premature to conclude that sensitivity studies based on climate equilibrium simulations can be reliably used to predict regional patterns of climatic changes. Such studies must be approached with great caution, even "as an approximate guide for predicting the latitudinal pattern of sea surface temperature trends," particularly in the Southern Hemisphere. However, to further narrow uncertainties and to test relationships between transient and equilibrium simulations, we believe that the use of the following hierarchical approach would be helpful. (i) The response to actual time-dependent CO2 increase scenarios must be simulated (as opposed to inferred) and compared to instant equilibrium or lagged equilibrium estimates. (ii) Simulations with idealized geography (like the sector model of Bryan et al.) should be extended to include the actual fractions of land and ocean at different latitudes. (iii) Simulations with interactive deep oceans should eventually use realistic global geography in both latitude and longitude, as in (2). Without further simulations we cannot know the extent to which the neglect of explicit transient calculations will prove a serious omission in estimating regional climatic response to increasing CO₂.

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References and Notes

- 1. S. Manabe and R. T. Wetherald, J. Atmos. Sci.
- S. Manabe and R. J. Stouffer, J. Geophys. Res. 85, 5529 (1980).
- 3. S. H. Schneider and S. L. Thompson, ibid. 86,
- 3135 (1981). K. Bryan, F. G. Komro, S. Manabe, M. J. Spelman, Science 215, 56 (1982).
- We require this information in order to apply Duhamel's equation, which translates the stepfunction response into a transient climatic response [see C. R. Wylie, Jr., Advanced Engineering Mathematics (McGraw-Hill, New
- neering Mathematics (McGraw-Hill, New York, 1960), p. 338].

 6. Figures 2 and 3 of (4) give the normalized step-function responses and necessary scale factors, respectively. The equilibrium doubling response is taken as one-half the quadrupling response
- See (3) for an explanation of a very similar approach.
- 8. Even slower scenarios are considered plausible by A. Lovins, H. Lovins, F. Krause, and W. Bach [Least Cost Energy (Brick House, Ando-
- ver, Mass., 1981), p. 161]. E. N. Lorenz, J. Atmos. Sci. 36, 1367 (1979); I. M. Held, ibid. 35, 572 (1978).
- We estimate the step-function response by assuming that the e-folding response time τ of temperature to a perturbation can be approximated by $\tau = R/\lambda$, where R is the thermal inertia and λ is the thermal damping coefficient (3). We estimate these parameters from (4) and then use them to construct a response function for 60°S. For estimating the zonal mean thermal inertia. we use an arithmetic average of land and ocean values. [This is the "infinite wind" limit derived by S. L. Thompson and S. H. Schneider, J.

Geophys. Res. 84, 2401 (1979)]. The ocean thermal inertia is estimated by integrating the temperature perturbation at 60° over depth [see (4), figure 3] to get an equivalent mixed layer depth of 625 m. [The technique for determining an equivalent mixed layer depth is described in (2).] For the model of Bryan et al., \(\) falls in the range of 1 to 2 W m⁻² K⁻¹, typical of climate models (3). We make a global estimate for \(\) in the model of Bryan et al. of about 1.3 W m⁻² K⁻¹ by dividing their given ocean surface heating increase of 6.5 W m⁻² by their global temperature increase of about 4.9 K for a CO₂ quadrupling. By this process, we assume that λ for 60° is probably about the same as the global value. This assumption appears reasonable since the albedo-temperature feedback in the model of Bryan et al. is weakened as a result of "excessive warming at high latitudes" in their control case [(4), p. 57]. With R estimated from the effective mixed layer depth and an assumption

of a 50 percent land fraction, we get a time constant of 32 years for latitude 60° in the model of Bryan et al. This independent estimate of the time constant is close to what we estimated visually from figure 2 of Bryan et al. With this encouragement, we estimate the time constant for a realistic land/sea fraction at 60°S to be 60 years. Finally, to scale the step-function response for 60°S, we assume an equilibrium temperature change for CO₂ doubling of 2.3 K

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Atom Pair Distribution Functions of Liquid Water at 25°C from **Neutron Diffraction**

Abstract. The structure of liquid water is described by three atom pair distribution functions $g_{OO}(r)$, $g_{OH}(r)$, and $g_{HH}(r)$. These functions have now been derived from neutron diffraction data on four mixtures of light and heavy water. They will provide a crucial and sensitive test for proposed models of liquid water.

