Water and Wastewater* (ref 3, page 213, section 314B, 3. Procedure). This method was prepared and published jointly by APHA, AWWA, and WPCF. The method selected is a classical EDTA titration. This method has four main categories: apparatus, reagents, procedures, and results. These categories can logically be converted to frames, each of which can have additional knowledge frames as slots. Finally, the frames can be linked together to form the SRM. The apparatus and reagents' frames will have numerous attributes that depend on the specific standard methods implemented.

Apparatus:

- (1) Glassware.
- (2) pH meter.

Reagents:

- (a) Buffer solution (pH = 10).
- (b) EDTA (0.01 N).
- (c) EBT (Eriochrome Black T).

Additional knowledge is required both from the user and system itself. To supply the required knowledge, information has been included from several articles and books. When the knowledge base is complete, the procedure's text is parsed and extracted, and the key words are mapped onto the knowledge base to create the complete procedure. For example, consider the keyword "Dilute". This key word is converted into a frame-structured procedure which has several attributes and slot values. While some of the slot values in this frame have to do with amounts of materials, many of the slot entries

depend on the configuration of the laboratory. The combination of these keyword commands can be used to build the analytical procedure. Part of the standard method text about the procedure is shown in following sentence in which the key word "dilute" will be emphasized.

"...

(3) Procedure:

(a) Pretreatment of polluted water and wastewater samples. ...

(b) Titration of sample.

... Dilute a 25-mL sample to about 50 mL with distilled water in a porcelain casserole or other suitable vessel. Add 1-2 mL of buffer solution."

In this system, several required attributes of the key word "dilute" have been implemented. This ensures the portability of the "dilute" command to different laboratories. The activation of the "dilute" function will require the local user to modify several slot values prior to executing the procedure.

To convert this procedure's text into the primitive robotic procedure some additional key words will have to be extracted, e.g., "Add". After the conversion by the system, the text:

"Dilute a 25-mL sample to about 50 mL with distilled water in a porcelain casserole or other suitable vessel. Add 1-2 mL of buffer solution."

will become the robot's executable procedure:

Dilute.sub

rem Dilute 25 ml sample to about 50 ml with distilled water in a porcelain casserole or other suitable vessel.

Add.sub

rem Add 1 to 2 ml buffer solution.

In the activated procedure "dilute", dilute.sub will have three attribute and two primitive robot commands. When dilute.sub is activated, the user will be asked to input the source of the diluent, the destination, and finally, the amount to complete the dilution. Notice that the questions generated allow the user to complete the dilution in his or her local environment as the source and destination will be given in terms of the local configuration.

The frame structured procedure for Dilute.sub is

FRAME : (Dilute)

origination : ?

destination : ?

amount : ?

procedure : Dilute

The "Dilute" command will be activated only after the required slots are filled. The "Dilute" procedure also includes two other primitive robot procedures, "getamount.sub" and "putamount.sub", to handle some of the details of the dilution process.

The same process used for converting the "dilute" key word is applicable to a key word like "Add". Indeed, adding a reagent to a sample is merely a special case of "dilute", and the converted procedure will use several of the same robot functions and procedures.

EXPERIMENTAL SECTION

Robotics System. A Zymate II robot was used to perform all the experimental manipulations. The robotics system included a robot arm with three removable hands, a vortex mixer, a solvent delivery system, a balance, and a centrifuge. The diagram for the laboratory robotics including the HP UV/VIS spectrophotometer is shown in Figure 1. The Zymate controller was used to communicate between the Zymate II and the microcomputer.

Microcomputer. An IBM-compatible PC running under MS-DOS 3.3 operating system was used. The microcomputer was equipped with one 360K floppy disk driver, one 20M hard disk, and 640K of RAM.

