

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.

QUINTIN JOHNSON

GORDON S. SMITH, EILEEN KAHARA
Lawrence Radiation Laboratory,
University of California, Livermore

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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

among the most saline and unproductive in the world's oceans, and I infer that similar environmental extremes have presented an effective ecologic barrier during the late Recent to species which might otherwise have lived there (6). Thus *Globigerinoides ruber* has reached such extreme dominances by default; it is virtually the only foraminifer to have survived in this region under such conditions, and even it is somewhat diminished in absolute abundance (7).

Again using 50-percent values as criteria, I have defined this second region of high dominance as the Southern Sargasso Central water (Fig. 2). The northern boundary of this area runs along 30°N, at present the approximate southern limit of winter overturn. Surface layers north of 30°N are thoroughly mixed in winter, resulting in an influx of nutrients and phytoplankton

and an increase of foraminiferal abundance (8). South of about 30°N the "seasonal" thermoclinic stratification apparently remains intact even through the winter, and the shallow waters consequently remain extremely impoverished through the entire year. The southern and western boundaries of the Southern Sargasso Central water are marked by a shallower permanent thermocline, faster currents, greater productivity, higher biomass levels, and a more abundant and diverse foraminiferal population (9). *Globigerinoides ruber*, while even more abundant in an absolute sense in these warm peripheral areas, has evidently not been able to so completely dominate the fauna as it has in the central waters (7). Thus by inference, the southwestern part of the Sargasso Central water seems to have been the most unreceptive warm-water mass in the North Atlantic.

The anticipated pole-to-equator diversity gradient is not only greatly subdued, but virtually eliminated by the vigorous subtropical North Atlantic gyre (Fig. 3) (10). Only within the frigid Polar-Subpolar water off Newfoundland are there sufficiently low diversities to suggest a planetary gradient. Moreover, no maximum diversity belt girdles the equator, and several very low diversity values appear there. An anomalous area of low diversity blankets the Sargasso Central water, coinciding with the uniquely high *Globigerinoides ruber* dominance. This supports the interpretation that those dominance values were caused by a low productivity and high salinity barrier to other species during the late Recent.

The prominent belt of high diversity associated with the subtropical North Atlantic gyre is not entirely explained by any one factor. In different sections

