

ing  $^{21}\text{Ne}$  for  $^3\text{He}$  as the noble gas and increasing the sensitivity of optical measurement of rotation of polarization at low frequencies to approach the spin-projection noise.

*This work was done by Michael Romalis, Tom Kornack, and Rajat Ghosh of Princeton University for Glenn Research Center. Further information is contained in a TSP (see page 1). Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-17942-1.*

## Utilizing Ion-Mobility Data To Estimate Molecular Masses

Potential applications include detecting biochemicals in pharmaceutical settings.

NASA's Jet Propulsion Laboratory, Pasadena, California

A method is being developed for utilizing readings of an ion-mobility spectrometer (IMS) to estimate molecular masses of ions that have passed through the spectrometer. The method involves the use of (1) some feature-based descriptors of structures of molecules of interest and (2) reduced ion mobilities calculated from IMS readings as inputs to (3) a neural network. This development is part of a larger effort to enable the use of IMSs as relatively inexpensive, robust, lightweight instruments to identify, via molecular masses, individual compounds or groups of compounds (especially organic compounds) that may be present in specific environments or samples. Potential applications include detection of organic molecules as signs of life on remote planets, modeling and detection of biochemicals of interest in the pharmaceutical and agricultural industries, and detection of chemical and biological hazards in industrial, homeland-security, and industrial settings.

The following background information is prerequisite to a meaningful summary of the present method.

- An IMS includes a drift tube that has length  $L$  and is filled with a drift gas (e.g.,  $\text{N}_2$  or  $\text{CO}_2$ ) at a pressure,  $P$ , which could be atmospheric or any other suitable pressure. Mixed into the drift gas is a trace amount of ionized molecules from a sample or environment of interest. An electric potential ( $V$ ) is applied between the ends of the drift tube.
- The mobility ( $K$ ) of the ions is given by  $K \equiv L^2/Vt$ , where  $t$  is the amount of time taken by the ions to drift along the tube from the inlet to a detector at the outlet.
- The correlation among the mobility, the mass ( $m$ ) of an ion, the mass ( $M$ ) of a drift-gas molecule, and the cross section ( $\Omega$ ) for collisions between an ion and a drift-gas molecule is given

by

$$K = \frac{3q}{16N} \left( \frac{2\pi}{kT} \right)^{1/2} \left( \frac{m+M}{mM} \right)^{1/2} \frac{1}{\Omega}$$

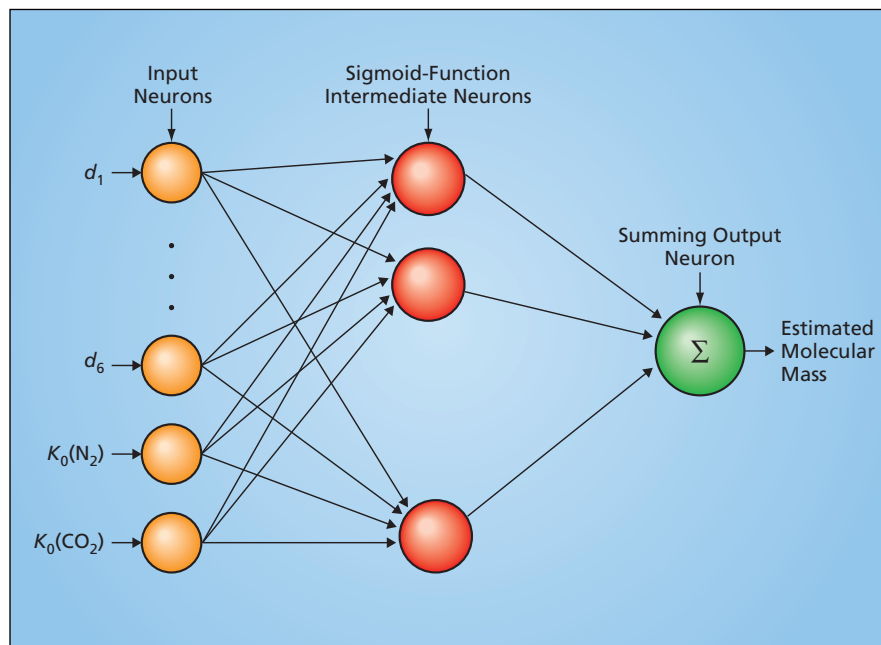
where  $q$  is the fundamental unit of electric charge,  $N$  is the density of the drift-gas molecules, and  $k$  is Boltzmann's constant.

- The reduced mobility ( $K_0$ ) is given by  $K_0 \equiv KT_S P / TP_S$ , where  $T_S$  denotes standard temperature ( $\approx 273$  K) and  $P_S$  is standard atmospheric pressure (represented by a mercury-barometer column height of 760 mm under normal Earth gravitation).
- In a previous study, it was found that there are some correlations between the molecular structure of each compound and the  $K_0$  value of ions of that compound in a given drift gas.

This concludes the background information.

The theoretical basis of the present developmental method can be summa-

rized as the hypotheses that there could be a correlation among molecular structure, collision cross section, and molecular mass, such that it should be possible to estimate the mass of an ion by  $m = \Phi(K_0)$ , where  $\Phi$  is a nonlinear function to be determined,  $\hat{\Omega}$  is an estimated collision cross section that one strives to make as nearly equal as possible to the observed collision cross section. The estimated collision cross section is expressed as  $\hat{\Omega} = g(W, S)$ ,  $g$  is another nonlinear function to be determined,  $W$  is a vector of weights in a parameter space (e.g., a vector of neural-network weights), and  $S \equiv (d_1, d_2, d_3, \dots)$  is a vector of feature-based numerical descriptors of the molecular structure. In this method, the applicable equations are not solved explicitly; rather, they are solved implicitly by means of a neural network (see figure). For each compound of interest, the inputs to the neural network are (1) a set of six feature-based descriptors extracted from a



A Neural Network processes six feature-based descriptors ( $d_1$  through  $d_6$ ) and reduced-mobility values for two drift gases [ $K_0(\text{N}_2)$  and  $K_0(\text{CO}_2)$ ] into an estimate of molecular mass.

much larger set of molecular-structure descriptors by means of principal-component analysis and (2)  $K_0$  values for that compound in two different drift gases.