Enormous effort has been invested in experimental determinations of the properties of liquid water, in attempts to interpret these properties in terms of molecular interactions, and in the development of models with which known properties can be correlated and unknown properties predicted. Despite the effort, our factual knowledge is meager and our understanding rudimentary. An example is the structure of liquid water, described by the three atom pair distribution functions $g_{OO}(r)$, $g_{OH}(r)$, and $g_{\rm HH}(r)$. Only the function $g_{\rm OO}(r)$ is known (1) with sufficient accuracy to test proposed models of liquid water.

Neutron diffraction is a unique tool for probing the structure of water, because the hydrogen atoms cannot be "seen" with adequate precision by other techniques (such as x-ray or electron diffraction). This was recognized in the pioneering work of Wollan and Shull (2), who, in 1946, measured the first neutron diffraction patterns of liquid water at the X-Pile in Oak Ridge. The existence of two stable hydrogen isotopes with different coherent scattering lengths suggests that one could perform the standard isotopic substitution experiments (3) on water and obtain the three partial structure functions. In practice, however, the very large incoherent cross section of light hydrogen obscures the structural information contained within the coherent scattering. This means that in order to

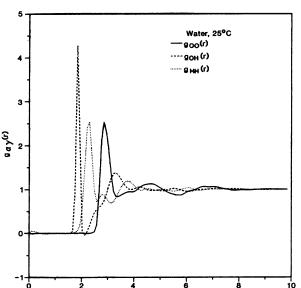


Fig. 1. Intermolecular atom pair distribution functions for liquid water at 25°C.

obtain sufficiently good statistics for the coherent scattering cross sections very large numbers of neutrons have to be counted. We have used a dedicated diffractometer at the High Flux Isotope Reactor to obtain neutron data of very high statistical accuracy for four mixtures of light and heavy water containing 0.01, 35.79, 67.8, and 99.75 percent deuterium (4). Another problem is the complex nature of the interaction of thermal neutrons with light nuclei such as hydrogen. Inelastic and recoil effects make extraction of the static coherent scattering function from the measured effective cross sections difficult. We have solved this problem by constructing the dynamic scattering function for sufficiently realistic models of water and integrating over the energy transfers (5). The static coherent scattering functions for the four mixtures were then analyzed to yield the three partial structure functions. Subtraction of the intramolecular terms vielded the three intermolecular structure functions for the atom pair interactions in liquid water. The accuracy of these results is very difficult to assess, because they were derived from experimental data with a very low signal-tonoise ratio. However, we have shown (4) that the partial structure functions meet all known consistency tests for diffraction data from liquids. The determination of the three atom pair distribution functions by Fourier inversion is complicated by sizable termination effects, which have been minimized by an empirical procedure (6). Only a brief description of the main results, shown in Fig. 1, will be given here.

The oxygen atom pair distribution function, $g_{OO}(r)$, derived from the neutron data is not significantly different from that obtained previously from x-ray diffraction (1). This curve contains information about the positional correlation between centers of molecules in liquid water. Principal features are an asymmetric distribution of nearest neighbors centered at 2.85 Å, which overlaps with the distribution of tetrahedrally coordinated second neighbors near 4.5 Å. This overlap of first and second neighbor distance distributions has been interpreted (7) in terms of a complex near neighbor coordination sphere which cannot be explained by tetrahedral coordination

