ameter. Radar studies have shown that the primaries usually spin in ~2 hours, near the spin period at which a cohesionless body can no longer be held together by gravity; are roughly spherical; and have low—albeit poorly constrained—densities. Orbits are almost circular and close (~5 primary radii). Because NEAs are more often binaries than other objects and traverse planetary orbits, the suspicion is that they formed when fragile rubble piles were tidally torn asunder (*12*), like comet Shoemaker-Levy 9 (*11*).

In the outer solar system, a satellite circles 617 Patroclus, one of six Trojans (the asteroids that orbit at Jupiter's distance) surveyed so far with adaptive optics. Seven trans-Neptunian objects (TNOs, residents of the Kuiper Belt or Centaurs), reflecting perhaps 1% of the TNO population, are binary (*2*). These outer solar-system binaries are distinctly different from those closer to the Sun, implying alternative formation mechanisms. The companions have comparable masses on eccentric, widely separated orbits. It remains unclear how such loosely bound objects can be formed. They may have been produced in the early solar system, when TNOs were more numerous.

Well-determined masses and shapes allow reliable estimates of density. Compared to the measured densities of carbonaceous (2.3 to 2.8 g/cm^3), stony (3 to 4 g/cm^3), or iron (5 to 6 g/cm^3) meteorites (*12*, *18*), asteroids (the putative source of meteorites) have remarkably low densities. For example, the main-belt asteroid 45 Eugenia's density is 1.2 (+0.6/-0.2) g/cm^3 (*2*), that of the NEA 2000UG11 is ~1.0 ± 0.5 g/cm^3 (*19*), and even the density of the "metallic" 22 Kalliope is just 2.3 ± 0.4 g/cm^3 (*2*). These low densities confirm estimates from spacecraft flybys and from direct gravitational tugs of other bodies. Asteroids must therefore contain significant pore space (40 to 60%) (*18*), suggesting an unconsolidated rubble-pile structure, as inferred from rotational studies (*20*).

As the mutual orbits of more solar-system binaries are tracked, we will be able to use the densities of the solar system's smallest members to understand their origins. Along with asteroid families, binaries are providing a code book to decipher the pivotal role of impacts in forming and destroying solar-system bodies. Like stellar binaries, solar-system pairs are revealing much about the processes that have given us today's rich world.

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PERSPECTIVES: LASER CHEMISTRY

Water Vapor Gets Excited

Peter F. Bernath

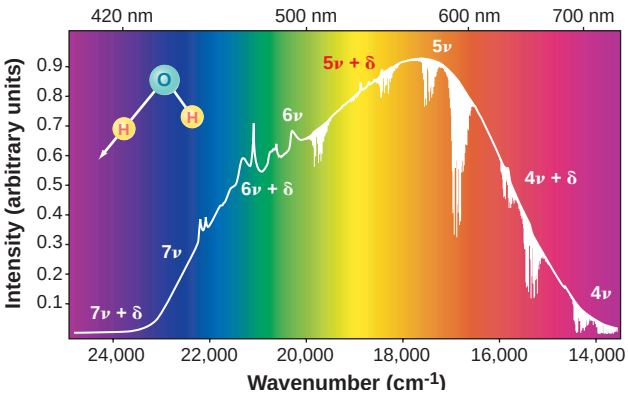
Water vapor is by far the most important greenhouse gas. By absorbing outgoing thermal radiation from Earth, it provides some 30 K of heating (*1*). Water vapor also absorbs about 10 to 20% of incoming solar radiation (*2*). The weak overtone bands of water (see the figure) play an important role in this absorption because the solar photon flux peaks at ~630 nm, in the yellow-red part of the visible spectrum. Both the amount of water vapor in our atmosphere and the strength and position of its absorption bands thus help to maintain Earth's energy balance (*1*).

The intensities of the absorption lines are determined by the electric dipole moment surface, which describes the charge distribution in the water molecule as a function of the two O–H bond lengths and the bond angle. A reliable dipole moment surface is thus essential for the calculation of a molecular spectrum from first principles. Several dipole moment surfaces are available for water (*3, 4*). On page 993 of this issue, Callegari *et al.* (*5*) report a clever method for testing their quality.

The prediction of the water spectrum on the basis of ab initio potentials and dipole moment surfaces is very important. Currently available experimental data cannot account for the atmospheric absorption of sunlight (*6*). In astronomy, the spectral energy distribution emitted from cool stars and brown dwarfs is strongly modulated by water absorption (*7*), which cannot be simulated with existing experimental data. Only theory can generate the many millions of weak absorption lines that are required to bring observations and simulations into agreement (*8*). Ab initio predictions of the water spectra have also been used to assign hot water spectra in sources such as sunspots (*9*).

The prediction of an absorption spectrum requires as minimum input a set of line positions, their intensities, and a lineshape function. Often these data are derived from experiment and tabulated in public databases (*10*). Water line positions can routinely be measured to eight significant digits, whereas line intensities typically have an accuracy of only 5%. Hence, empirical dipole moment surfaces deduced from experimental data have modest reliability (*4*). Dipole moment surfaces derived from state-of-the-art ab initio calculations (*5*) are probably more accurate.

