Sound and Fury in Jupiter

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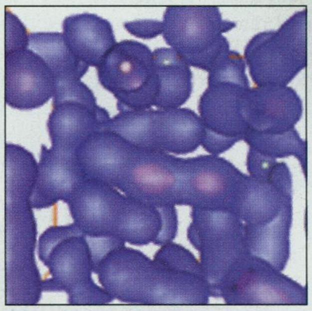
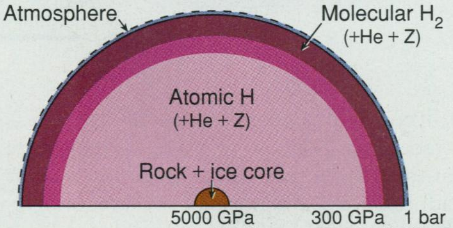
Jupiter is a ball of mostly hydrogen and helium 300 times more massive than the Earth. Its surface complexion is familiar and coming into sharper focus with the myriad studies of the comet Shoemaker-Levy 9 impacts last summer and the prospect for new planetary probes next year. However, the vast interior of the planet, below the cloud tops, remains hidden from view. Because of its size, the planet is gravitationally compressed to extraordinarily high pressures and temperatures, reaching ~5 TPa (50 Mbar) and ~20,000 K at its center, and produces states of matter unlike anything found here on or in the Earth. Thus, even an approximate picture of the jovian interior requires knowledge of the behavior of its major components under extreme conditions. This means understanding the nature of hot, dense hydrogen, particularly in the plasma state that is theoretically predicted to occur at depth and long thought to be the source of Jupiter's strong magnetic field. As demonstrated in the reports by Nellis *et al.* (*1*) and Alavi *et al.* (*2*) elsewhere in this issue, the confluence of new experimental and theoretical studies of hydrogen at high pressure, combined with astronomical observations, is opening up a new era of such investigations.

Under ambient conditions on Earth, hydrogen forms a gas of diatomic molecules, but it has been predicted since the early days of quantum mechanics to transform to a metal at sufficiently high pressures. It is a tale told by theorists: The known density and magnetic field of Jupiter arises from an interior consisting of atomic metallic hydrogen blanketed by a layer of nonconducting molecular hydrogen. Curiosity about both the jovian interior and the nature of this transition in hydrogen has spawned a large number of high-pressure experiments in recent years. Recently, Duffy *et al.* (*3*) measured the pressure dependence of the sound velocity of molecular hydrogen to record-high static pressures with a diamond-anvil cell. The results were used to construct both a sound velocity profile and a new equation of state (pressure-volume relation) for planetary modeling. Nellis *et al.* (*1*) now report new experiments to examine further the equation of state of hydrogen. In particular, they measured the temperature increase associated with shock compression and found evidence for molecular dissociation at lower pressures than previously thought. The two studies are largely consistent with each other and with the major features of existing models for Jupiter (*4*, *5*). However, both experimental studies differed sharply with models inferred from reported observations of free oscillations, or low-order "breathing" modes, of the planet (*6*).





Three views of the largest planet in the solar system. (**Top**) Image of Jupiter from the Voyager 1 spacecraft. (**Center**) View of the planet from within, magnified by a factor of 10^{17} relative to the top image. This is a snapshot of hydrogen from the simulation reported in (*1*) at high temperature and a pressure near 400 GPa (4 Mbar). The blue and red surfaces show regions of constant electron density, and the small spheres indicate the positions of the nuclei. (**Bottom**) Simplified view of the jovian interior, showing the molecular envelope, transition zone, and fluid atomic mantle, each containing hydrogen, helium, and a smaller amount of unknown heavier material denoted by *Z* (*4*, *5*). A rock-ice core of several Earth masses is thought to exist at the center (*4*).

The issue cannot be considered resolved, however, because of the extraordinary changes in hydrogen documented at still higher pressure. In addition to the new evidence for dissociation on shock compression, a large number of surprising effects have been observed in statically compressed hydrogen at 100 to 300 GPa (1 to 3 Mbar) (*7*). Although the molecular phase is stable to above 200 GPa (at low temperature), a series of phase transitions occur, giving rise to an unusually complex phase diagram, and there are extraordinary changes in optical properties indicating significant changes in bonding and electronic structure (*7*). These observations are particularly intriguing because this is also the pressure range in which numerous theoretical calculations have predicted closing of the band gap. However, accurate calculations for the molecular phase under these conditions (that is, before dissociation) have been especially difficult. With one electron and proton per atom, hydrogen is deceptively simple. As textbook problems in physics, theoretical calculations for molecular hydrogen and for the atomic metal at ultrahigh pressure (>1 TPa) now boast high accuracy. But the dense molecular phase has been a great challenge, if not a conundrum, for theory.

Recently, this situation has changed markedly. Not only has theoretical work on hydrogen progressed significantly, but such studies are steadily pushing the envelope of condensed-matter theory in general (*2*, *8*–*10*). The emerging view is that accurate calculations under these conditions require techniques that go beyond standard approximations in condensed-matter physics. The problem for hydrogen is that the electronic properties depend strongly on the position of the nuclei but the positions are ill-defined because the protons are dynamic, and competing configurations are very close in energy. Moreover, because the band gap is small, electronic excitations must be taken into account for the high-temperature fluid. In short, the interactions are complex: The dynamics of both electrons and protons must be considered together under conditions in which the system straddles the fine line between the molecular and atomic, between insulator and metal.