In a numerical-simulation test of the method, the neural network was trained

by use of descriptors,  $K_0$  values, and molecular masses pertaining to 65 organic compounds, then interrogated by use of descriptors and  $K_0$  values pertaining to 10 other organic compounds. The molecular masses generated by the neural network were found to differ from the

correct values by root-mean-square errors of no more than a few percent.

*This work was done by Tuan Duong and Isik Kanik of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1). NPO-44576*

## Optical Displacement Sensor for Sub-Hertz Applications

NASA's Jet Propulsion Laboratory, Pasadena, California.

A document discusses a sensor made from off-the-shelf electro-optical photodiodes and electronics that achieves  $20 \text{ nm}/(\text{Hz})^{1/2}$  displacement sensitivity at 1 mHz. This innovation was created using a fiber-coupled laser diode (or Nd:YAG) through a collimator and an aperture as the illumination source. Together with a germanium quad photodiode, the above-mentioned displace-

ment sensor sensitivities have been achieved. This system was designed to aid the Laser Interferometer Space Antenna (LISA) with microthruster tests and to be a backup sensor for monitoring the relative position between a proof mass and a spacecraft for drag-free navigation. The optical displacement sensor can be used to monitor any small displacement from a remote loca-

tion with minimal invasion on the system.

*This work was done by Alexander Abramovici, Meng P. Chiao, and Frank G. Dekens of Caltech for NASA's Jet Propulsion Laboratory. For further information, download the Technical Support Package (free white paper) at [www.techbriefs.com/tsp](http://www.techbriefs.com/tsp) under the Physical Sciences category. NPO-30681*

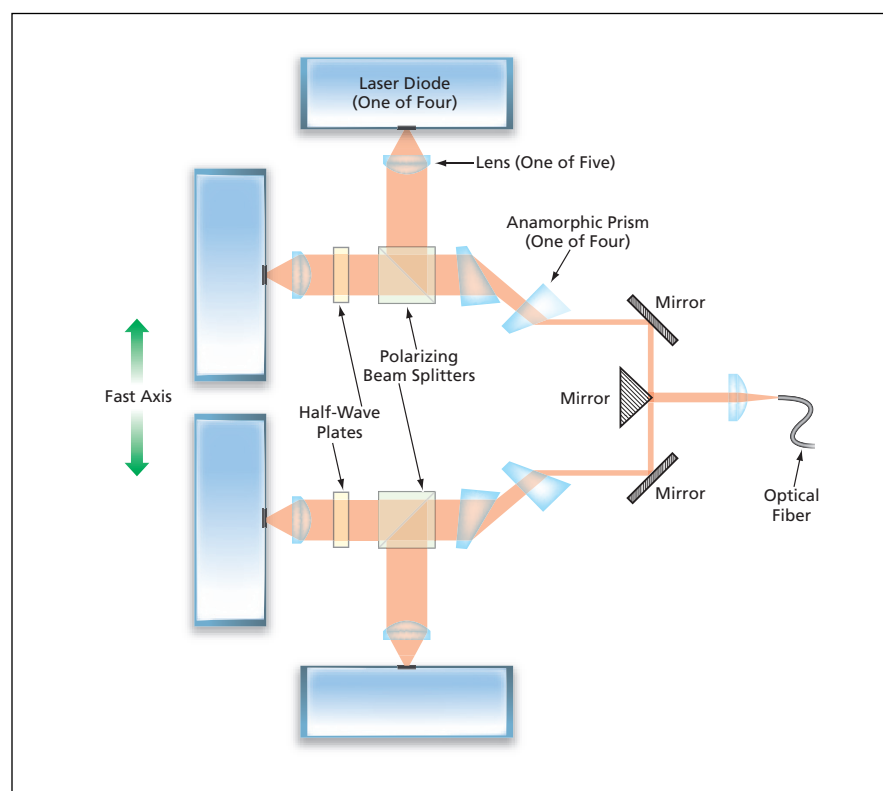
## Polarization/Spatial Combining of Laser-Diode Pump Beams

Four beams are combined into two, which are then combined into one.

NASA's Jet Propulsion Laboratory, Pasadena, California

The figure depicts a breadboard version of an optical beam combiner that makes it possible to use the outputs of any or all of four multimode laser diodes to pump a non-planar ring oscillator (NPRO) laser. This apparatus could be an alternative to the one described in the immediately preceding article. Whereas that one utilizes spatial (beam-shaping) beam-combining techniques, this one utilizes a combination of polarization and spatial beam-combining techniques. In both that case and this one, the combined multiple laser-diode pump beams are coupled into an optical fiber for delivery to the NPRO pump optics.

As described in more detail in the immediately preceding article, the output of each laser diode has a single-mode profile in the meridional plane containing an axis denoted the "fast" axis and a narrower multimode profile in the orthogonal meridional plane, which contains an axis denoted the "slow" axis. Also as before, one of the purposes served by the beam-combining optics is to reduce the fast-axis numerical aperture (NA) of the laser-diode output to match the NA of the optical fiber. Along the slow axis, the unmodified laser-diode NA is already well



Four Laser-Diode Beams are polarization-combined into two, then narrowed along the fast axis, then combined into one beam incident on an end face of an optical fiber.