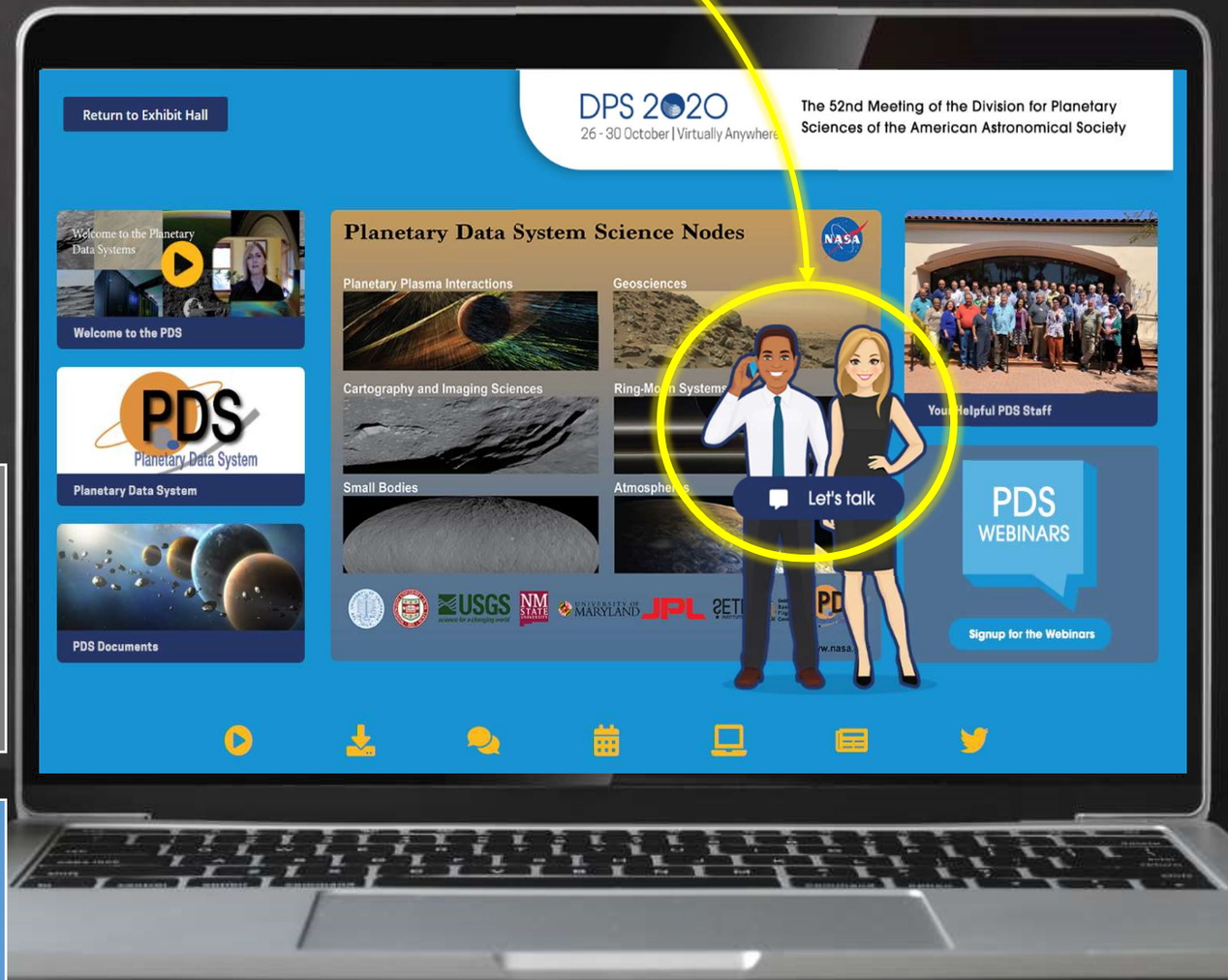
Mars Rover In Situ X-ray Compositional Data Sets and Analysis Tools

Scott VanBommel
Planetary Data System Geosciences Node
Payload Uplink/Downlink Lead, MER and MSL APXS

McDonnell Center for the Space Sciences
Department of Earth and Planetary Sciences
Washington University in St. Louis

To enter a tutorial session, click on “Let’s talk” at the **PDS Exhibitor Booth** at the DPS web site.



Webinars

Introduction to PDS Geosciences Node Data Sets and Analysis Tools
Monday, October 26
12:00 to 12:30 PM EDT

Introduction to PDS Geosciences Node Orbital Data Explorers and Landed Mission Analyst Notebooks
Wednesday, October 28
2:00 to 2:30 PM EDT

Tutorials

MRO CRISM Hyperspectral Data Sets and Analysis Tools
Monday, October 26
2:30 to 3:30 PM EDT

Mars Rover In Situ X-ray Compositional Data Sets and Analysis Tools
Tuesday, October 27
3:00 to 4:00 PM EDT

Content and Use of PDS Geosciences Node Orbital Data Explorers
Wednesday, October 28
4:00 to 5:00 PM EDT

Content and Use of PDS Geosciences Node Landed Mission Analyst Notebooks
Thursday, October 29
3:00 to 4:00 PM EDT