What molecular properties of water determine the positions and strengths of the absorption lines? From a theoretical perspective, the line positions are determined by the changes in the total electronic energy as a function of the two OH bond lengths and the bond angle, captured in the potential energy surface (*11*). Simi-



Now you see it. The visible absorption spectrum of water, recorded with a high-resolution Fourier transform spectrometer and a long-path absorption cell. The overtones are the small modulations of the spectrum. **(Inset)** The water overtone O–H stretch. [Adapted from (*15*)]

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larly, the dipole moment surface determines the line intensities (*3, 11*).

In contrast to the ab initio calculation of line intensities, line positions from ab initio potential energy surfaces are still far from spectroscopic accuracy. Problems include the breakdown of the Born-Oppenheimer approximation (which enables the separation of nuclear and electronic motions) because of the light, rapidly moving hydrogen atoms. Furthermore, relativistic and quantum electrodynamic effects make nonnegligible contributions to the energy levels (*7, 12*).

Despite this somewhat discouraging news on the theoretical front, Partridge and Schwenke have shown that a small empirical adjustment of the high-quality ab initio potential surface yields calculated line positions to better than 0.05 cm^{-1} on average (*11*). This result is somewhat deceptive, however, because such spectroscopic accuracy is achieved for calculations within the range of data used to derive the correction only; the quality of the predictions deteriorates rapidly for line positions beyond the range of the available experimental data.

Callegari *et al.* (*5*) have devised a highly precise method for testing the reliability of dipole moment surfaces that does not require the measurement of line intensities. The trick is to apply an electric field to a sample of water vapor and monitor the splitting of the lines. The field causes each rotation-vibration level to split into components because of the partial removal of the degeneracy associated with spatial quantization of rotation.

This Stark effect is well known. Average dipole moments have previously been measured in the low-lying vibrational states of water (*13*). Callegari *et al.* (*5*) have now found a way to measure small Stark splittings in very weak water overtone transitions.

The authors use a sequence of three powerful laser pulses—the first to excite the overtone transition, the second to dissociate H_2O into H + OH, and the third to monitor the OH free radical—for the ultrasensitive detection of visible water bands. Because the Stark splittings are relatively small compared to the laser line widths, the interference of two coherently excited molecular wave functions was monitored with the "quantum beat" method (*14*).

The work is a tour de force in modern chemical physics. As is often the case, the take-home message depends somewhat on your personal perspective. The good news is that the best current dipole moment functions for water are generally in good agreement with experimental observations. However, discrepancies of up to about 10% indicate that there is room for improvement. Such work is already under way (*5*).

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PERSPECTIVES: GENOMICS

Gene Duplication and Evolution

Michael Lynch

In the transmittance of genetic material from parent to offspring, accidents occasionally happen. Such accidents may result in the duplication of a chromosomal segment that then becomes separated from the original segment, ending up in a different chromosomal location. A number of human genetic disorders are known to be associated with the increased expression of genes contained within such duplications. However, evolutionary biologists have long been enthralled with the idea that duplicate genes could provide the ultimate substrate on which evolution could work. There are two ways in which gene duplication could generate a substrate suitable for adaptive evolution. Either one member of the duplicate gene pair could take on a new function, or two duplicate genes could divide the multiple functions of the ancestral gene between them, with natural selection then refining each copy to a more restricted set of tasks (*1*). On page 1003 of this issue, Bailey and colleagues (*2*) contribute to our understanding of gene duplication by calculating the number of segmental duplications in the human genome.

The most common fate of duplicate genes appears to be the simple silencing of one member of the pair. The average time before silencing of one duplicate gene pair member is ~4 million years in animals (*3, 4*). By restoring the content of a genome to its original state, the silencing of duplicate genes has little direct effect on adaptive evolution. But, because either the ancestral or the descendant copy can be silenced, recurrent duplication of genes at unlinked chromosomal locations can passively give rise to small-scale chromosomal rearrangements (*5, 6*). When combined with geographical isolation, these small-scale gene rearrangements may contribute to the emergence of new reproductively isolated species.

Consider a pair of unlinked copies of an essential gene in an ancestral species. If, because of functional redundancy, one random member of the duplicate gene pair is destined to become silenced in each population, there is a 50% chance that different copies will be silenced in two geographically isolated populations, thereby resulting in different chromosomal locations for the gene (see the figure). The contribution of this process to the evolution of genetic incompatibility between the two populations depends on the rate at which gene duplication takes place. Thus, it is noteworthy that all recently characterized eukaryotic genomes harbor substantial numbers of very young gene duplicates, many showing less divergence than gene copies (alleles) at the same chromosomal position (locus).

By applying demographic principles and genome sequence analysis to species-wide surveys of duplicate genes, scientists have calculated an average duplication rate of ~1% per gene per million years (*3*). This estimate holds up under a reanalysis of additional and better curated genome sequences (*4*). Using a new statistical approach to infer the presence of duplicated regions in pools of random human genome sequences, Bailey *et al.* estimate that at least 5% of the human genome consists of segmental duplications. They calculate that the span of the segmental duplications in the human genome ranges from tens to

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