Alavi *et al.* (*2*) have developed a new technique to handle just this type of problem: first-principles molecular dynamics with excited electrons. This is an extension of previously developed techniques, in which the classical equations of motion for the protons are solved together with the wave functions of the electrons [see (*2*)]. This study represents an important extension of previous calculations of hydrogen (*8*), which predicted some surprising changes in the dense molecular fluid at high pressures and temperatures (see figure). With the new extension, they are able to examine the role of electronic excitations induced by high temperatures, an effect that had been neglected in previous work. In the present paper, Alavi *et al.* (*2*) used the technique to calculate the sound velocity of hydrogen at high pressures and temperatures.

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At low pressure, the calculated sound velocity profiles match the experiment exceptionally well, and at high pressures, the results are close to the extrapolated experimental curves, despite the dramatic changes in the material that begin at 100 GPa (*7*). The agreement reinforces the conclusions of the diamond-cell (*3*) and shock-wave studies (*1*). Small differences between the latter two at the highest pressures arise from the uncertainty in fitting intermolecular interaction potentials to the experimental data. Indeed, the degree of molecular dissociation obtained from the analysis of the shock-wave data depends strongly on the form of the potentials. It must be admitted that the new calculations are also not without attendant approximations; in particular, the zero-point (quantum) motion of the protons is neglected, the electronic part is carried out within the local density approximation, and adiabatic corrections are approximate. In addition, all calculations were performed at 1000 K, whereas the temperature in Jupiter rises steeply with depth (reaching ~10,000 K at 300 GPa). Nevertheless, the emerging consensus—from diamond-cell experiments, shock-wave compression, and now theory—is highly encouraging, but signifying what?

One of the conclusions of all three studies is the need to revise either the interpretation of purported observations of the jovian free oscillations or existing interior models for the planet. The models predict a significantly larger characteristic free-oscillation frequency than indicated by the observations (*3*). One way to force agreement is to dissolve significantly more He (or other elements heavier than H) into the jovian mantle, but the amounts required would likely make the planet too dense. Recently, Lederer *et al.* (*11*) reported that at least some of the observations could be albedo features (relative variations in brightness of the planet's surface) rather than global oscillations: a portion of the frequency spectrum seems to be contaminated by variations in Jupiter's complex and highly turbulent atmosphere, which is coupled to the rapid rotation rate of the planet.

The implications of this new insight on dense hydrogen run deeper than this. Perhaps most compelling is that abrupt dissociation of hydrogen and the presence of distinct molecular and atomic (plasma) layers within the planet is probably overly simplistic. There is likely to be a transition zone between the two regions (perhaps loosely analogous to that in the mantle of the Earth) in which the molecular-atomic transition takes place, perhaps with no discrete boundary in Jupiter. At 150 to 400 GPa, the theoretical calculations predict evanescent stringlike structures that rapidly exchange protons and electrons at high temperatures (*2, 8*). In the language of chemical physics, this is a regime of intense reactive scattering. Moreover, electron transfer and dissociation at lower pressures imply that a portion of the planet's magnetic field may be generated at much shallower depths than previously thought. Nellis *et al.* (*1*) suggest that this also produces an unusual temperature profile at intermediate depths, which in turn controls the style of convection. Interestingly, an intermediate transition zone has also been proposed from analysis of observational data for the planet (*4*). How these changes in hydrogen are related to the complex phase diagram documented experimentally at lower temperatures is not yet fully established, but the calculated high-temperature charge-transfer processes likely parallel the charge-transfer states identified spectroscopically for the solid (*7*). With continued efforts to characterize dense hydrogen and hydrogen-helium (and more complex) mixtures, a chemical understanding of the interiors of the gas giants may emerge to complement that which is now developing for their atmospheres.

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Glycobiology: More Functions for Oligosaccharides

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Glycosylation is a major feature of the extracellular portion of CD2, a leukocyte antigen on T cells that mediates cellular adhesion. CD2 consists of two immunoglobulin G (IgG) superfamily domains, a V set (amino terminal) and a C2 set. The protein has three glycosylation sites—one in the adhesion domain that is characterized by the glycoforms $[\text{-(GlcNAc)}_2\text{-(Man)}_{5\text{–}8}]$. The nuclear magnetic resonance (NMR) solution structure of this adhesion domain, described on page 1273 of this issue (*1*), is the first example in which both the polypeptide and the attached oligosaccharide are defined.

The solution structure reveals that the core monosaccharides GlcNAc2 interact with the polypeptide, and as a result much of the remainder of the oligosaccharide is conformationally restricted. On the basis of the new structure and site-directed mutagenesis studies, the authors conclude that the glycan stabilizes an exposed cluster of five positive charges from surface lysines (Lys^{69}, Lys^{71}, Lys^{64}, and Lys^{55}, with Lys^{61} at the center), mainly through hydrogen bonds and van der Waals contacts (Fig. 1A). Elimination of the N-linked glycan leads to partial or complete unfolding and loss of counterreceptor (CD58) binding. The authors suggest that glycosylated Ig domains such as CD2 are not rigid protein scaffolds but have conformations that result from an interplay of dynamic interactions between the polypeptide and attached glycan. Interestingly, if the central Lys^{61} is replaced by glutamic acid (as in rat CD2), the negative charge allows the formation of a salt bridge with Lys^{69}, and rat CD2 is stable even without an attached oligosaccharide.

The concept that an oligosaccharide might have a structural role by susbstituting for one or more amino acids has been noted in the closely related structures of the variable domain of trypanosome variant surface glycoproteins (*2*). An α helix in one structure is replaced in another by the first three monosaccharides of an oligosaccharide, which bury the same core amino acids as the α helix.

The elegant biosynthetic glycan-processing pathway in the cell allows, in principle, the same oligosaccharide to be attached to quite different proteins without having to code the information into the DNA of the individual proteins. However, the orientation of the attached oligosac-

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