Outline

Missions Overview

APXS Overview

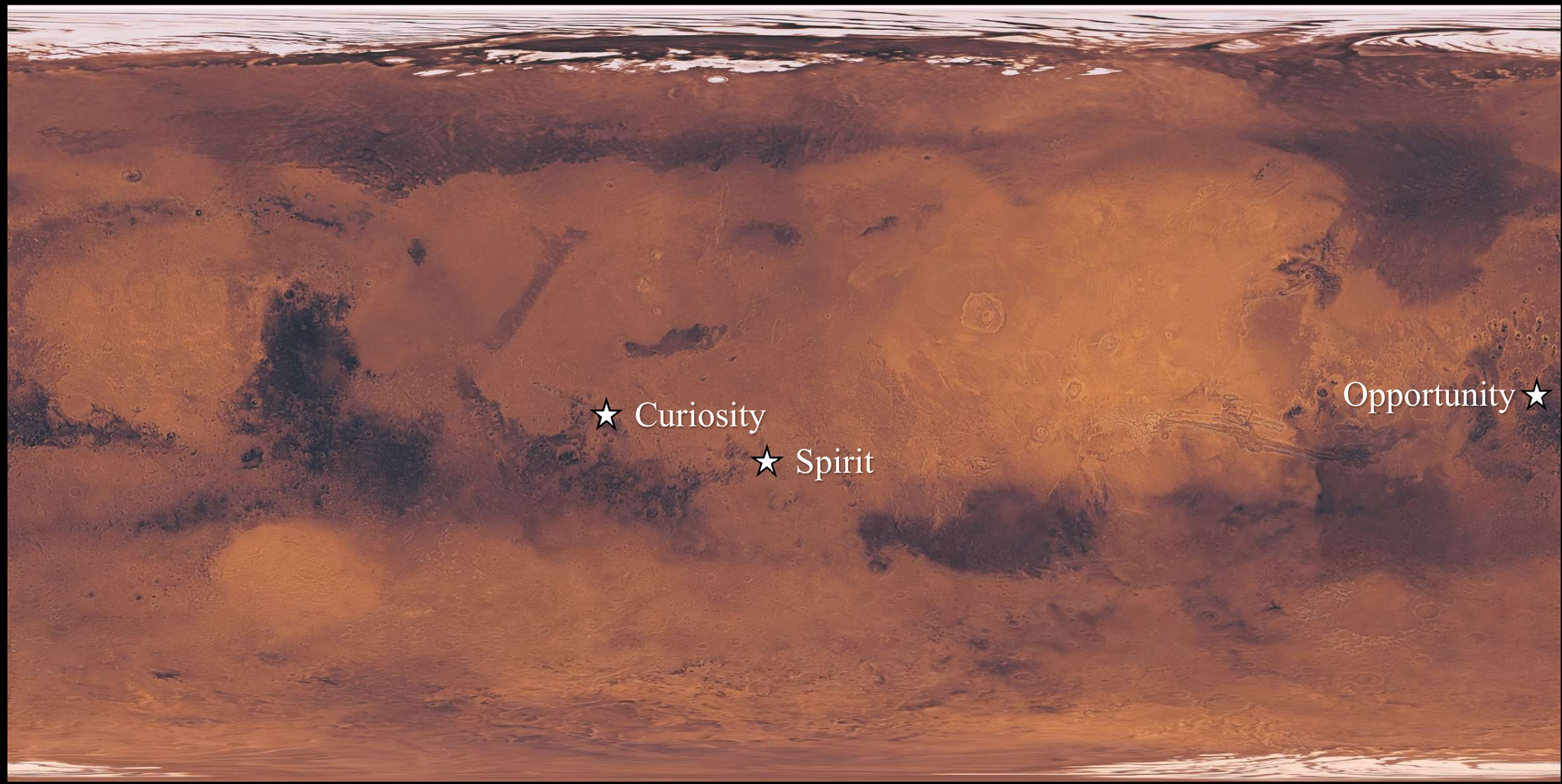
APXS Data: Considerations

APXS Data: Availability

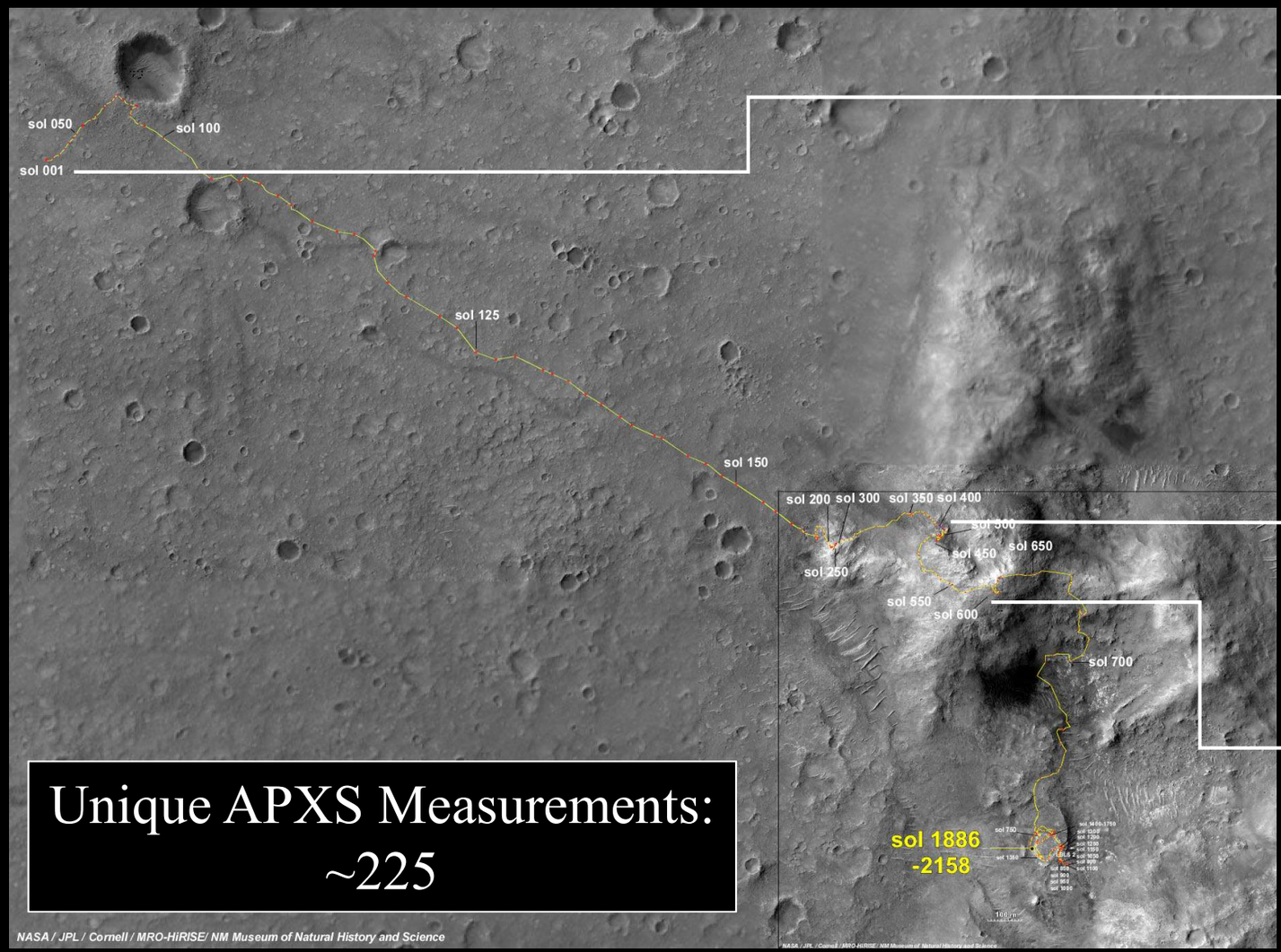
Analytical Techniques:
Deconvolution & Emulation

Analytical Techniques:
PCA

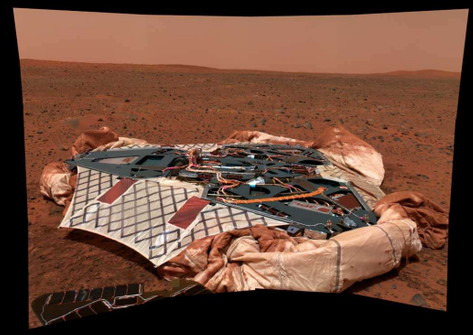
Missions Overview

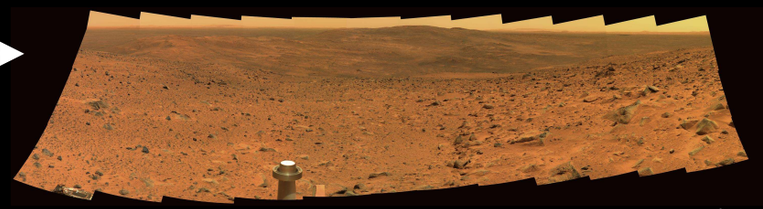


Mission Overview: Spirit



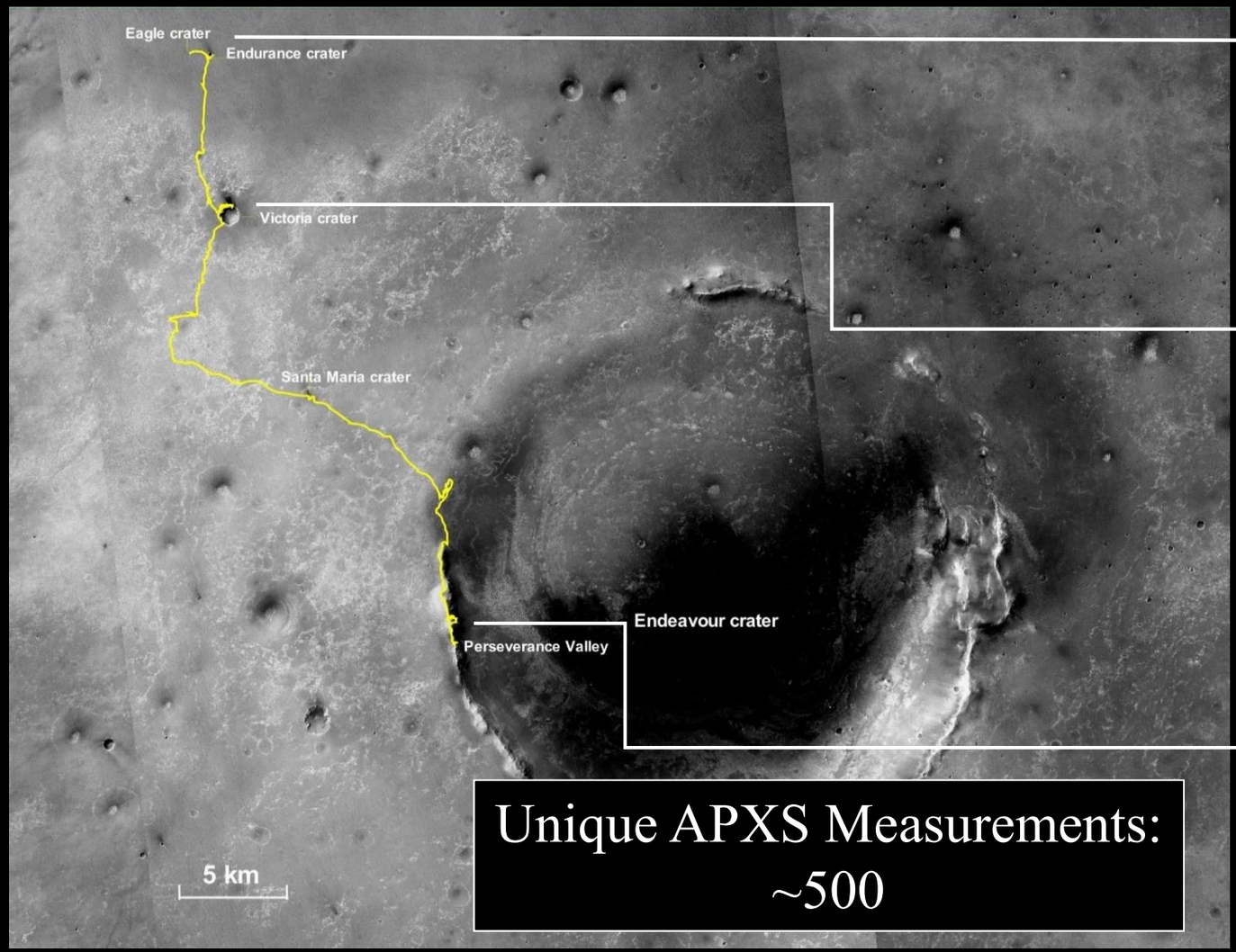
Unique APXS Measurements: ~225

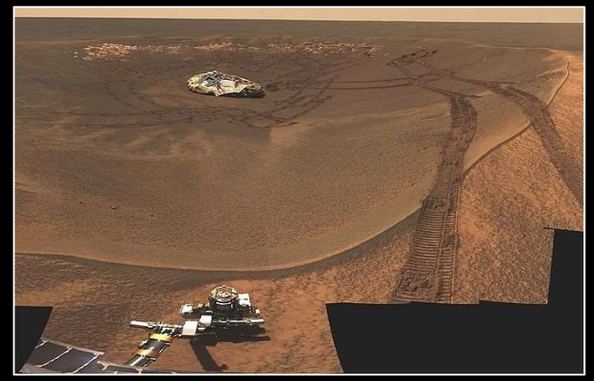


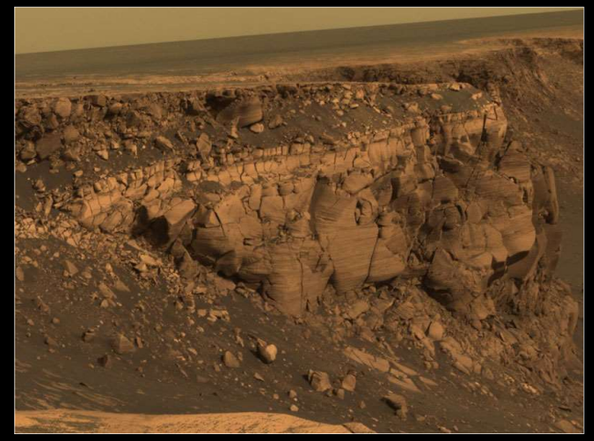


MER Contact Science Target List: https://pds-geosciences.wustl.edu/mer/urn-nasa-pds-mer_cs_target_list/