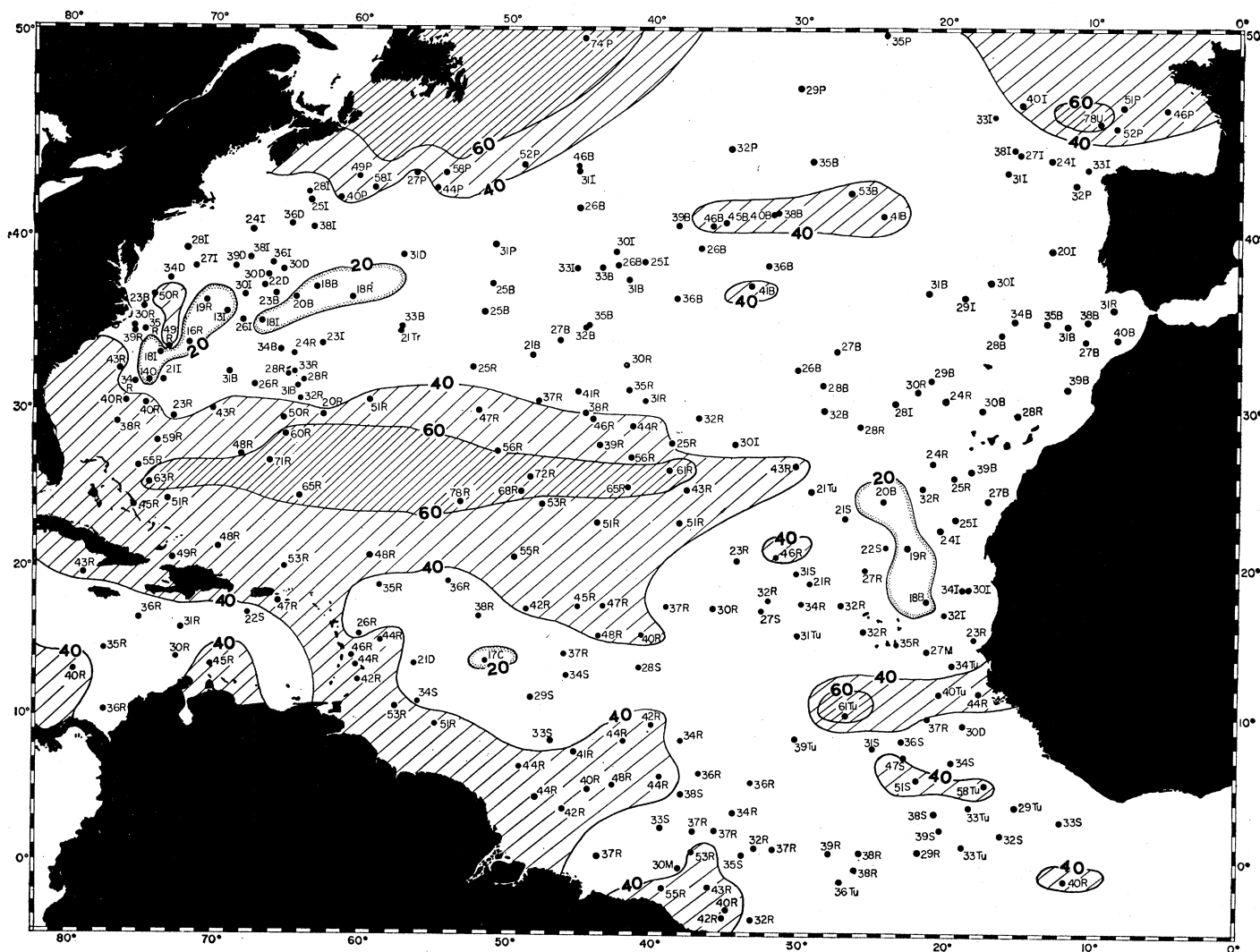


Fig. 1. Species dominance of planktonic Foraminifera in North Atlantic surface sediments, showing the percent of the dominant species in each core. The letter after each percentage figure gives the name of the dominant species, thus: P, *Globigerina pachyderma*; R, *Globigerinoides ruber*; B, *Globigerina bulloides*; I, *Globorotalia inflata*; D, *Globoquadrina dutertrei*; S, *Globigerinoides sacculifer*; Tu, *Globorotalia tumida*; M, *Globorotalia menardii*; C, *Globigerinoides conglobatus*; O, *Pulleniatina obliquiloculata*; U, *Orbulina universa*; Tr, *Globorotalia truncatulinoides*.

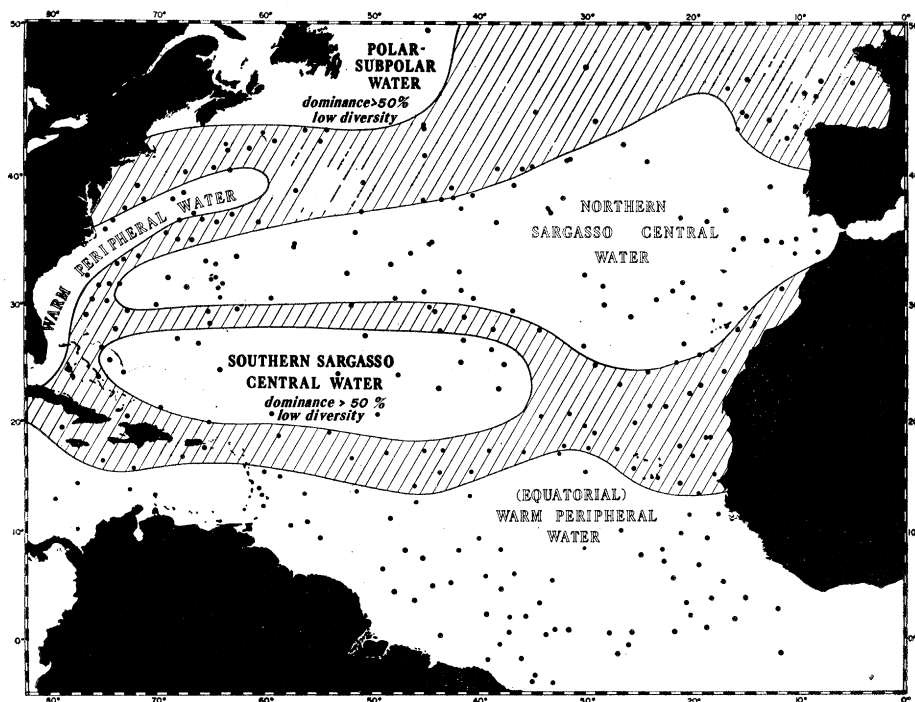


Fig. 2. Paleoecologically significant late Recent water masses of the North Atlantic, defined by planktonic Foraminifera in surface sediments. The Polar-Subpolar water and the Southern Sargasso Central water are defined by dominance maximums and diversity minimums, both of which indicate prohibitive late Recent environments. Transitional waters between distinct masses are diagonally ruled. The two water masses not discussed in the text (Northern Sargasso Central water and Warm Peripheral water) are defined on the basis of characteristic suites of environmentally related species rather than by dominance and diversity patterns (Ruddiman, 2).

