DETERMINATION OF ICY SATELLITE SURFACE COMPOSITION FROM SPACECRAFT OBSERVATIONS: MISSION-CRITICAL CRYOGENIC LABORATORY SPECTRAL MEASUREMENTS.

J. B. Dalton, III[1], [1]Planetary Ices Group, Jet Propulsion Laboratory, MS 183-301, 4800 Oak Grove Drive, Pasadena, CA 91109-8001.

Introduction: The bulk of our knowledge regarding icy satellite surface composition is derived from visible to near-infrared (VNIR) reflectance spectroscopy, much of it from spacecraft observations. Spectra of planetary surfaces can be modeled either as linear (areal) mixtures, or as nonlinear (intimate) mixtures, to yield estimates of relative abundance of surface compounds. Linear mixture analysis of planetary surface composition requires access to reflectance spectra of the candidate compounds. Nonlinear mixture analysis requires the real and imaginary indices of refraction (optical constants), which may be estimated from reflectance spectra, or derived from a combination of reflectance and transmittance measurements.

Characterization of Surface Compounds: To date, most candidate species proposed as icy satellite surface constituents have not yet been sufficiently characterized to enable such models. Most infrared spectra of candidate icy satellite surface materials published to date were measured in the mid-infrared (MIR) for purposes of understanding the interstellar medium. In order to constrain abundances of surface materials from spectral observations of icy bodies, cryogenic laboratory measurements for all candidate materials are needed with the following characteristics:

Required quantities. First, useful measurements must be of either reflectance or optical constants (real <u>and</u> imaginary indices of refraction). These are the quantities which enable quantitative abundance modeling. By themselves, transmittance, absorbance, absorption coefficient, line strength, optical depth, or other quantities which cannot be converted to reflectance (primarily due to poorly constrained scattering processes) are of limited usefulness.

Required wavelength range. Second, measurements are needed across the full spectral range of typical spacecraft instruments (298 to 5500 nm would cover the Galileo and Cassini cameras and spectrometers). While a compound may only have strong absorption features in part of the wavelength range, it still contributes to the continuum everywhere, including the vicinity of diagnostic features of other compounds. Deconvolving the observations requires laboratory measurements across the full range, for all proposed constituents, particularly where they may coexist.

Required sample thickness. Third, measurements must be conducted with samples sufficiently thick to yield useful absorption features, shapes and strengths. The overtones and combinations which make up most of the VNIR spectral signatures are far weaker than the MIR fundamentals. However, reflected sunlight from cold icy bodies in the outer solar system exhibits insufficient spectral contrast and inadequate signal to enable the identification of surface materials in the MIR so remote-sensing instrumentation for icy bodies concentrates upon the VNIR, where there is more available signal. Yet, a thin film ($<\sim 10$ microns) in the laboratory does not engender sufficient path length for the weak VNIR absorptions to manifest. This is not a problem for a planetary regolith several meters to kilometers thick, but does present a challenge for laboratory work.

Required temperatures. Fourth, measurements must be temperature-appropriate to the bodies of interest. Most of the candidate compounds (especially ices) display marked spectral changes with temperature. Differences of as little as 5-10 K can be distinguished in laboratory spectra of many materials. In order to explain planetary observations, laboratory measurements in the 50-150 K range will be critical.

Important Candidate Materials: Names and/or chemical formulae (where applicable) for 122 materials proposed as surface materials for icy worlds of the outer Solar System are given in the table. Each of these has either been observed in comets, interstellar molecular clouds, or on icy bodies or asteroids, produced in the lab by chemical, photolytic, radiolytic, or other means, or predicted on the basis of numerical simulations. A search of the published literature reveals a dearth of temperature- and wavelength-appropriate spectral measurements of these materials which can be used for quantitative abundance modeling. This represents a major opportunity for laboratory spectroscopists to conduct measurements which will be of paramount importance in interpreting the available data from modern imaging spectrometers on recent (Galileo), current (Cassini, New Horizons) and planned spacecraft m issions.

Conclusion: Scientific return from spacecraft- and ground-based observations of planetary surfaces will be significantly enhanced by the proper application of cryogenic laboratory spectroscopy. With these measurements in hand, investigators may identify materials, derive their abundances, map their distributions, and infer their roles in the evolution of these enigmatic bodies.