Mission Overview: Opportunity



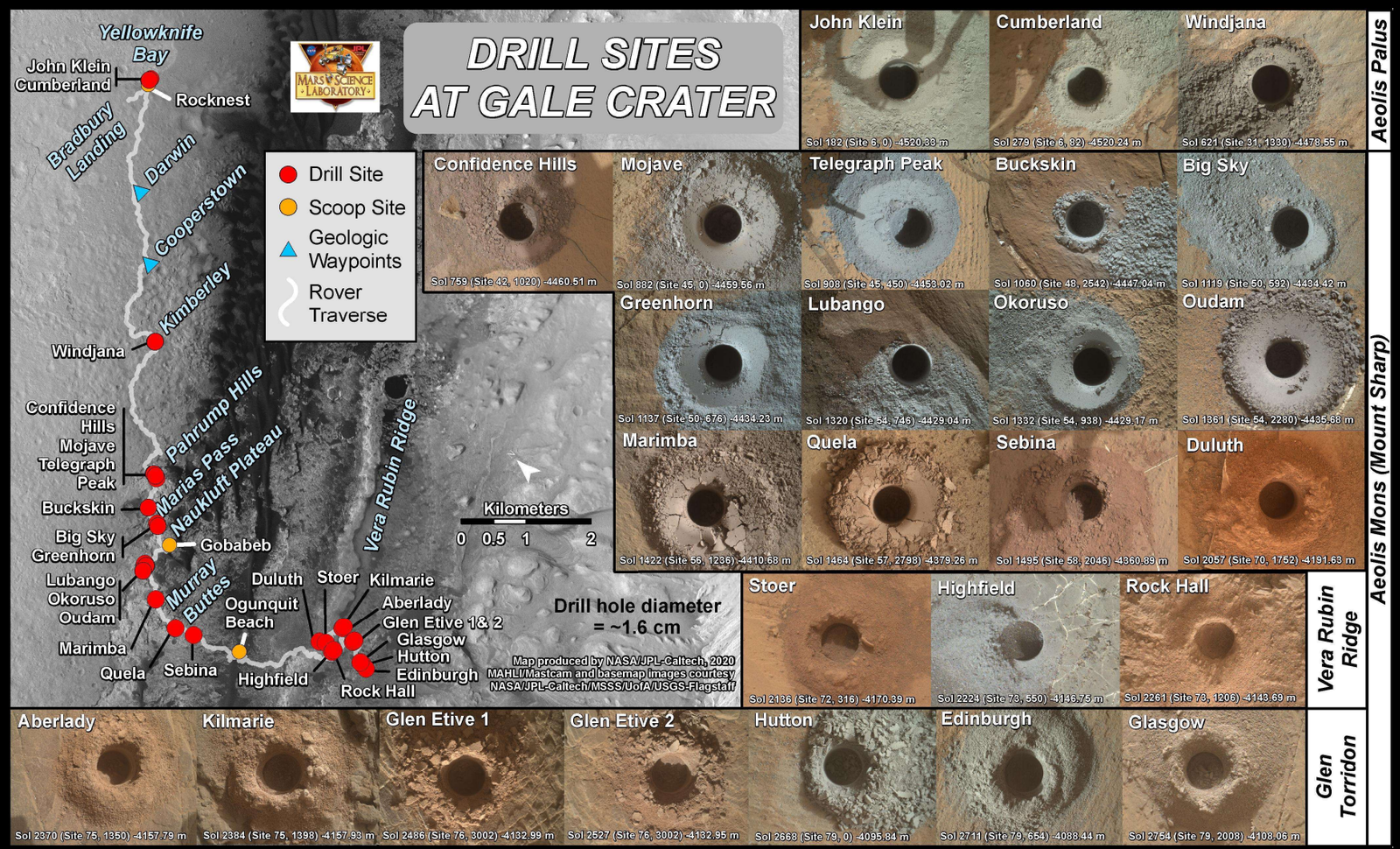




Unique APXS Measurements: ~500

MER Contact Science Target List: https://pds-geosciences.wustl.edu/mer/urn-nasa-pds-mer_cs_target_list/

Mission Overview: Curiosity

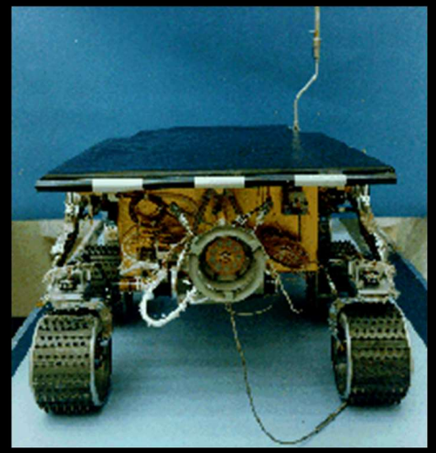


Unique APXS Measurements: ~950

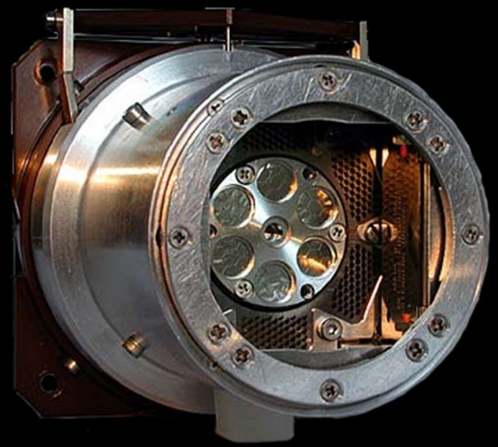
MSL APXS Data Supplement (to sol 2301): https://pds-geosciences.wustl.edu/msl/urn-nasa-pds-msl_apxs_supplement_sols_0_2301/

APXS Overview

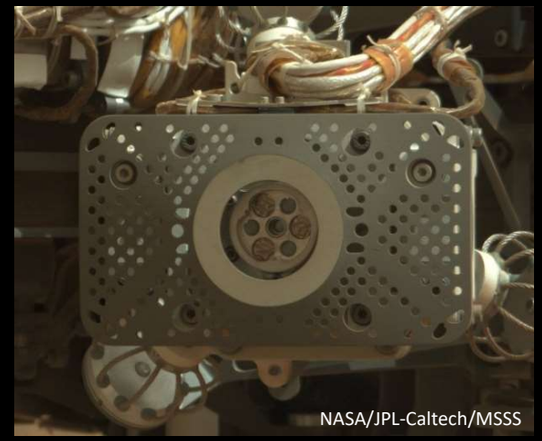
1997 – Mars Pathfinder
(Sojourner)

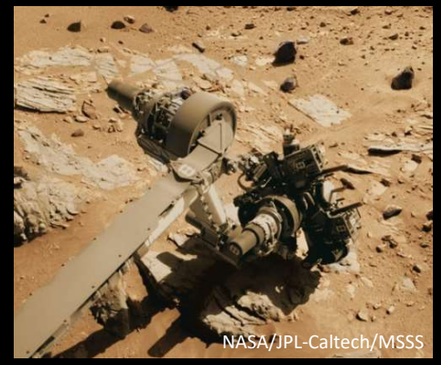


2004 – MER
(Spirit, Opportunity)

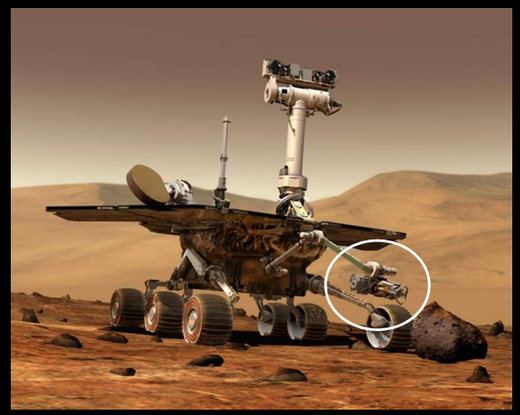


2012 – MSL
(***Curiosity***)