The function $g_{HH}(r)$ describes the distance distribution between hydrogen atom pairs in different water molecules and, hence, contains information about orientational correlations in the liquid. Principal features are a near neighbor distribution centered at 2.29 Å which

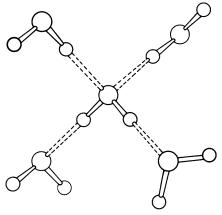


Fig. 2. Model for the average orientation of pairs of near neighbor molecules in liquid water. Large local and instantaneous deviations from this average configuration occur in the liquid.

overlaps with the distribution of second neighbors near 3.9 Å. The function $g_{OH}(r)$ shows a narrow distribution of first neighbors near 3.2 Å. A nearest neighbor O···H distance of 1.86 Å, a corresponding O···O distance of 2.85 Å, and an intramolecular O-H distance of 0.96 Å (4) suggest that most water molecules are connected to their nearest neighbors through nearly straight hydrogen bonds as shown in Fig. 2.

The oxygen atom pair distribution function $g_{OO}(r)$ derived from x-ray diffraction has already provided a crucial test of water models in computer experiments (8). The functions $g_{OH}(r)$ and $g_{\rm HH}(r)$ derived in this study will provide an even more sensitive test of proposed models for liquid water. This should help lead eventually to a realistic statistical mechanical theory of liquid water.

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References and Notes

- 1. A. H. Narten, M. D. Danford, H. A. Levy, Discuss. Faraday Soc. 43, 97 (1967); A. H. Narten and H. A. Levy, J. Chem. Phys. 55, 2263
- E. O. Wollan and C. G. Shull, Clinton Lab. Mon. Prog. Rep. Mon P-113 (May 1946); ibid., Mon P-220 (November 1946).
 J. E. Enderby and G. W. Neilson, Adv. Phys. 22 (2080)
- W. E. Thiessen and A. H. Narten, J. Chem.
- Phys., in press.
 5. L. Blum, M. Rovere, A. H. Narten, ibid., in
- 6. A. H. Narten, W. E. Thiessen, L. Blum, in
- 7. A. H. Narten and H. A. Levy, Science 165, 447
- D. W. Wood, in Water: A Comprehensive Treatise, F. Franks, Ed. (Plenum, New York, 1979), vol. 6, p. 279.
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Laboratory Cultivation of *Prochloron*, a Tryptophan Auxotroph

Abstract. Laboratory cultures have been established of the didemnid symbiont Prochloron, a unique prokaryotic alga that synthesizes chlorophylls a and b but no phycobilin pigments. Cell division in Prochloron cultures occurs under acidic conditions (pH 5.5) in the presence of tryptophan. The alga is a naturally occurring tryptophan auxotroph that survives in nature by close association with the host, Diplosoma similis. The metabolic dysfunction that renders Prochloron auxotrophic may involve only the initial step of the tryptophan biosynthetic pathway.

The unicellar prokaryotic alga Prochloron sp. (1), found in nature in symbiotic association with one family of colonial didemnid ascidians (Urochordata), has received considerable attention from botanists. This unusual alga synthesizes chlorophylls a and b and lacks phycobilins, thus resembling higher plants rather than blue-green algae (2). The alga has been placed in a new division, the Prochlorophyta, to reflect these characteristics (3). Efforts to study this alga have been hampered by the inability of investigators to maintain cultures of Prochloron. We report here on conditions that allow the cultivation of Prochloron, and offer an explanation for the difficul-

ties encountered in previous attempts at culturing the organism.

Our efforts to establish suitable culture conditions for *Prochloron* were based on attempts to duplicate conditions found in its Hawaiian host, Diplosoma similis Fluiter (formerly D. virens) (4). Since crushed colonies of this didemnid ascidian liberate acid (5, 6), it is possible that the algal cells normally exist in an acidic environment rather than the alkaline surroundings in which cyanophytes are commonly observed (7, 8). It also appears that Prochloron depends on some generally available metabolite rather than a compound of restricted distribution, as the alga has been observed with



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