Astro-1 Honors 2020
Class 5: In Situ Resource Utilization — Finding and extracting water and other volatiles on the Moon

Dr. Jatila van der Veen
Project Scientist, Physics Department, UCSB
Adjunct Professor of Astronomy, SBCC
The Moon may have substantial deposits of $\text{H}_2\text{O}$, $\text{NH}_3$ (ammonia), $\text{CO}_2$, $\text{H}_2\text{S}$ (hydrogen sulfide), and other volatiles in the PSRs at the poles.

How do we know this? Mainly from lunar orbiters and probes that were crashed into the surface intentionally, so that orbiters could study the plumes that were ejected.

Methods:
- Molecular spectroscopy
- Thermal emission spectroscopy
- Raman spectroscopy
- UV reflection and absorption
- IR reflection and absorption

What do we mean by spectroscopy?
The fundamental frequency gives us the lowest tone we can hear for a particular length of string.

Multiples of the fundamental frequency produce higher tones.

If we can identify these characteristic frequencies, we can use this information to identify the substance.
Tacoma Narrows Bridge – wind set it vibrating in its normal modes until one day it collapsed.

https://www.youtube.com/watch?v=qbOjxPCfaFk

The Sun vibrates in normal modes
Spectrum of sound waves in the Sun

Frequencies are in milliHertz, around 10,000 times below audible frequencies for human ears.
Here is the sound of pressure waves sloshing around inside the Sun, recorded by the BiSON group in Birmingham, UK, http://bison.ph.bham.ac.uk/, compressed around 10,000 times to the range of human hearing.
The simplest mathematical representation of a wave \( F(t) = A \sin (\omega t) \) represents a periodic displacement of some medium with amplitude “A” and angular frequency \( \omega \). The simplest wave form looks something like this:

A single frequency of 440 Hz sounds like this:

The spectrum of this wave would look something like this, a single spike:
Atomic spectra

A spectrum of vibrations is produced when energy falling on an atom causes the electrons to oscillate in characteristic frequencies, called NORMAL MODES, and absorb, transmit, or emit energy at precise wavelengths/frequencies that are characteristic of that substance. Thus a spectrum is like a ‘fingerprint’ of a substance.

You have seen this phenomenon for the hydrogen emission spectrum in class.
H-atom absorbs energy in ‘just the right’ amounts so that electrons oscillate between their rest energy level and higher energy levels. The total color is magenta (pinkish-purplish). When the light is seen through a diffraction grating, the individual colors are visible.
Analogy: Represent the Hydrogen visible spectrum with SOUND. For each wavelength, calculate the frequency. Then we map each frequency to a sound within the range of human hearing.

\[ c = \lambda f \]

For all light waves, speed is constant = \(3.0 \times 10^8\) m/sec
\[ f = \frac{c}{\lambda} \]

<table>
<thead>
<tr>
<th>Spectral line</th>
<th>H-(\alpha)</th>
<th>H-(\beta)</th>
<th>H-(\gamma)</th>
<th>H-(\delta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength</td>
<td>656 nm</td>
<td>486 nm</td>
<td>434 nm</td>
<td>410 nm</td>
</tr>
<tr>
<td>Frequency</td>
<td>(4.57 \times 10^{14}) Hz</td>
<td>(6.17 \times 10^{14}) Hz</td>
<td>(6.91 \times 10^{14}) Hz</td>
<td>(7.32 \times 10^{14}) Hz</td>
</tr>
<tr>
<td>Assigned tone</td>
<td>457 Hz</td>
<td>617 Hz</td>
<td>691 Hz</td>
<td>732 Hz</td>
</tr>
</tbody>
</table>

Here is the ‘sound’ of excited hydrogen – the combination of four visible frequencies.
Here’s the *spectrum* of the Hydrogen Balmer series represented in sound – four peaks for each of the four frequencies: 457 Hz, 617 Hz, 691 Hz, and 732 Hz.

Here’s what the sound of four frequencies played simultaneously looks like:
Here is the ‘sound’ of just the H-α line at 656 nm or 457 Hz corresponding to just the H-α (red) line.
Here’s a visualization of the normal modes of a hydrogen atom. The electron is excited by an input of energy of ‘just the right amount’ to make it jump to higher energy levels. The energy states of the electron in a hydrogen atom are visualized as ‘orbitals’ of different shapes. Every time the electrons go from a higher to a lower energy state, they emit photons that are of an energy that exactly matches the difference in energy levels.
Molecules produce absorption and emission spectra when excited so as to vibrate in their normal modes.