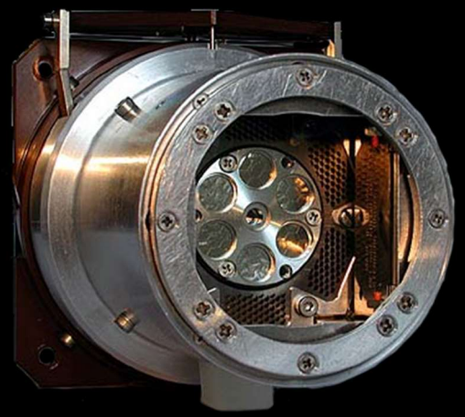




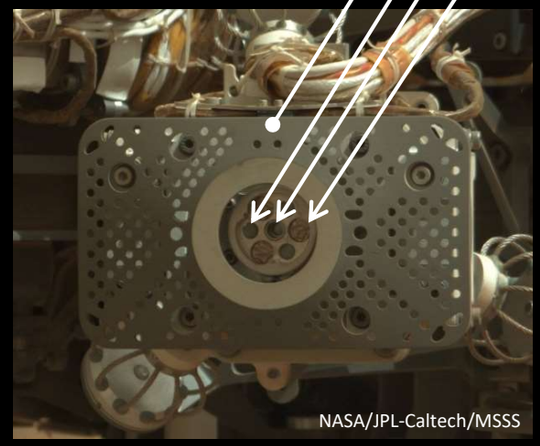
APXS Overview

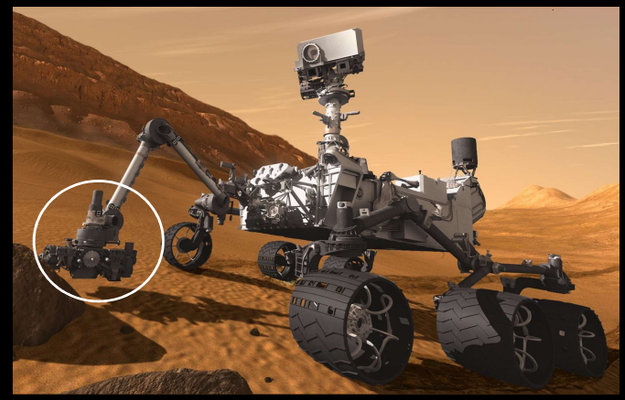


MER



MSL

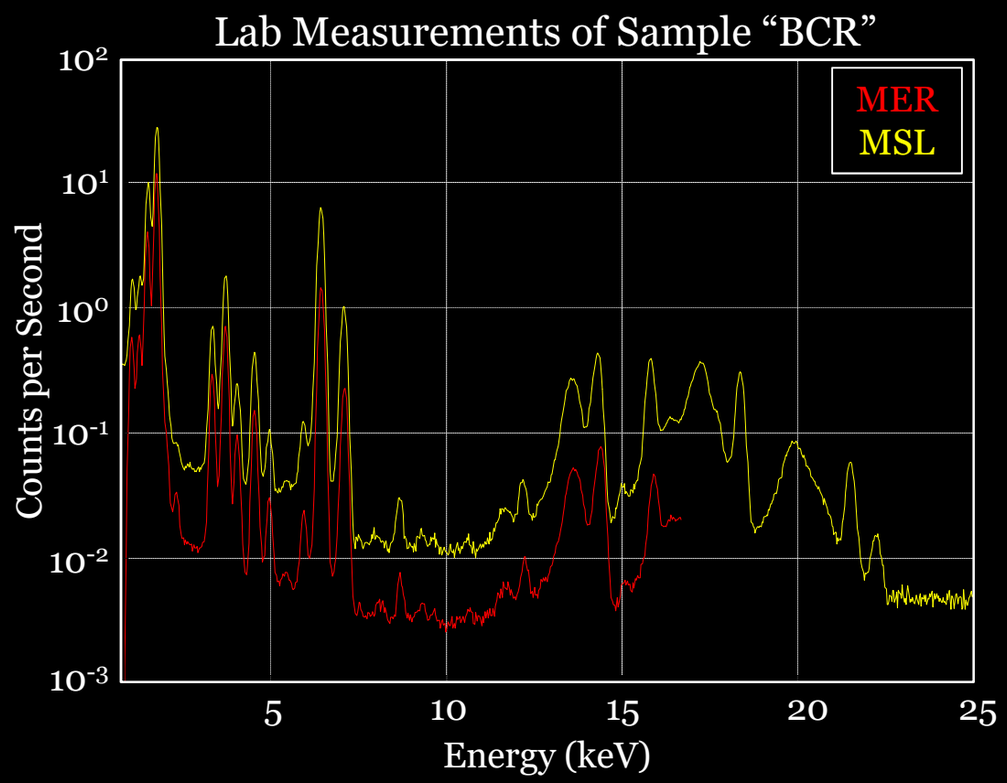




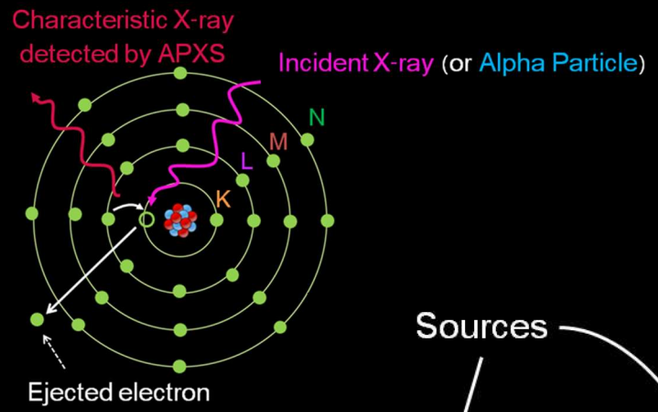
Specifications	
Sample Separation	30 mm (Contact)
In-Contact FOV	35 mm ⌀
Energy Range	0.9 – 16 keV
Resolution	160 eV (FWHM)
Operating Temp	-130°C to -40°C
Power Dissipation	2.8 W

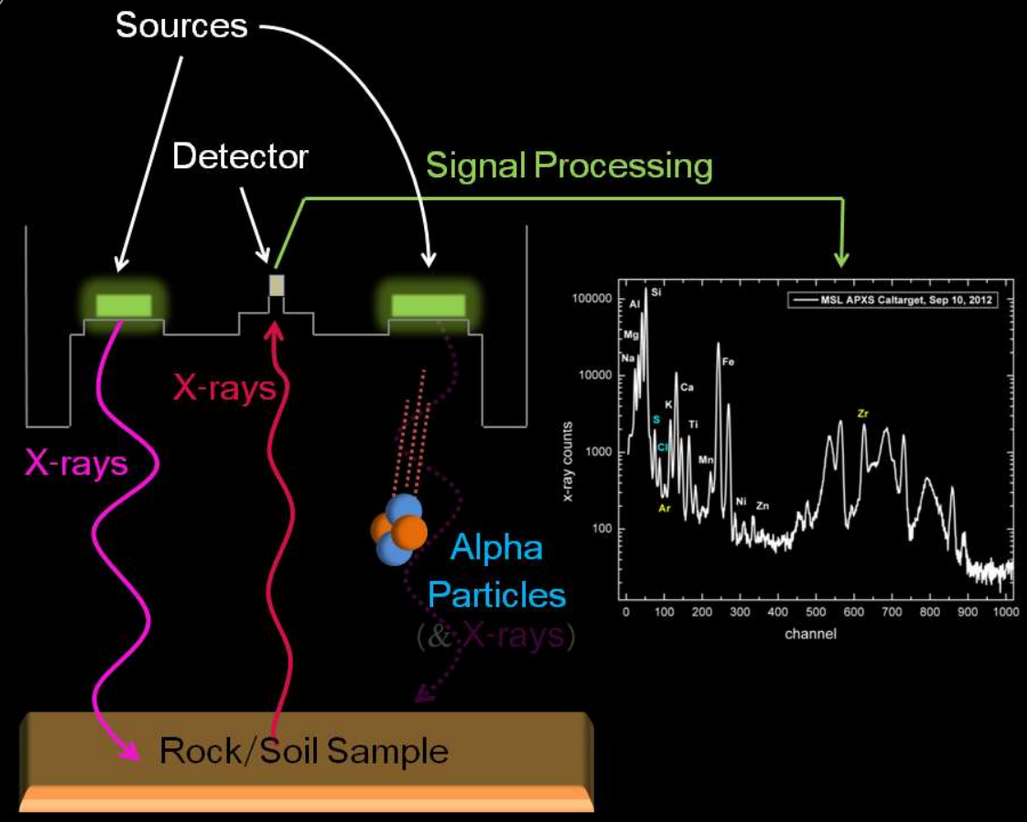
Specifications	
Sample Separation	18 mm (Contact)
In-Contact FOV	15 mm ⌀
Energy Range	0.7 – 25 keV
Resolution	140 eV (FWHM)
Operating Temp	-130°C to -5°C
Power Dissipation	5 W (+3 w/Peltier)