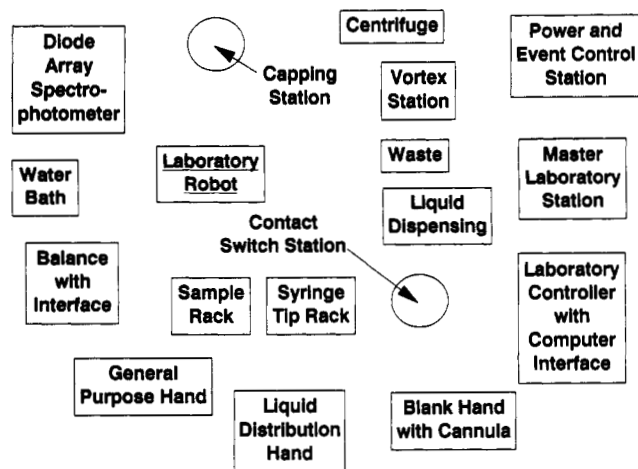


Figure 1.

Table I. Comparison of SRMs and Manual Operations^a

2 mL	calcium (1.0 mg Ca ²⁺)
4 mL	distilled water
1 mL	buffer solution (pH = 10)
2 drops	EBT (0.5 g in 100 g of ethylene glycol monomethyl ether)
EDTA	0.005 N as titrant
titrant	0.215 mL added each time by robot

	SRMs	manual operation
experiment 1, mL ^b	1.90	2.00
experiment 2, mL	1.88	1.95
experiment 3, mL	1.90	1.95
average, mL	1.893	1.967
mg of CaCO ₃	0.947	0.984
SD	0.009	0.0223
% SD	0.48	1.13

^a The list contains the chemicals and the titration parameters for the comparison. ^b Indicates the amount needed to titrate the unknown. The amount for robotic method is based on calculation, while the manual operation used visual indicator detection to determine the end point.

Spectrophotometer. An HP 8451 diode array spectrophotometer was used to collect all UV/VIS absorbance spectra. The spectrophotometer has a wavelength resolution of 4 nm over the range from 190 to 820 nm.

Verifying the Water Hardness SRM. To verify that the SRM for water hardness was valid, two identical samples were analyzed in triplicate, one with the SRM and the other manually (see Table I). Both the SRM and the manual determination were carried out in strict accordance with the stipulated procedure.³ For the SRM, the end point determination was carried out spectrophotometrically. As is normally true for an analysis procedure adapted to a robot, the operational details of the SRM will be quite different from the traditional titration methods.

In the SRM, the titration was carried out in a test tube. This test tube can hold approximately 14 mL of solution. A 2-mL portion of sample was transferred to the reaction test tube and diluted to 6 mL with deionized water. Approximately 2 mL of buffer was added to maintain the pH value at 10. The sample was thoroughly mixed in a vortex mixer after each addition of titrant. After each addition of titrant, approximately 2 mL of the sample was transferred from the reaction test tube to a circular spectrophotometer cell, and the absorbance was measured. Following the absorbance measurement, the solution in the absorbance cell was transferred quantitatively back to the reaction vessel. The same cell was used throughout a complete titration. Clearly, a more expedient and accurate way to carry out this titration would be to measure the absorbance directly in the reaction vessel. A laboratory seeking to put this SRM into routine use should

