

months from tide and wave action and in summer months from tides and the North Equatorial Current. The surface movement of waterborne radioactivity from Bikini and Eniwetok atolls would therefore be westward toward the Philippine Islands, with the possibility of some movement back toward the east in the Equatorial Countercurrent and possibly eastward at shallow depth in the Cromwell Current (13). Both Christmas Island and Penrhyn Atoll lie in the path of the westward-moving South Equatorial Current and consequently would be unlikely recipients of waterborne radioactivity emanating from Bikini and Eniwetok lagoons.

Nickel-58 comprises some 68 percent of stable nickel, and we have considered the possibility of the production of ^{59}Ni (half-life, 80,000 years) both by (n,γ) interactions with stable nickel, (p,n) reactions with stable cobalt, and (p,α) reactions with ^{56}Fe (92 percent abundance). Based on abundances, cross sections, and decay constants, we calculated an activity ratio of ^{63}Ni to ^{59}Ni of approximately 600 for the (n,γ) production of ^{59}Ni . Nickel-59 decays by electron capture and is determined by measuring the 6.9-keV x-ray which results from the de-excitation of its daughter, ^{59}Co . A 3000-minute count of the most radioactive clam kidney from Eniwetok Atoll in an anticoincidence shielded x-ray counter gave a positive indication of ^{59}Ni (at a counting error of 1 S.D.), with an upper limit of some 0.1 disintegration per minute per gram of dry weight. No ^{59}Ni was detected in 1000-minute counts of soil samples obtained from either atoll. It is probable, therefore, that no large amounts of ^{59}Ni were produced, and that the presence of small amounts of ^{59}Ni precludes its usefulness as a tracer in oceanic processes.

A realistic assessment of the total ^{63}Ni present at Bikini and Eniwetok atolls is not possible from the data presented here, although knowledge of such an inventory and of the rate at which it is injected into the North Equatorial Current would help one to determine its usefulness as a downstream tracer for these waters. However, the giant clam *Tridacna* sp. appears to be an excellent indicator organism, which could be used to delineate the downstream penetration of ^{63}Ni .

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Automatic Determination of Crystal Structure

Abstract. Several crystallographic computer programs have been organized into one large automatic program for solving crystal structures. The emphasis of this organization has been to produce a noninteractive system, that is, to have all decisions made by the computer. Input data are the raw intensity data, cell constants, space group, chemical formula, and other miscellaneous items. The output is a stereo picture of the contents in a unit cell. The program, operating in a noninteractive mode, has successfully solved compounds of unknown structure; in addition, for a test compound of completely unknown composition, this program deduced the correct structure with an average error in bond distance of 0.05 angstrom and an average error in bond angle of 7° .

It is generally recognized that there is a very important unsolved problem in crystallography—the phase problem. By this we mean that diffraction experiments do not permit one to obtain the structure factor and yield only its magnitude $|F|$. The great number of crystal structures that have been solved indicates that the problem is not insurmountable. For the most part these structures have been solved by the Patterson technique (1). More recently the symbolic addition procedure (2) is becoming the method of choice, especially for organic compounds with no heavy atom. This latter technique can be reduced to a formalism in which one starts with phases for a small number of reflections and generates relations between these and a large enough set of other reflections so that a Fourier map based on these phases permits a trial model to be obtained. If, in carrying out the symbolic addition, the program is unable to clearly distinguish the best starting combination of phases, one can calculate all possible E-maps (usually a small number) and attempt to obtain a correct trial model from one of these.

It is of interest to discover if one can use such a structure-solving capability together with other crystallographic

programs to obtain a completely automatic structure-solver. In this connection we desire a noninteractive system which may be used by the noncrystallographer, rather than an interactive one for the professional crystallographer similar to those already described (3). Based on our experience so far, the answer is clearly yes.

We have constructed an automatic structure-solving program consisting, in the main, of standard crystallographic programs as subroutines. These subroutines have been integrated together with decision-making subroutines so as to eliminate the decisions which were previously reserved by the crystallographer for himself. The user supplies raw data, space group, and other miscellaneous items; the program produces a stereo plot of the best trial model.

At present, the algorithms for the solution of the structure are relatively unsophisticated; it is anticipated that they can be made more clever as additional experience is gained. For greater flexibility, it is possible to interrupt the program in order to overrule decisions made by it. This has usually proved to be unnecessary; in fact the "hands off" policy may sometimes be the best approach. The structure of PaOCl_2 (4) was easily solved by this program after

attempts to interpret the Patterson map failed as a result of bias resulting from an inaccurate chemical formula. In another example, the crystal structure of Ga_2Mg (5) had previously been solved by conventional Patterson methods only after a great amount of difficult work, again because of incorrect formulation. We have rerun this problem using the automatic program. Even with the incorrect formula, this problem turned out to be trivial.