APXS Overview



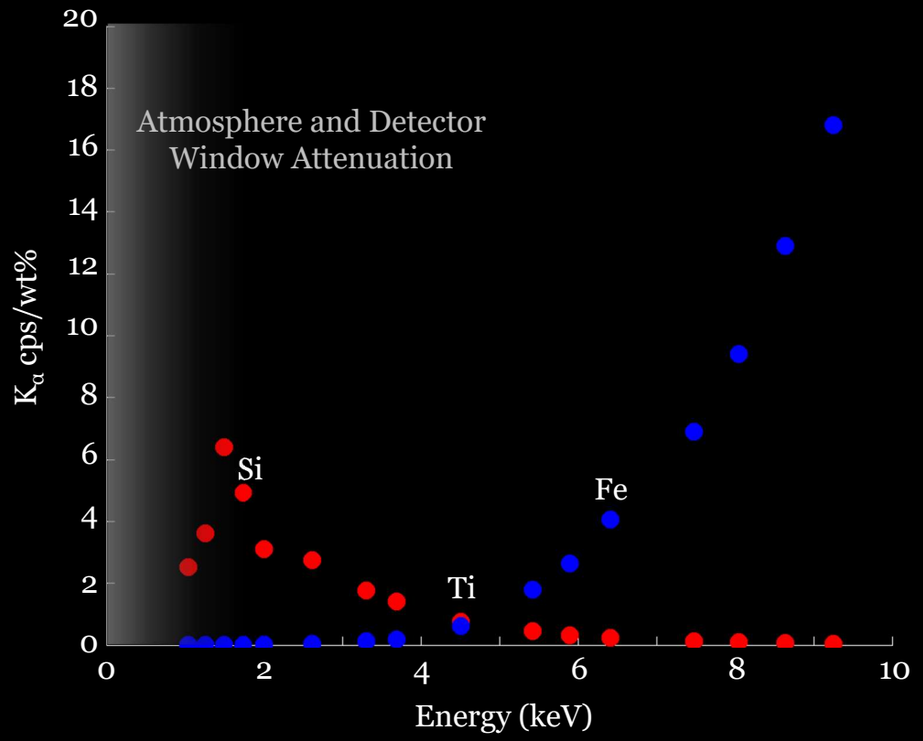
	MER	MSL
Sensitivity (Relative)	1	~3
Operable Peltier Cooler	No	$\Delta T=30^{o}C$
Meaningful APXS Calibration Target	No	Yes
Alpha Detectors (for RBS)	Yes	No
Proximity Mode	No	Yes



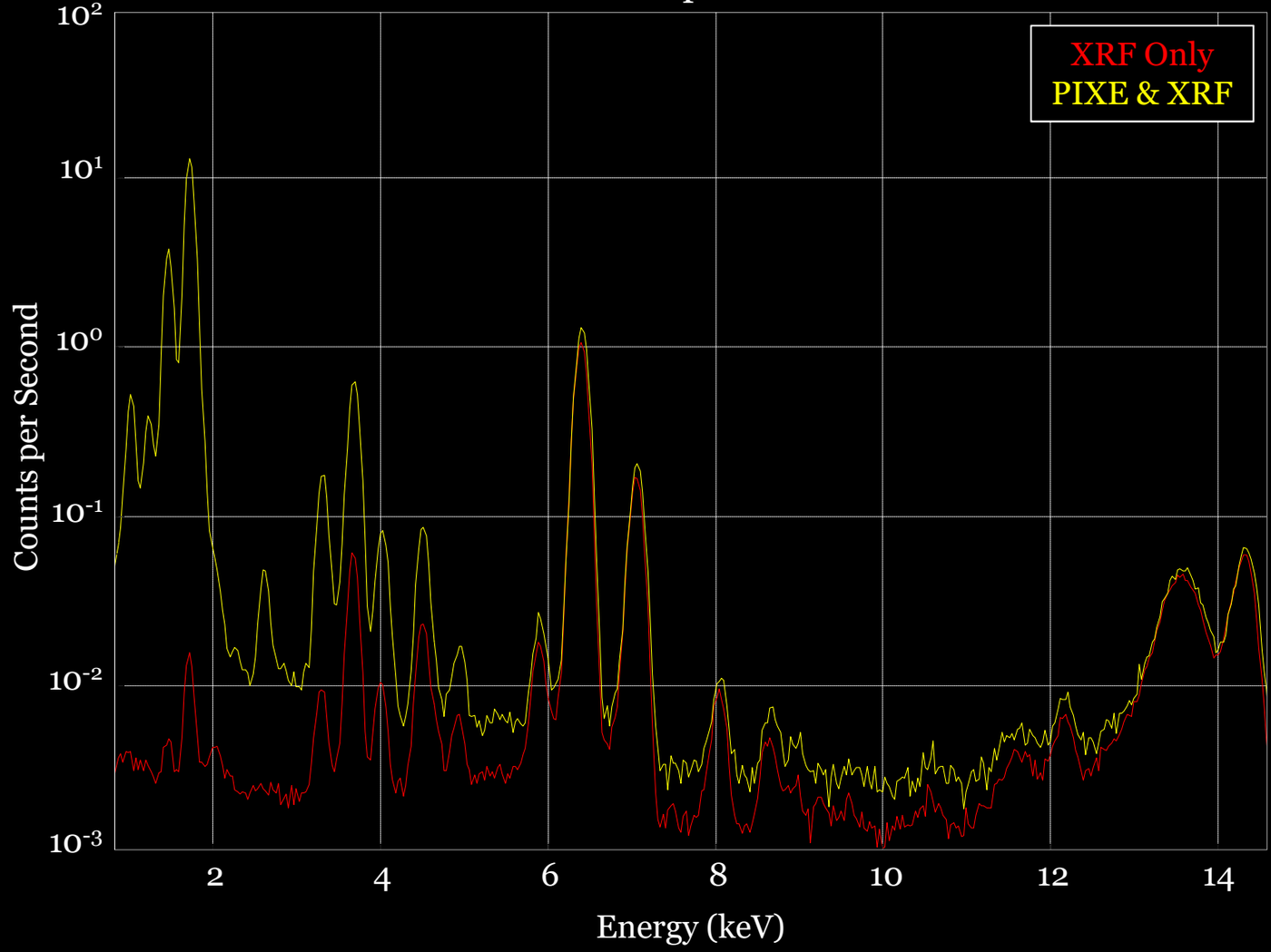


APXS Overview

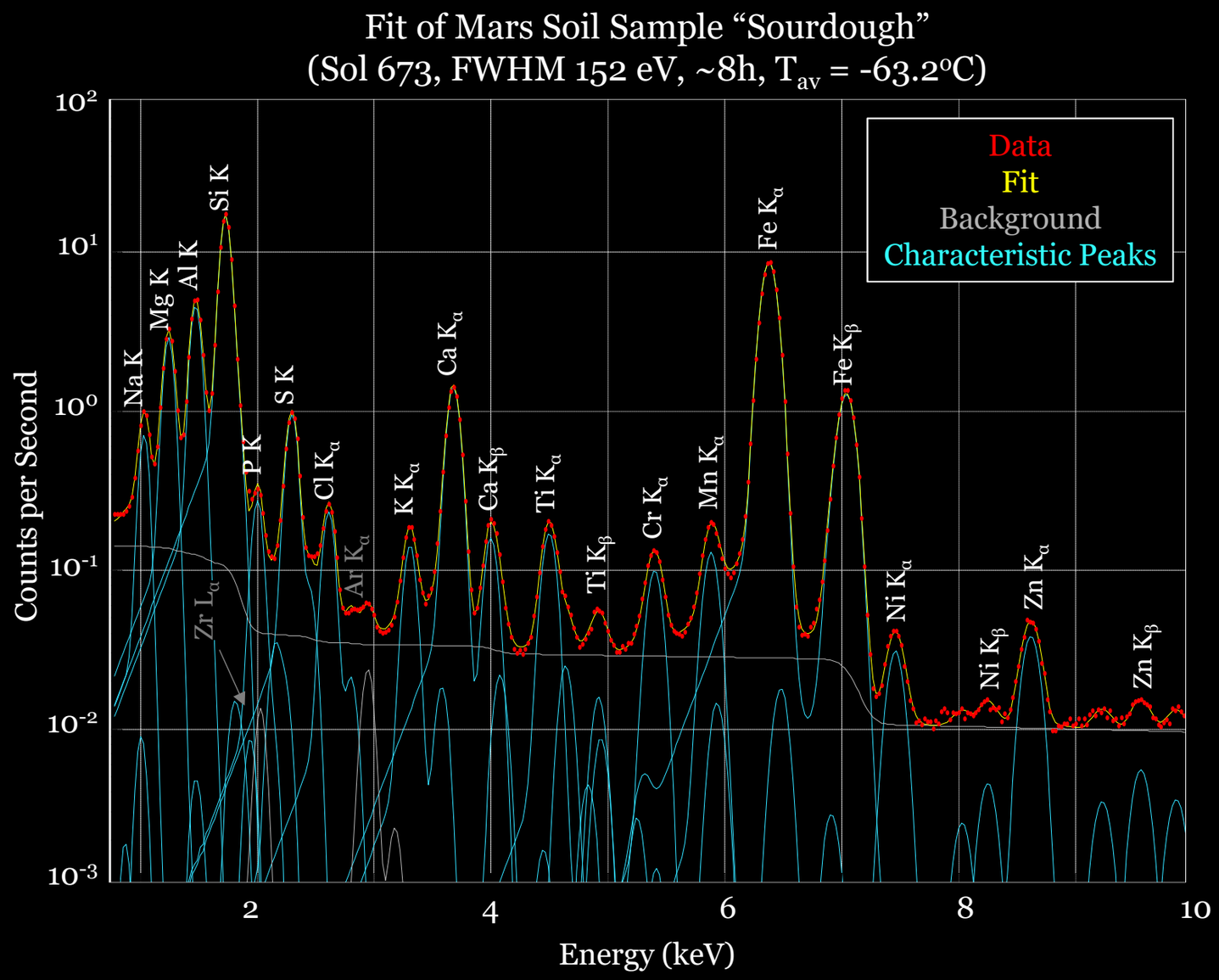
Excitation by Alpha and X-rays on APXS Target