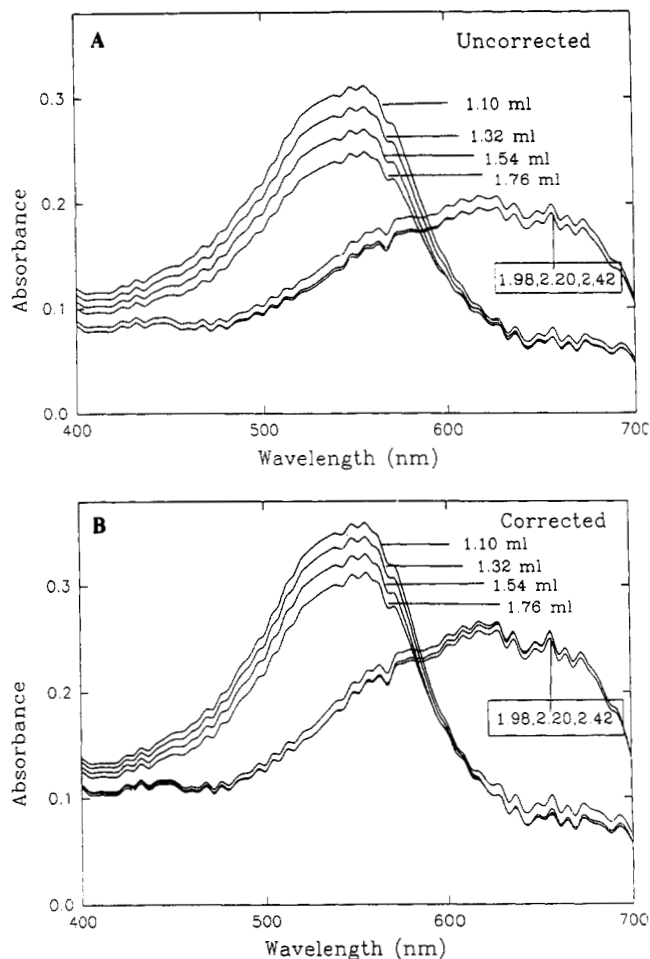


Figure 2.

make the necessary hardware modifications. However, consistent with the philosophy of the SRM, the details of the implementation of the spectrophotometric titration are specified in terms of the local robot environment.

The absorbance of the sample, after each addition of titrant, was stored in a file for subsequent analysis. The method of end point detection used was admittedly approximate but deemed to be adequate for the purpose of this determination. The absorbance spectrum of the EBT indicator as a function of volume just prior to and just following the equivalence point is shown in Figure 2, parts A and B. Figure 2B is corrected for the dilution that occurs during the titration. Absorbances at 548 nm (absorbance maximum for the metal indicator complex) and at 616 nm (absorbance maximum for the free indicator) were plotted as a function of volume in Figure 3. Note that the splined curves placed through the points only indicate the general shapes of the curves. The end point was taken as the intersection of the two curves. As a practical matter, the two points closest to the equivalence point in each curve were used to describe a straight line, and the intersection of these two lines was taken as the end point. If a laboratory were optimizing this SRM for highest accuracy, most sophisticated end point detection algorithms would have to be used.

RESULTS AND DISCUSSION

A Turbo Pascal program has been written for the purpose of creating SRMs from the standard methods procedures. This program assists the user by linking the available robot functions to the key words in the procedure. The details of the conversion of the standard methods into a robot executable SRMs are shown in Appendix 1. The original standard method for determining water hardness was modified to be more amenable

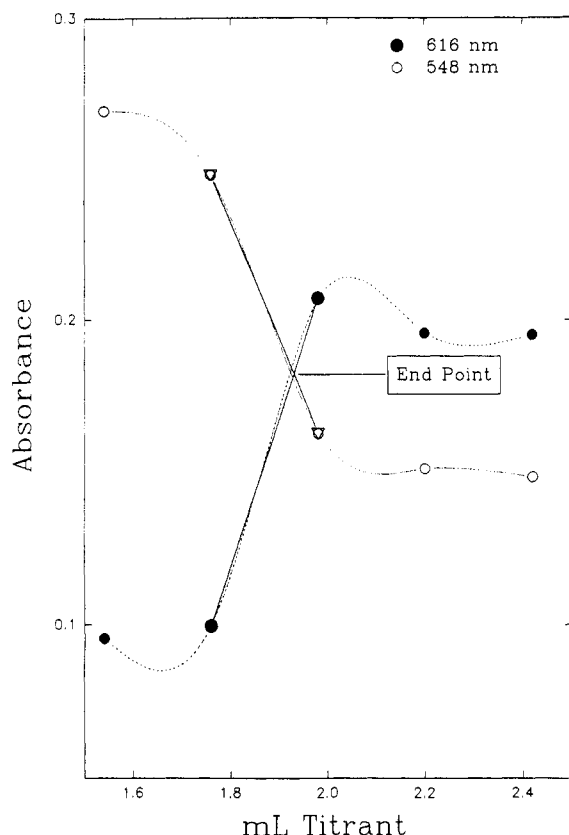


Figure 3.

to robot implementation. The SRM is based on this modified procedure. The translation of this modified script to an SRM is partially a manual operation with the system identifying key words in the script and requesting system specific information from the user. The key word extraction and implementation for this demonstration is detailed in Appendix 2.