These results suggested that the information contained in the raw intensity data alone might be sufficient to solve the structure without knowledge of the chemical composition. In order to test this hypothesis, we used the completely automatic structure-solver. Raw data, cell constants, and space-group information for an unknown structure were supplied to one of us. No other information (for example, on the chemical formula) was provided. An arbitrary density was chosen from which an approximate number of atoms per cell could be calculated. This could also be done by the program if desired.

Starting from these meager data, the program drew a stereo picture of the contents within the unit cell after one uninterrupted calculation taking 19 minutes on an IBM 7094. This stereo picture together with the summary parameters served as the trial structure for least-squares refinements which led to a discrepancy index (R factor) of 8 percent. The refined bond data indicated that the chemical formula was $\text{C}_4\text{H}_4\text{O}_4$ (fumaric acid), and the source (6) was found. Although the molecule is a simple one, this structure was solved entirely by the computer without assistance from the crystallographer and without knowledge of the composition.

Comparisons made between the trial model of the structure-solving program and the refined model of Bednowitz and Post (6) show that the average errors are only 0.05 Å for bond lengths and 7° for bond angles.

In the current version, this program has been used to solve four previously unknown structures with up to 20 atoms in the asymmetric unit. For one of these it was necessary to interfere in the decision-making step because the algorithm which selects the starting reflections arrived at a bad combination. This indicates that more work is required. Indeed, it is anticipated that this program would probably fail on many structures. The results thus far were obtained for structures for which it was reasonable to expect the symbolic

addition step to function effectively. Such would probably not be the case for structures in which a substructure feature is pronounced. The current version also requires that the structure have a center of symmetry.

Later versions of this and similar programs could be coupled directly to an automatic diffractometer under computer control, and the entire procedure could be made automatic. In view of the apparent power of the symbolic addition procedure to solve structures when the formula is unknown, it is not even unreasonable to expect that someday such a system could be used by chemists seeking to discover the formula as well as the structure of some newly prepared material.

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Recent Planktonic Foraminifera: Dominance and Diversity in North Atlantic Surface Sediments

Abstract. *Foraminiferal dominance values above 50 percent and associated diversity minimums in surface sediments of the North Atlantic coincide with past extremes of temperature, productivity, or salinity in overlying surface waters. These parameters delimit a cold Polar-Subpolar water mass and an impoverished, saline Southern Sargasso Central water mass for the late Recent. Anticipated pole-to-equator diversity and dominance gradients in the open ocean are virtually eliminated by the stronger trends of the vigorous subtropical North Atlantic gyre.*

That the number of species (diversity) of virtually all forms of animal and plant life diminishes toward the colder regions of the earth is a central

tenet of ecology. This diversity gradient has been used in open oceans to define ancient pole positions, while minor departures from the regional gradient have been attributed to local environmental features, particularly oceanic circulation (1). In contrast, the tendency of any one species to comprise a large fraction of the total fauna varies in the opposite sense, increasing toward polar regions. This parameter is termed dominance. Dominance-diversity trends of planktonic Foraminifera in and around the subtropical North Atlantic gyre have been evaluated from 290 surface sediment samples (2).

Dominance is highest in cores from two areas of the North Atlantic—beneath the cold polar-subpolar waters off Newfoundland and beneath the southern part of the Sargasso Sea in the west-central Atlantic (Fig. 1). The dominant species in the northern area is *Globigerina pachyderma*, which is recognized as the most typical cold-water planktonic foraminifer (3). Temperature appears to explain the dominance of *G. pachyderma*; no other species is as well adapted to these frigid waters. It accounts for more than half of the population in an area extending southward just to the Polar Front (4).

Dominances of any species of planktonic Foraminifera that exceed 50 percent in sediments of the open ocean seem to indicate past extremes of temperature, salinity, or productivity in the overlying waters. On this basis, I have defined Polar-Subpolar water as an ecologically distinct mass during the late Recent interval represented by surface sediment samples (Fig. 2).

The warm-water species *Globigerinoides ruber* accounts for the other maximum-dominance area at 20° to 30°N (Fig. 1). It also contributes many of the high values from 0° to 20°N, but only in shallow cores unaffected by differential solution (5). The Sargasso Sea values of well over 50 percent are unique at low latitudes for planktonic Foraminifera in surface sediments. Top sediment samples represent mixed averages spanning as much as several thousand years, and it is presumably rare that any one species can predominate at such high percentages in warm open-ocean areas for such long periods. Moreover, the southern Sargasso Sea region is sufficiently warm through much of the year that it should be receptive to the same variety of species typically found in tropical waters. However, the shallow layers of these central waters are at present