Lab Measurements of Sample "SSK1" with MER APXS

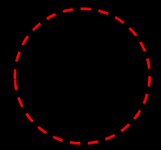


APXS Overview



APXS Data Considerations

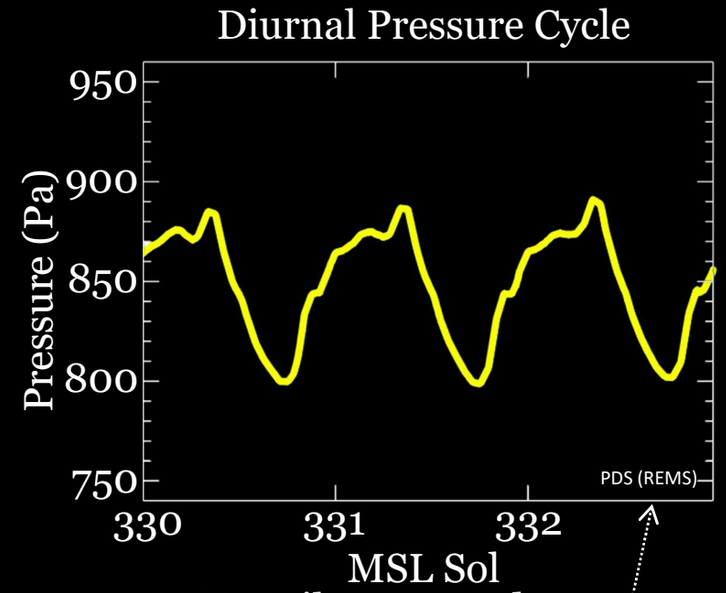
- Temperature
- Sample Proximity
- Measurement Duration
- Heterogeneities