Normally, the robotic procedures derived are a combination of the unit robot operations. These unit operations are combinations of the robot positions sequenced in such a way as to accomplish some task. The four unit operations which we have used to assemble the dilution procedure, *dilute.sub* are listed in Appendix 3. This subroutine is assembled in response to the key word "Dilute", which was extracted from the original script. All key words identified are handled in much the same way. The amount of user interaction required depends on the nature of the operation and the specifics of the local robot environment. After the implementation of all the key words for the water hardness analysis, the SRM created will consist of an ordered series of robot instructions capable of performing the analysis.

In the experimental part, the EDTA concentration had been changed from 0.01 N to 0.005 N, mainly because of the restriction of the robotic equipment. The test tube can hold approximately 14 mL of solution, but using the Zymate Z620 vortex to mix the solution in the tube, the content of the tube can not exceed 9 mL. The reason for diluting the sample to 8 mL is to allow a visual decision on the change of the colors for EDTA titration. The titration increments of the EDTA by using the robotic system can be rearranged from 0.1 mL to 10 mL depending on the sample's hardness and the concentration of the EDTA. For this experiment, increments of the 0.215 mL of EDTA is the optimum for the robotic system used.

The results from the SRM and the manual analysis are compared in Table I. The end points in the titrations were determined spectrophotometrically for the robot determination (the SRM) and visually in the manual determination using

EBT as the indicator. There is about a 4% difference between the manual operation and the SRM, which is within the expected error for this type of determination. The sensitivity could be improved by modifying the basic SRM structure to use some other standard method, like atomic absorption, which is more sensitive. Because of the modularity of these procedures, modifications can be made easily.

To make the SRM more efficient and easier to use, some modifications in the original method are required. For this experiment the adjustment is to change the sample size and the EDTA concentration. For the SRM, it is possible to duplicate every step of the manual-operated standard method. AI techniques can help the developer of standard methods to retain the principles of the standard methods and implement the equivalent robotic procedures instead. These robotic procedures can replace part of the human operation to avoid human exposure to a dangerous environment or to speed up tedious and repetitive manual operations. This paper does not advocate the use of a robot to replace every step of standard methods that are manual, but to provide an option that can overcome the variability among laboratories. It is very common in standard methods that instruments are not specified. The same concept can be applied to the robotic system, which needs only to specify the functions to be performed. Consistent with this feature, the robotics that are used for the standard methods need not to be specified.

CONCLUSION

This work has demonstrated a working model of a system for the creation of SRM's. This model is a PC-based program written in TURBO PASCAL and uses a frame-based knowledge base and a highly interactive procedure parsing utility.

The primary purpose of SRMs is to overcome the variability among laboratories and to provide an optional method amenable to conversion from the original manual method. The ideal system should include the automatic parsing of standard procedures into SRM's. However, this is a very difficult problem that is not yet solved. Not only is it difficult to process the natural language of chemical procedures, it is also difficult to map procedures intended for manual operations into procedures amenable for automation by a laboratory robot.

ACKNOWLEDGMENT

Funding for this project was provided by a grant from the National Science Foundation.

APPENDIX 1

Original Standard Method.

"(3) Procedure

...

(b) Titration of sample:

... Dilute a 25-mL sample to about 50 mL with distilled water in a porcelain casserole or other suitable vessel. Add 1-2 mL of buffer solution. ... Add 1-2 drops of indicator solution. ... Add standard EDTA titrant slowly, ... At the end point the solution normally is blue."