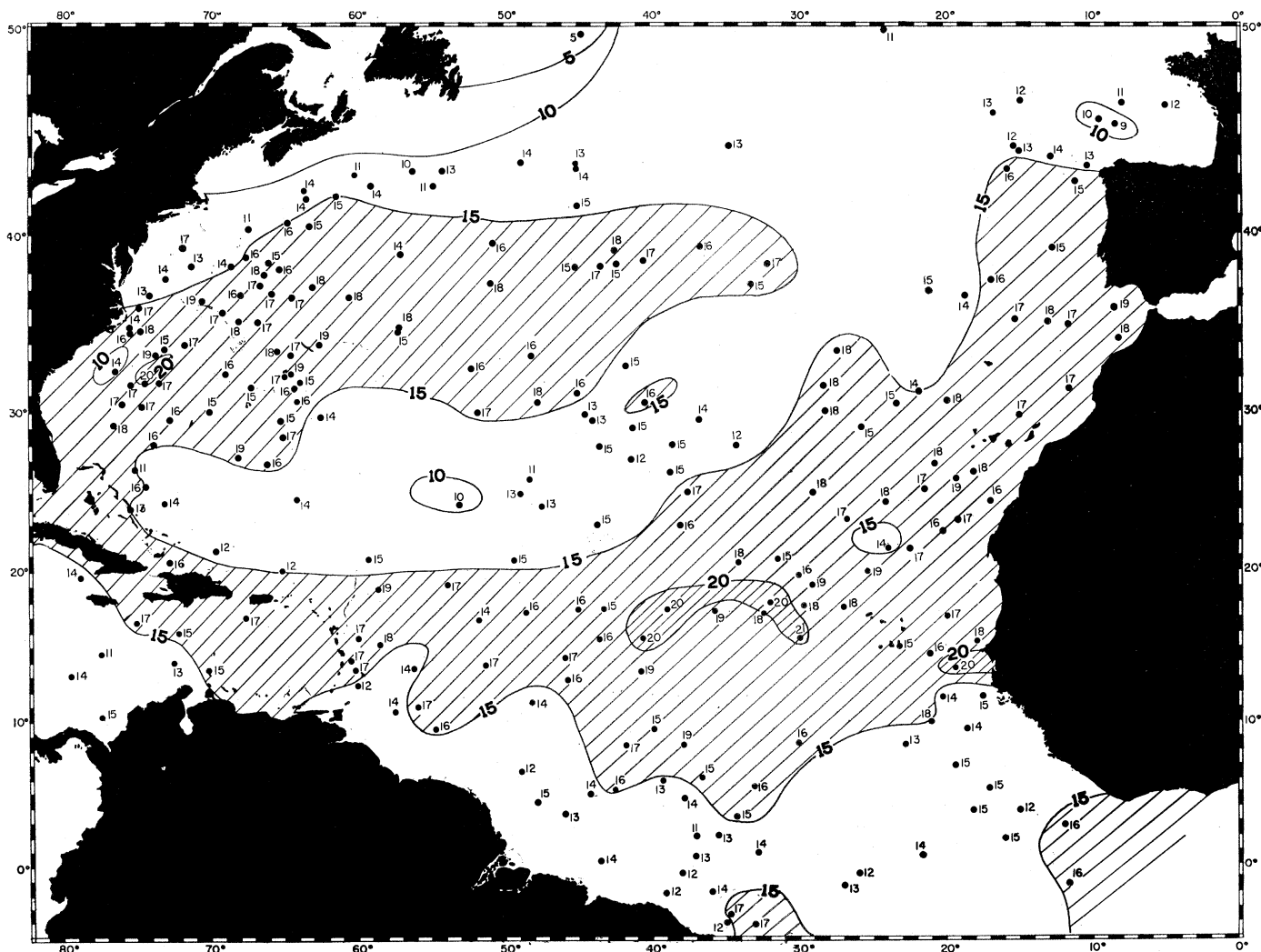


Fig. 3. Species diversity showing number of species in each core top more abundant than 0.2 percent of the planktonic foraminiferal fauna. High diversity defines peripheral areas of the subtropical North Atlantic gyre; diversity is lowest in the Southern Sargasso Central water and north of the Polar Front.