Normal modes for molecules in solids are vibrations. Normal modes for molecules in liquids include vibrations, rotations, and librations. Normal modes for molecules in gases also include translations.

For water, $\text{H}_2\text{O}$, the main “springs” that are doing the vibrating are the O-H bonds.
Water absorbs over a wide range of electromagnetic radiation with rotational transitions and intermolecular vibrations responsible for absorption in the microwave (≈ 1 mm - 10 cm wavelength) and far-infrared (≈ 10 µm - 1 mm), intramolecular vibrational transitions in the infrared (≈ 1 µ- 10 µ) and electronic transitions occurring in the ultraviolet region (< 200 nm).

http://www1.lsbu.ac.uk/water/water_vibrational_spectrum.html
DFT Investigations of the Vibrational Spectra and Translational Modes of Ice II

https://www.mdpi.com/1420-3049/24/17/3135/htm

Theoretical study of ice II – modeling normal modes of vibration and predicting the spectra that should be seen in different methods of spectroscopy.
Absorption spectrum for water

Note the peak at ~3 microns.
Our goal is to find water, minerals, and volatiles. How?

- **Orbiting spacecraft**: active multispectral reflectance measurements in the ultraviolet to near-infrared spectral range and/or passive multispectral emission measurements in the thermal infrared, for definitive detection and mapping of water and other volatiles within several micrometers of the surface.

- **Impactor probes**: targeted, well characterized impacts to kinetically excavate the subsurface, observed from a separate Moon- or Earth-based platform in the ultraviolet to microwave spectral range to detect ice and vapor released at several distinct sites.

- **Penetrator probes**: targeted, instrumented probes capable of detecting ices and quantifying their depth distribution at several distinct sites using neutron spectroscopy, mass spectroscopy, and/or tunable laser spectroscopy.

- **Landers and rovers**: instrumented platforms with a drill or excavator, capable of measuring the composition and abundance of ices at the surface and subsurface within a relatively confined region of the Moon.
Any light elements or compounds deposited on the lunar surface by possible out-gassing or comet fragments and meteorites are subject to direct exposure to the vacuum of space. Over the course of a lunar day, about 29 Earth days, all exposed surfaces of the moon are bathed in sunlight with daylight temperatures reaching up to 250°F (121°C). Any ice exposed to sunlight for any length of time would turn into water vapor, break apart and be lost to space.

Water could only exist in areas of permanent shadow and those areas exist at the lunar poles. Some of these crater floors have not seen sunlight for possibly billions of years. Temperatures within these craters do not go above –280°F (–173°C) so they act as ‘cold traps’ where even light elements or compounds don’t have enough energy to evaporate.
Cabeus Crater, near South Pole, was the site of the LCROSS impact site, intended to observe water and volatiles in the ejecta plume.
LCROSS plume [https://www.youtube.com/watch?v=ewW09qodWVU](https://www.youtube.com/watch?v=ewW09qodWVU)
LCROSS

- Volatiles in LCROSS plume ejected from Cabeus Crater impact (9th Oct. 2009).
- Excavated top few metres of material at impact site (84.675°S, 311.275°E), deeper than neutron data represent (>~ 0.7 m).
- Mean H₂O in plume detected as 5.6 ± 2.9 % (155 ± 12 kg).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Molecules cm⁻²</th>
<th>% Relative to H₂O(g)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>5.1(1.4)E19</td>
<td>100.00%</td>
</tr>
<tr>
<td>H₂S</td>
<td>8.5(0.9)E18</td>
<td>16.75%</td>
</tr>
<tr>
<td>NH₃</td>
<td>3.1(1.5)E18</td>
<td>6.03%</td>
</tr>
<tr>
<td>SO₂</td>
<td>1.6(0.4)E18</td>
<td>3.19%</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>1.6(1.7)E18</td>
<td>3.12%</td>
</tr>
<tr>
<td>CO₂</td>
<td>1.1(1.0)E18</td>
<td>2.17%</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>7.8(42)E17</td>
<td>1.55%</td>
</tr>
<tr>
<td>CH₄</td>
<td>3.3(3.0)E17</td>
<td>0.65%</td>
</tr>
<tr>
<td>OH</td>
<td>1.7(0.4)E16</td>
<td>0.03%</td>
</tr>
</tbody>
</table>