Modified Text from Original Method.

Titration of sample:

- (1) Dilute a 2-mL sample to about 6 mL in test tube.
- (2) Add 1 mL of buffer solution.
- (3) Add 2 drops (EBT or murexide) of indicator.
- (4) Titrate from red to pure blue color. The duration of the titration should not exceed 5 min.
- (5) Perform titrations on each of the samples provided.

Converted Executable SRM:

- (1)

Dilute.sub
 rem Dilute 2 mL sample to about 6 mL in test tube
 stop.sub
 (2)
 add.sub
 rem Add 1 mL buffer solution
 stop.sub
 (3)
 add.sub
 rem Add 2 drops (EBT or murexide) indicator
 stop.sub
 (4)
 titrate.sub
 rem Titrate from red
 rem to pure blue color
 stop.sub
 The duration of the titration should not exceed 5 min
 stop.sub
 (5) Perform titrations on each of the samples provided
 stop.sub

APPENDIX 2

Key Word Extracted from Modified Text.

add
 dilute
 measure
 titrate
 titration
 titrations

Key Word Implementation.

Dilute.sub : Dilute, Add.
 Frame : (Dilute)
 origination : ?
 destination : ?
 amount : ?
 procedure : getamount.sub, putamount.sub.
 Titrate.sub : titrate, titration, titrations
 Frame : (TITRATE)
 apparatus : ?
 reagent(add) : ?
 location : ?
 indicator : ?
 location : ?
 absorbance : ? (for spectrophotometer)
 pH : ?
 titrant : ?
 location : ?
 amount(add) : ?
 number(add) : ?
 procedure : getamount.sub, putamount.sub,
 getspec.sub, putspec.sub, get-
 tube.sub, puttube.sub, vortextos-

pec.sub, spectovortex.sub, mix.sub

APPENDIX 3

Primitive Robot's Procedure (Movement) Implementation.

Getamount.sub
 attblk.sub
 hand3
 blank.rack
 r.down.to.blank.rack
 valve.c = 0
 mls
 timer(3) = 6
 wait for timer(3)
 blank.rack
 Putamount.sub
 hand3
 blank.rack
 r.down.to.blank.rack
 vol.c = 0
 mls
 timer(3) = 6
 wait for timer(3)
 blank.rack
 parkblk.sub
 Attblk.sub
 clear.blank.hand
 band3pos1
 hand3pos2a
 hand3pos3
 clear.blank.hand
 Parkblk.sub
 clear.blank.hand
 hand3pos3
 hand3pos2p
 hand3pos1
 clear.blank.hand

Registry No. H₂O, 7732-18-5; Ca, 7440-70-2.

REFERENCES AND NOTES

- (1) Sawyer, C. N.; McCarty, P. L. *Chemistry for Environmental Engineering*, 3rd ed.; McGraw Hill: New York, 1980; pp 514-519.
- (2) Minear, R. A.; Keith, L. H. *Water Analysis*; Vol. 1, Academic Press: New York, 1982; Vol. 1, pp 1-44.
- (3) *Standard Methods for the Examination of the Water and Wastewater*, 16th ed.; American Public Health Association: Washington, DC, 1985.
- (4) Strimaitis, J. R.; Hawk, G. L., Eds. *Advances in Laboratory Automation Robotics*; Zymark Corp.: Hopkinton, MA, 1989; Vol. 5, pp 139-165.
- (5) Hunt, V. D. *Artificial Intelligence and Expert Systems Sourcebook*; Chapman & Hall: New York, 1986; pp 113-114.
- (6) Barr, A.; Feigenbaum, E. A.; Cohen, P. R. *The Handbook of Artificial Intelligence*; William Kaufmann: New York, 1981; Vol. 1, pp 216-222; Vol. 3, pp 557-562.
- (7) Fresenius, W.; Quentin, K. E.; Schneider, W., Eds. *Water Analysis*; Springer-Verlag: Berlin, Heidelberg, 1988.