of the periphery of the gyre, four conditions contribute to its existence. (i) Nutrient-biomass levels are high, sustaining an abundant and diverse flora and fauna (9). Because foraminifers are as likely as other zooplankton to have species-specific food sources among the plankton on which they feed, their compositional diversity should mirror both the abundance and variety of food in the peripheral waters of the subtropical gyre (11). Locally, cool upwelling waters off coastal Saharan Africa at 20°N furnish very high nutrient and biomass concentrations, and diversity in that area is high. The winter overturn of the Northern Sargasso Central water above 30°N apparently boosts its diversity above the Southern Sargasso Central water minimum (8). (ii) Salinities are intermediate, neither so low (as off Guiana) nor so high (as in the southern Sargasso Sea) as to prohibit species from inhabiting those regions. (iii) Currents of sufficient velocity exist to carry equatorial foraminifers northward to northeastward and more northern species southward to southwestward within the general clockwise circulation of the subtropical gyre. These latitudinal displacements occur primarily in the Gulf Stream and the Canaries Current regions, where a mixed fauna with greater diversity results (12). (iv) Strong physical oceanographic gradients allow temporal overlap of water masses and create laterally mixed faunas in the sediments below. The particularly abrupt Gulf Stream gradients must encourage temporal mixing within the meander belt. The southernmost portion of the peripheral belt of high diversity may be in part due to seasonal and long-term mixing. Along latitudes 15° to 20°N several typically equatorial and central water species overlap. Because no species is wholly indigenous to those latitudes, the high diversity there seems better attributed to this overlapping effect.

Within compact, well-defined gyres such as that in the North Atlantic, prohibitively severe conditions may override and blur planetary dominance and diversity gradients. The resulting dominance maximums and diversity minimums among planktonic fauna can constitute valid criteria by which to detect paleoecologically significant water masses, along with the major features of ocean circulation.

WILLIAM F. RUDDIMAN*
Lamont-Doherty Geological
Observatory, Palisades,
New York 10968

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* Present address: U.S. Naval Oceanographic Office, Chesapeake Beach, Maryland 20732.

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Lecithin Aerosols Generated Ultrasonically above 25°C

Abstract. DL-Dipalmitoyl- α -lecithin, suspended in 0.15-molar sodium chloride solution by sonic cavitation at 20 kilohertz, can be aerosolized by an 800-kilohertz ultrasonic generator only at temperatures above 25°C. The aerosol thus produced is exceptionally stable against evaporation even at particle radii of 0.1 to 0.6 micron; this suggests applicability to the therapy of pulmonary disorders.

Synthetic DL-dipalmitoyl- α -lecithin (DPL) dispersed in 0.15M aqueous sodium chloride (saline) by a sonic cavitation generator (Branson Heat Systems sonifier W185D, 20 khz) can be readily aerosolized ultrasonically (Macrosonics Corporation Ultramist III, 800 khz) above a threshold temperature of about 25°C, without the addition of albumin, glycol, or other materials. The aerosol particles ultrasonically generated from 2 percent DPL (by weight) suspended in saline in air saturated with water vapor at 37°C have radii ranging from 0.1 to approximately 0.6 micron, whereas the control saline gives particles larger by a factor of 10, as estimated by Stokesian settling velocity. The aerosolized lecithin particles are exceptionally stable against evaporation.

The Laplace equation

$$P_e = 2\sigma/r$$

relates the excess pressure P_e inside a drop of radius r to its surface tension σ . For a drop of pure water ($\sigma = 72$ dyne/cm) with $r = 0.2$ micron, $P_e = 7.2$ atm.

The Poynting equation for the actual vapor pressure P^* of a liquid of molal volume $\bar{V}$ and standard (1) vapor

pressure P^0 under an excess pressure P_e at temperature T gives

$$P^* = P^0 \exp(P_e \bar{V}/RT)$$

where R is the gas constant. The solution for $P_e = 7.2$ atm and $T = 310^\circ\text{K}$ gives $P^* \approx 1.005 P^0$. With pure water aerosols, approximately 0.2 micron in radius, such a driving force ($P^* - P^0$) in combination with a large surface-to-volume ratio would lead to rapid evaporation and disappearance, even in air at 100 percent relative humidity (2). That our lecithin aerosol particles of this size do not rapidly evaporate suggests that $P^* \approx P^0$; thus $P_e \approx 0$, and $\sigma \approx 0$. This implies that, in disruption of the geysers (3) in the ultrasonic aerosol generator, the rapidly decreasing surface area of the ejected matter leads to minima in surface tension near zero. This has been observed by Kuenzig *et al.* (4) and Fujiwara *et al.* (5) for lecithins in albumin by measurement of surface tension on a Wilhelmy balance and by cinephotomicrography on rapidly changing sessile bubbles in pure saline suspensions of DPL at 27°C or above (6).

We measured (6) the surface tension of DPL suspensions in saline as pendant drops of constant area as a