Colaprete et al. (2010), *Science*

See https://www.youtube.com/watch?v=up1h-ziAK5E
LRO Diviner  Multispectral camera observed LCROSS impact from lunar orbit
The OH emission lines strength plotted as a function of time. Before impact the line is flat (no OH). After impact the line strength grows and remains above the pre-impact baseline for several minutes.
Hydrogen deposits at the lunar poles measured by the LAMP instrument on the LRO.

UV reflectivity map of the lunar south pole measured by the LAMP instrument on LRO.

Lyman-α line is the first spectral line in the UV spectrum of hydrogen.
Diviner Observed Average Temperature

Reflectivity

North Pole

South Pole
Preliminary analysis of Chandrayaan-2 Imaging Infrared Spectrometer (IIRS) data
Shortwave-infrared spectroscopy has revealed an OH/H$_2$O absorption band at high latitudes (>60° on both hemispheres) on the Moon, and, in one case, at both lunar terminators [Clark, 2009; Pieters et al., 2009; Sunshine et al., 2009], though it is hydrocarbons, etc. The classic theory (WMB) envisioned exposed ice in large cold craters (cf. Vasavada et al., [1999]). Two variants of the classic storage geometry have been proposed: 1) the ice may be buried, and thus last at somewhat higher temperatures [Schorghofer, 2008; Paige et al., 2010], and 2) small shadows from large boulders and small craters near the poles may also act as cold traps resulting in a patchy distribution of ice with the resulting cumulative area being of comparable size to that of the large cold traps [Hayne et al., 2013a].

It remains unclear whether water ice in the PSRs could be exposed on the surface or only buried beneath the surface. If buried, it may have a layered structure, might be mixed with regolith by impact gardening, or distributed as impact ejecta. Some type of inhomogeneity can be expected in all cases.
So: How do we look for water remotely?

By looking for reflection, emission, and absorption of H, OH, and H$_2$O spectra according to what we understand of them by observation in the lab and modeling.

Why is water the signature of life?
Liquid water is required for life to start and for life to continue. No enzymes work in the absence of water molecules. No other liquid can replace water. We are very fortunate, therefore, that our planet is so well endowed. Water is a common material in the Universe, being found as widely dispersed gaseous molecules and as amorphous ice in tiny grains and much larger asteroids, comets and planets, but water needs particularly precise conditions to exist as a liquid as it does on Earth. It is most likely that this water arrived from multiple sources, such as comets and asteroids, somewhat after solid planet Earth was formed [1015].

Water possesses particular properties that cannot be found in other materials and that are required for life-giving processes (but see also [1153]). These properties are brought about by the hydrogen-bonded environment particularly evident in liquid water [1423]. Hydrogen bonds are roughly tetrahedrally and arranged such that when strongly formed the local clustering expands, decreasing the density. Such low-density structuring naturally occurs at low and supercooled temperatures and gives rise to many physical and chemical properties that evidence the particular uniqueness of liquid water. If aqueous hydrogen bonds were actually somewhat stronger, then water would behave similar to a glass, whereas if they were weaker then water would be a gas and only exist as a liquid at sub-zero temperatures.

http://www1.lsbu.ac.uk/water/water_anomalies.html
### Consequences of changes in water’s hydrogen bond strength

How much variation in water’s hydrogen bond is acceptable for life to exist? A superficial examination gives the range of qualitative effects as indicated below.

<table>
<thead>
<tr>
<th>Water hydrogen bond strength</th>
<th>Main consequence</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Hydrogen-bonding at all</td>
<td>No life</td>
</tr>
<tr>
<td>Hydrogen bonds slightly weaker</td>
<td>Life at lower temperatures</td>
</tr>
<tr>
<td>No change</td>
<td>Life as we know it</td>
</tr>
<tr>
<td>Hydrogen bonds slightly stronger</td>
<td>Life at higher temperatures</td>
</tr>
<tr>
<td>Hydrogen bonds very strong</td>
<td>No life</td>
</tr>
</tbody>
</table>

**If the hydrogen bonds in water were just a wee bit different, life as we know it would not exist.**