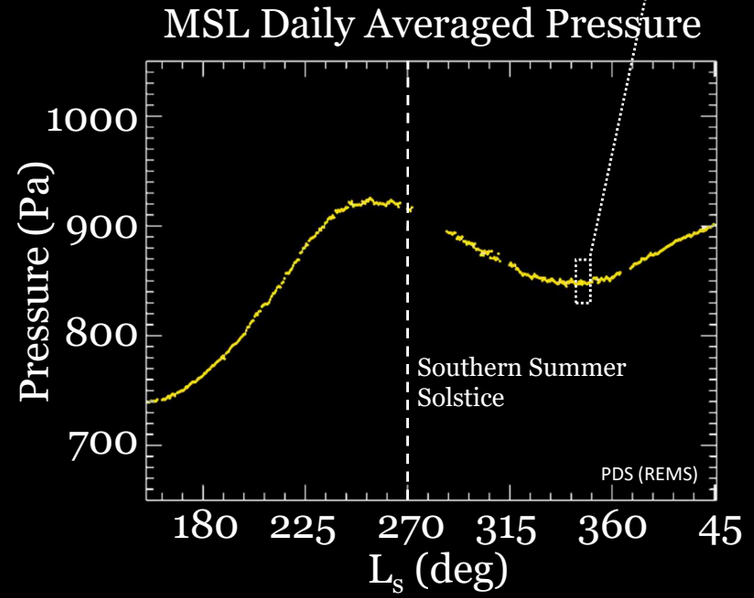


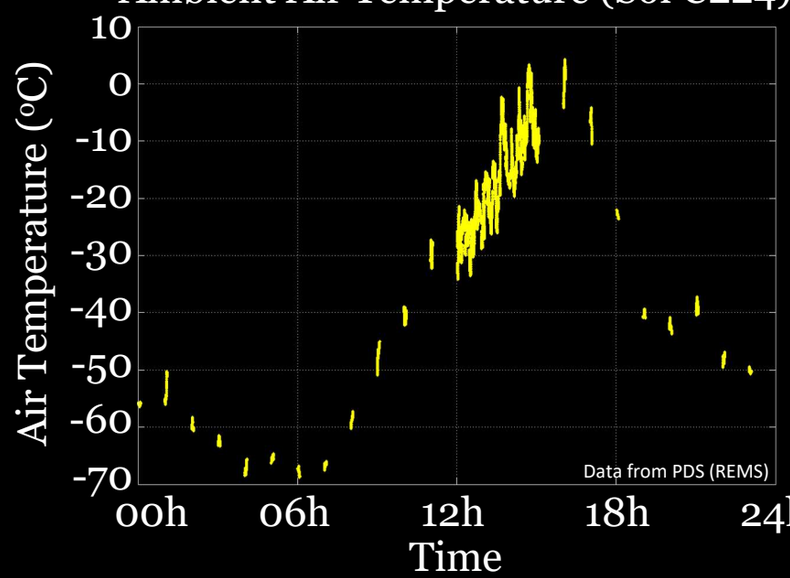
MSL APXS FOV

Image above captures an area approximately 3.5 cm x 5.0 cm in size

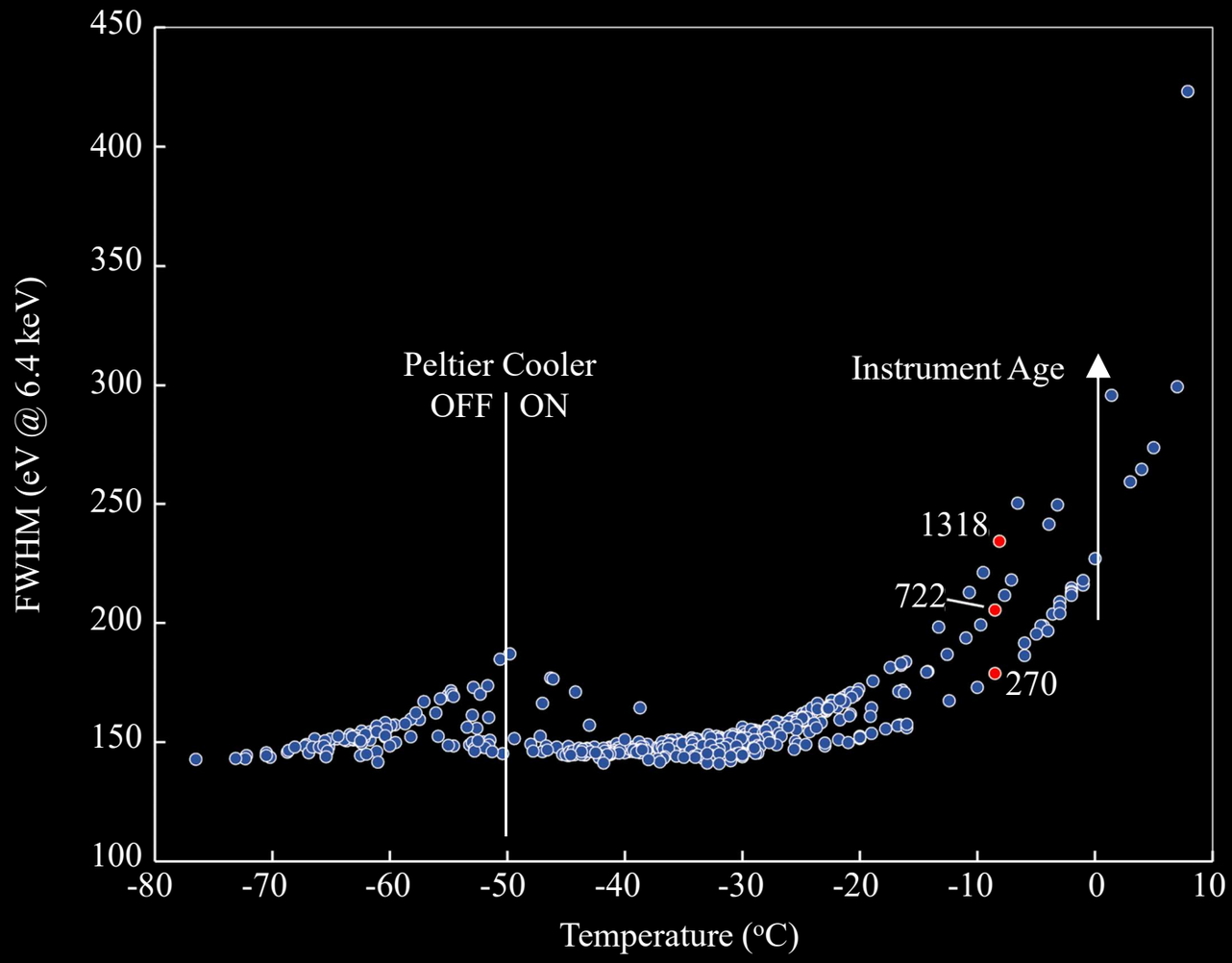
Credit: NASA/JPL-CalTech/MSSS

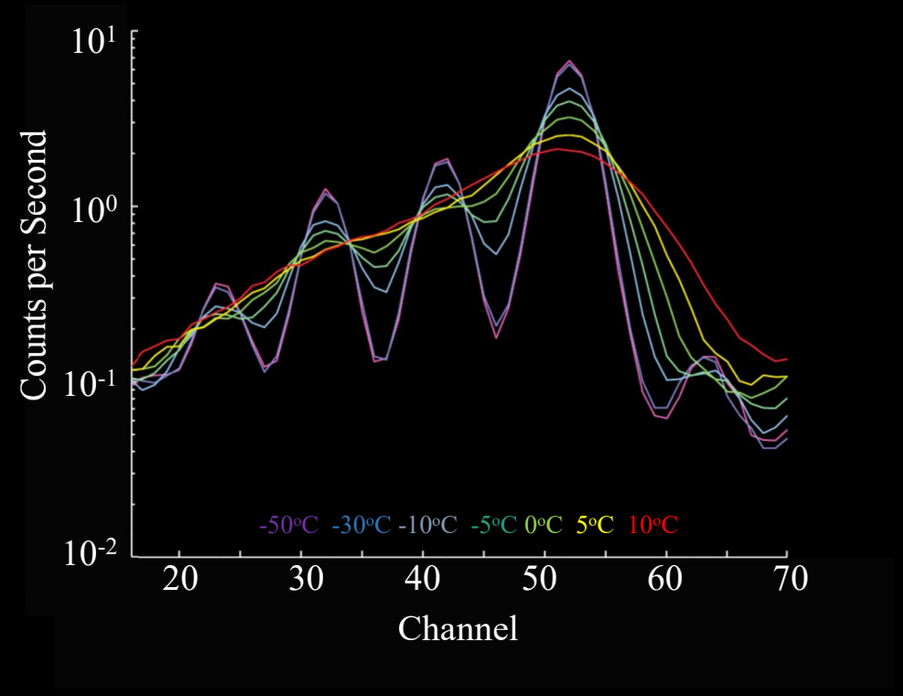






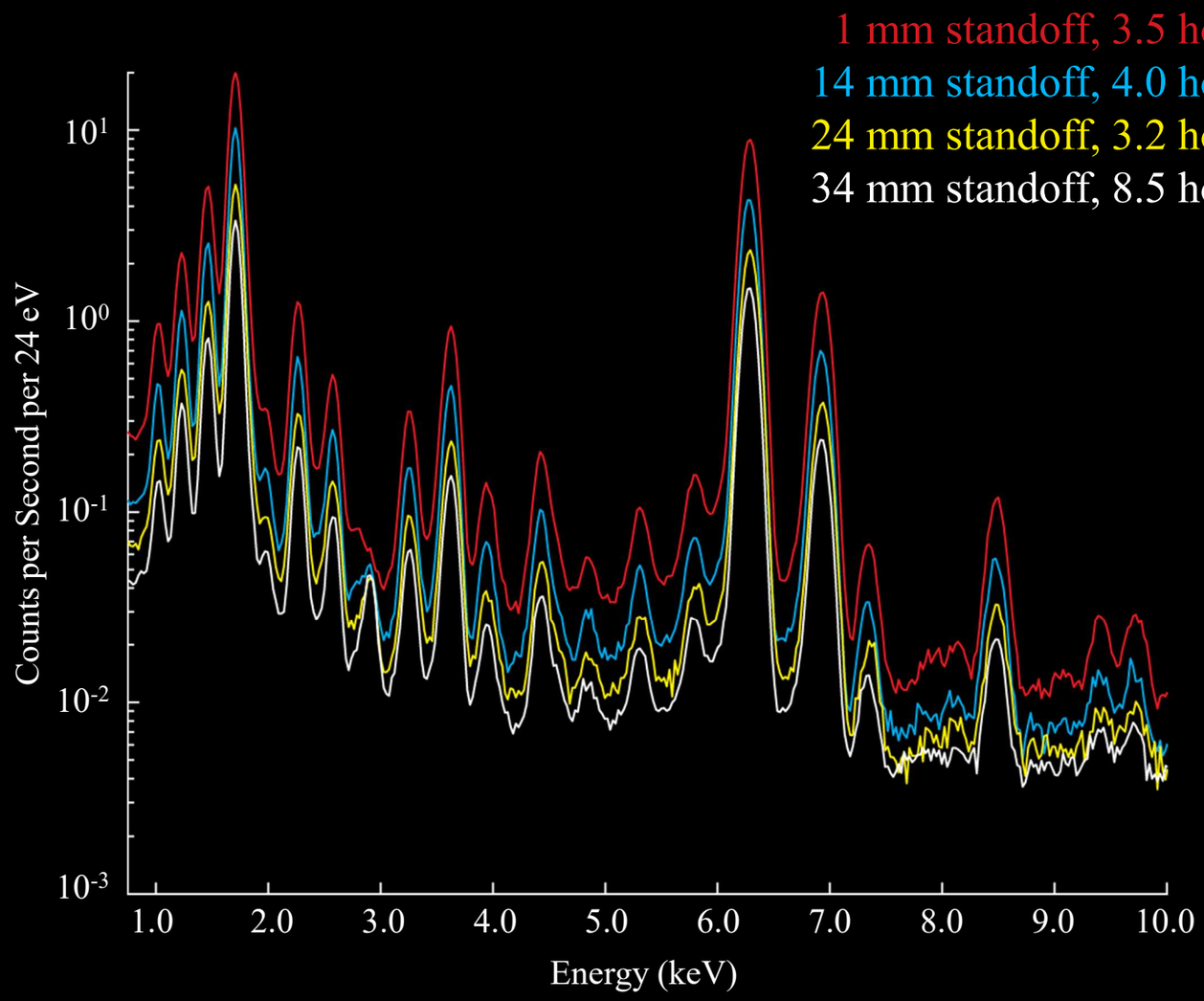
APXS Data Considerations: Temperature





More info: VanBommel et al., 2019, NIM:B, 441, 79-87.

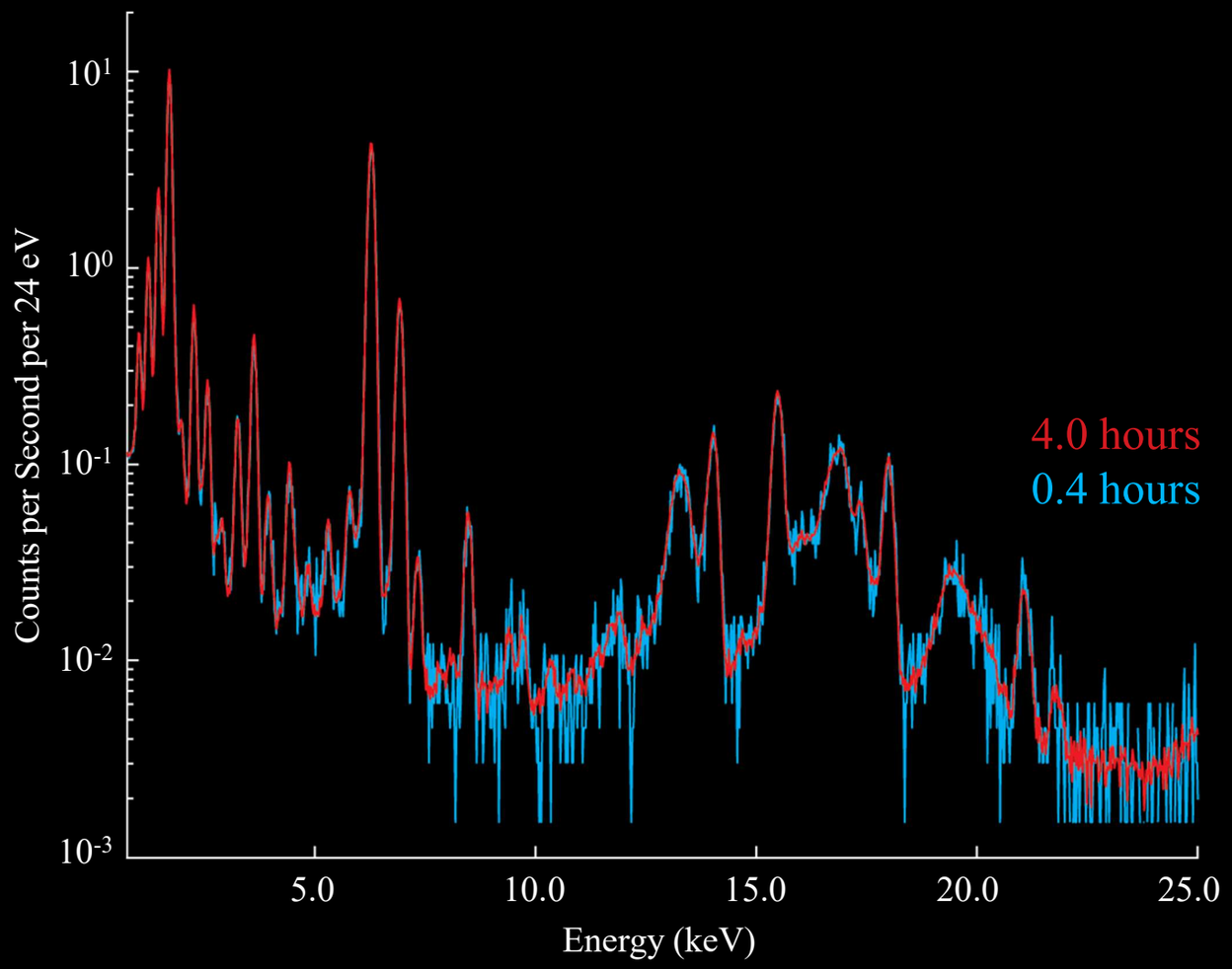
APXS Data Considerations: Sample Proximity



- Standoff (sample proximity) primarily affects statistical count rates
- Some elements have a standoff-dependent background
- Higher standoff means more attenuation of low-Z X-rays by the atmosphere (e.g., Na, Mg)
- For every 1 cm further from the sample, count rates are approximately halved

More info: VanBommel et al., 2019, Acta Astronaut., 165, 32-42.