Proposed Icy Satellite Surface Compounds			
Water	H_2O	Hydrogen Sulfide	H_2S
Deuterium Oxide	D_2O	Sulfur Dioxide	SO_2
Heavy Water	HDO	Sulfur Trioxide	SO_3
Hydrogen Peroxide	H_2O_2	Sulfuric Acid	H_2SO_4
Oxygen	O_2	H_2SO_4 Hydrates	$H_2SO_4 \bullet 8H_2O$, $H_2SO_4 \bullet 6.5H_2O$
Carbon Monoxide	CO	Sulfur	S_2
Carbon Dioxide	CO_2	Methyl Clathrate	$CH_4 \bullet H_2O$
Carbon Trioxide	CO_3	CO_2 Clathrate	$CO_2 \bullet H_2O$
Formyl ion	HCO	$H_2O \bullet$graphite	…
Formaldehyde	H_2CO	Bisodium Sulfate	Na_2SO_4
Formic Acid	H_2CO_2	Bisodium Carbonate	Na_2CO_3
Carbonic Acid	H_2CO_3	Calcium Carbonate	$CaCO_3$
D-Carbonic Acid	D_2CO_3	Magnesium Sulfate	$MgSO_4$
Carbon Suboxide	C_3O_2	Dodecahydrate	$MgSO_4 \bullet 12H_2O$
Methanol	CH_3OH	Epsomite	$MgSO_4 \bullet 7H_2O$
Ethanol	CH_3CH_2OH	Hexahydrite	$MgSO_4 \bullet 6H_2O$
Acetone	$(CH_3)_2CO$	Pentahydrite	$MgSO_4 \bullet 5H_2O$
Methyl Formate	$HCOOCH_3$	Starkeyite	$MgSO_4 \bullet 4H_2O$
Glycolaldehyde	CH_2OHCHO	Bassanite	$2CaSO_4 \bullet H_2O$
Ethyl Acetate	$CH_3CO_2CH_2CH_3$	Beryl	$Be_3Al(SiO_2)_6$
Dimethyl Carbonate	$(OCH_3)_2CO$	Bloedite	$Na_2Mg(SO_4)_2 \bullet 4H_2O$
Ethylene Glycol	$(CH_2OH)_2$	Bronzite	$(Mg,Fe^{2+})_2(Si0_3)_2$
Methane	CH_4	Dolomite	$(Ca,Mg)(CO_3)_2$
Acetylene	C_2H_2	Burkeite	$Na_6CO_3(SO_4)_2$
Ethylene	C_2H_4	Calcite	$CaCO_3$
Ethane	C_2H_6	Cordierite	$Mg_2Al_4Si_5O_{18}$
Propane	C_3H_8	Eugsterite	$Na_4Ca(SO_4)_3 \bullet 2H_2O$
Propdiene	C_3H_4	Gaylussite	$Na_2Ca(CO_3)_2 \bullet 5H_2O$
1,3-Butadiyne	C_4H_2	Goethite	FeOOH
Carbon Trimer	C_3	Gypsum	$CaSO_4 \bullet 2H_2O$
Cysteinesulfonic Acid	OCS	Hematite	Fe_2O_3
Nitrogen Oxide	NO	Jarosite	$KFe_3(SO_4)_2(OH)_6$
Nitrogen	N_2	Kaolinite	$Al_2Si_2O(OH)_4$
Ammonia	NH_3	Leonite	$K_2Mg(SO_4)_2 \bullet 4H_2O$
Ammonia hydrate	$NH_3 \bullet H_2O$	Lepidocrocite	FeOOH
Hydrazine	N_2H_4	Magnetite	$Fe(II)Fe(III)_2O_4$
Hydrogen Isocyanide	HNC	Mirabilite	$Na_2SO_4 \bullet 10H_2O$
Hydrogen Cyanide	HCN	Montmorillonite	$(Na,Ca)_{0.3}(Al,Mg)_2Si_4O_{10}(OH)_2 \bullet nH_2O$
Poly-HCN	poly HCN	Nahcolite	$NaHCO_3$
Acetonitrile	CH_3CN	Nontronite	$Na_{0.3}Fe^{3+}_2Si_3AlO_{10}(OH)_2 \bullet 4H_2O$
Ethylamine	CH_3CH_2CN	Natron	$Na_2CO_3 \bullet 10H_2O$
Vinyl Cyanide	CH_2CHCN	Olivine	$(Mg,Fe)_2SiO_4$
Propinonitrile	C_2H_5CN	Palagonite	…
Methylcyanoacetylene	CH_3C_3N	Iron Sulfide	FeS
Cyanoacetylene	HC_3N	Pyroxene Bronzite	$Mg_{0.8}Fe_{0.2}SiO_3$
Cyanogen	C_2N_2	Iron Oxide	FeO
Dicyanoacetylene	C_4N_2	Plagioclase	$(Na,Ca)(Si,Al)_4O_8$
Ammonium Nitrate	NH_4NO_3	Picromerite	$K_2Mg(SO_4)_2 \bullet 6H_2O$
Hydroxylamine	NH_2OH	Amorphic SiO_2 Quartz	SiO_2
Cyanate ion	OCN-	Pirssonite	$Na_2Ca(CO_3)_2 \bullet 2H_2O$
…	XCN-	Amorphic Pyroxene	$(Mg,Fe)SiO_3$
Isocyanic Acid	HNCO	Polyhalite	$K_2Ca_2Mg(SO_4)_4 \bullet 2H_2O$
Methyl isocyanate	CH_3NCO	Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$
Formamide	$HCONH_2$	Ortho-Pyroxene	$XY(Si,Al)_2O_6$
…	HCO_2NH_2	Clino-Pyroxene	$XY(Si,Al)_2O_6$
Urea	H_2NCONH_2	Serpentine	…
Thiourea	H_2NCSNH_2	Syngenite	$K_2Ca(SO_4)_2 \bullet H_2O$
…	$HCOO^- + NH_4$	Tholin	*e.g.*, $C_3H_5N_2$
Ammonium Hydrosulfide	NH_4HS	Kerogen	$C_{200}H_{300}SN_5O_{11}$
Thiocyanic Acid	HNCS, HSNC	Trona	$Na_3CO_3HCO_3 \bullet 2H_2O$

Table I. Candidate Icy Satellite Surface Compounds. These compounds have been predicted to occur on the the icy worlds of the outer solar system. Though hundreds of measurements have been performed, and the literature contains numerous examples of high-quality spectra at various temperatures, wavelength ranges, spectral resolutions, and sample thicknesses, to date only three compounds (H_2O, NH_3 , and CO_2) have been sufficiently characterized to permit quantitative abundance modeling of spacecraft observations across the full wavelength range of the visible to near infrared imaging and imaging spectrometer systems carried by spacecraft such as Galileo, Cassini, and New Horizons.