X-ray Fluorescence Analysis Simulation

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X-ray Fluorescence Analysis Simulation simulates the qualitative and quantitative X-ray fluorescence (XRF) analysis of an unknown containing 3 to 5 elements randomly selected from a list of 24 elements. The percentages in the quantitative analysis do not total 100% as there are always inert ingredients, thus all components must be determined. The simulation does not encompass such interelement effects as absorption and enhancement. The limited resolution (2° 2θ) does lead to some interesting spectral interferences that require switching analyzing crystals and/or X-ray tube targets in order to complete the analysis. Three analyzing crystals [lithium fluoride (LiF), ethylenediamine d-tartrate (EDT), and potassium acid phthalate (KAP)] and two target materials [tungsten (W) and chromium (Cr)] are available in the program.

While the program is more an analysis simulation than an instrument simulator, it does approximate a wavelength dispersive X-ray instrument with a resolution of 2° 2θ. A schematic of the operation of such an instrument is available through the Help menu. Students are expected to keep careful notes of all data collected and to devise appropriate standards for each element in order to do the quantitative analysis.

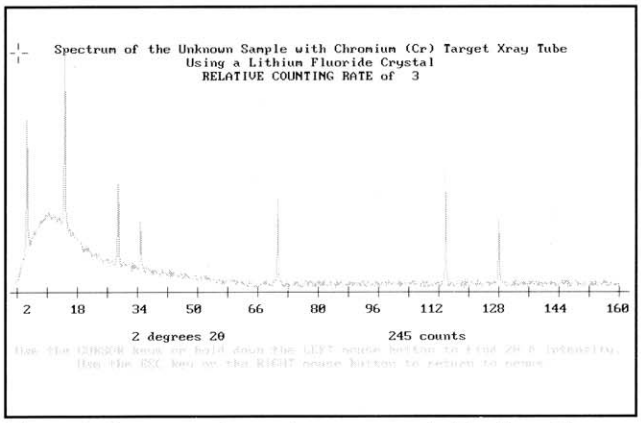

Figure 3. Spectrum of an unknown generated by X-ray Fluorescence Analysis Simulation.

The author has used some form of X-ray Fluorescence Analysis Simulation in his instrumentation class for about twelve years. The present program is modeled on one written by Breneman (*2*) but has been extensively rewritten to take advantage of the graphics ability of present-day computers. The students always enjoy the program when they understand what is necessary to perform an analysis. A four-component unknown will take the average student about two hours. Since it is used as a laboratory exercise, it is wise to provide students with advice and encouragement. A few students have actually come back and asked to use the program as a game.

In using the program as a laboratory exercise, it is helpful to emphasize that careful notes are necessary to prevent confusion. It is also useful to require students to discuss the differences between the nominal answer from the program and their answer. While this difference can not be more than ±10%, they should be made aware of the effect of noise and background on their answers.

Hardware and Software Requirements

Programs in Series B of *JCE: Software* require an IBM PC-compatible microcomputers with 640K RAM, one disk drive, and a VGA or compatible graphics adapter. PC- or MS-DOS version 3.1 or later is also required.

Both REACT and X-ray Fluorescence Analysis Simulation support a Microsoft compatible mouse; a mouse is recommended but not required.

REACT requires 350 K of free disk space for installation onto a hard disk drive; X-ray Fluorescence Analysis Simulation requires about 230 K.

Citations

1. Reaction courtesy of John Camp, a Texas High School teacher.
2. Breneman, G. L. *J. Chem. Educ.*, **1979** *56*, 303.

About This Issue

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How to Use These Programs

The programs in this Series B issue are for IBM PC-compatible computers.

REACT is designed for use in general chemistry and advanced high school chemistry courses. It might also be used as a resource in more advanced college courses such as Analytical Chemistry. It is a very useful tool anytime you need access to thermodynamic data or need to do quantitative calculations involving chemical reactions.

The program can be operated directly from the keyboard, or by using the mouse to point and click on selections. It includes a Library section from which one can select reactants and products from an alphabetical scrolling text box. A convenient alternative is to select a reaction from the saved files included with REACT. When the reaction is assembled, a single click balances the equation and displays its standard thermodynamic properties. The effect of temperature is easily investigated by typing new values into the temperature box. Another click takes you to the Equilibrium screen where you may enter initial concentrations or pressures of all species and have REACT determine the equilibrium values. The reaction may also be linked to other reactions allowing investigation of dissociation of multiprotic acids and other complex processes.

Students can set up such questions easily, and REACT solves them very quickly. Thus, the program can serve as an enjoyable and efficient learning tool for exploring practical problems as well as esoteric thermodynamic and equilibrium questions, allowing more time for thought about and discussion of the meaning of the results.