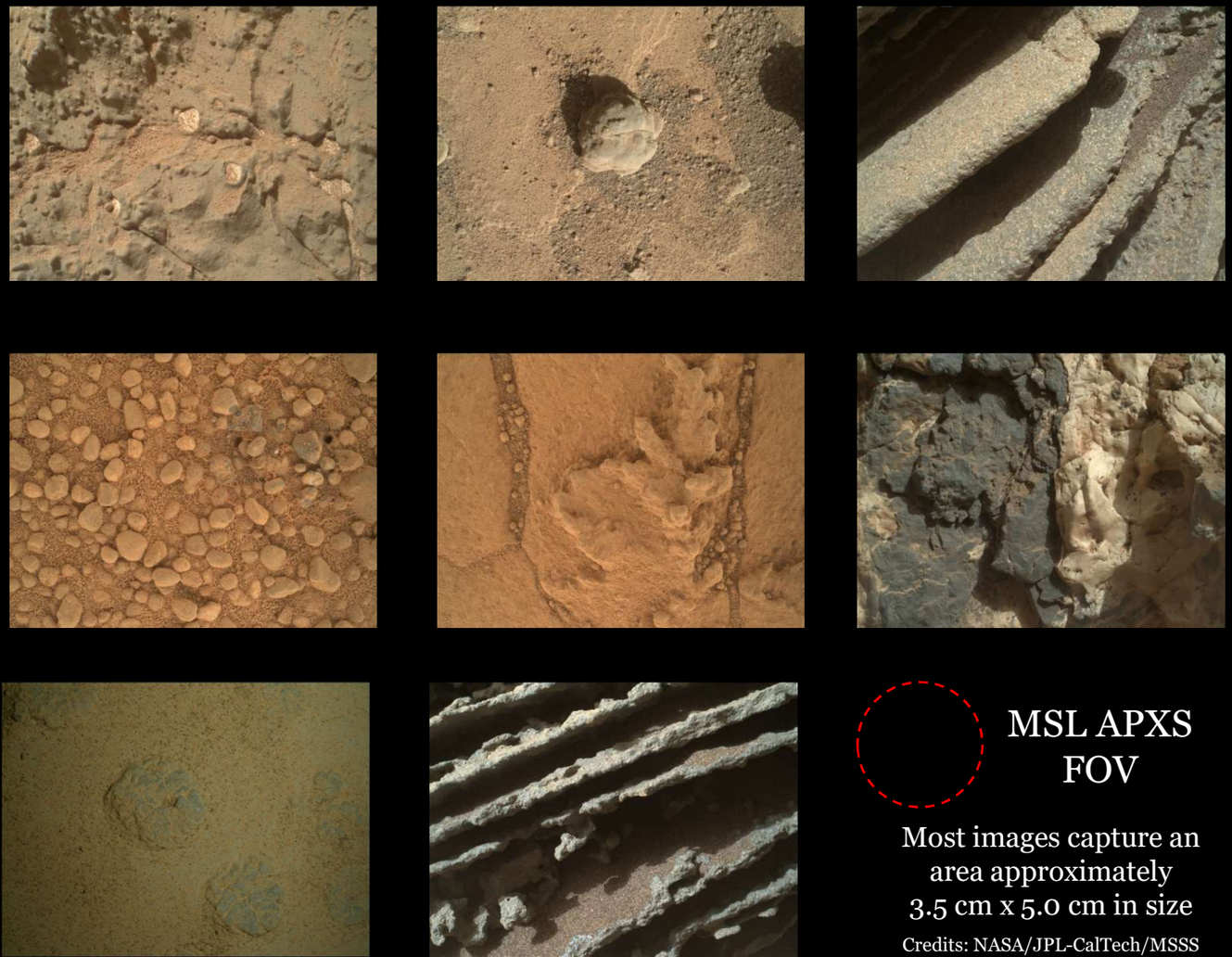
APXS Data Considerations: Measurement Duration



- Short-duration measurements are useful tactically in order to return geochemical data decisionally
- Short-duration measurements provide reliable results for major oxides
- Typical APXS measurements are 1-2 hours in length, or longer
- Overnight (4+ hour) measurements provide a high degree of confidence for trace elements

More info: VanBommel et al., 2019, Acta Astronaut., 165, 32-42.

APXS Data Considerations: Heterogeneities



MSL APXS FOV

Most images capture an area approximately 3.5 cm x 5.0 cm in size

Credits: NASA/JPL-CalTech/MSSS

- Targets are often interrogated with minimal sample preparation
- Chemical heterogeneities exist on a lateral scale smaller than a typical APXS field of view
- Vertical layering may also be present, affecting characteristic X-rays differently as a function of Z
- Surface dust is pervasive and skews low-Z compositions, as well as S and Cl, towards a known endmember composition

APXS Data: Availability

- APXS data are available online through the PDS Geosciences node
- APXS data are reported in wt% oxides with a few exceptions (Cl, Ni, Zn, Br)
- Sixteen (16) elements and oxide concentrations are reported for each APXS measurement in wt% (unless otherwise noted): Na_2O, MgO, Al_2O_3, SiO_2, P_2O_5, SO_3, Cl, K_2O, CaO, TiO_2, Cr_2O_3, MnO, FeO, Ni (µg/g), Zn (µg/g), Br (µg/g)
- Precision errors are reported, see data documentation for accuracy errors

MER APXS Concentration Data Availability (PDS3, PDS4)

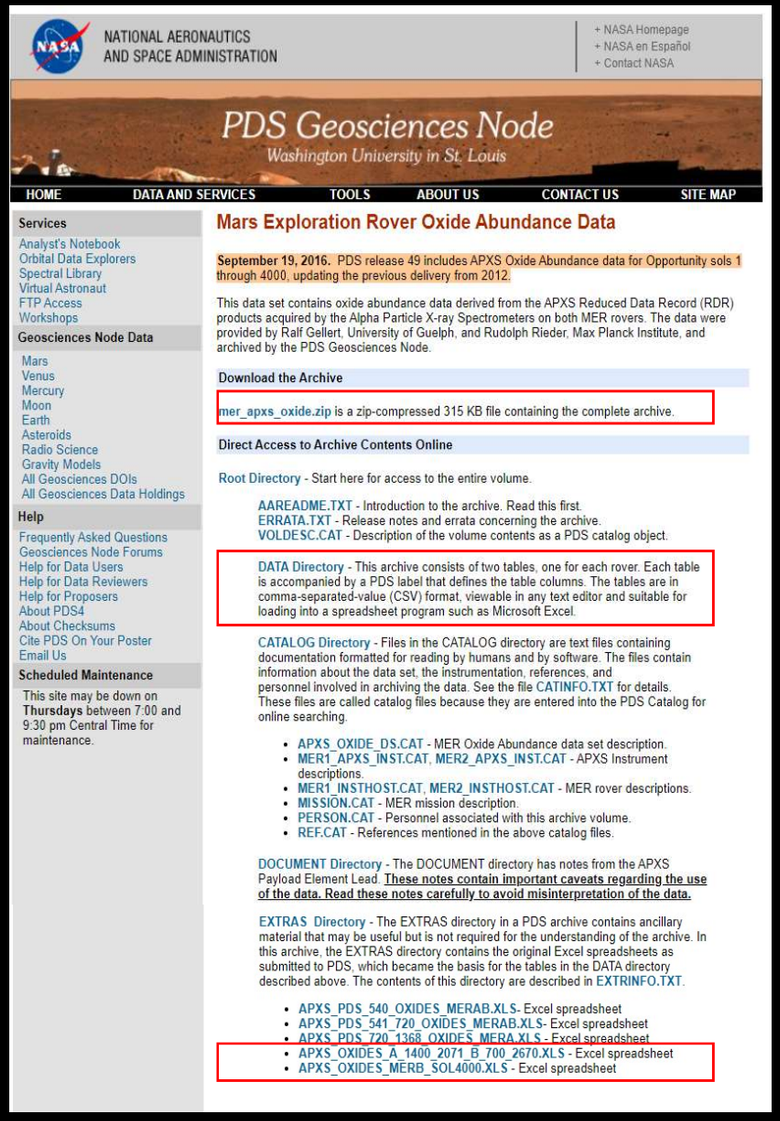
- Spirit & Opportunity: https://pds-geosciences.wustl.edu/missions/mer/mer_apxs_oxide.htm

MSL APXS Concentration Data Availability (PDS3)

- Curiosity: https://pds-geosciences.wustl.edu/msl/msl-m-apxs-4_5-rdr-v1/mslapx_1xxx/extras/

APXS Data: Availability

MER



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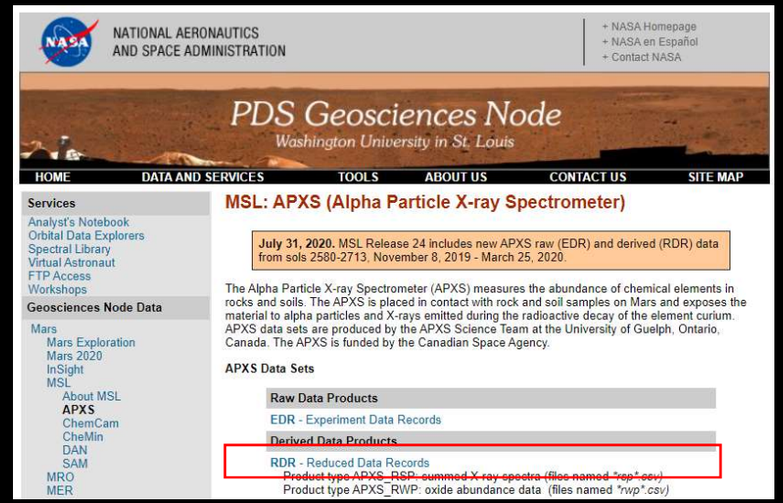
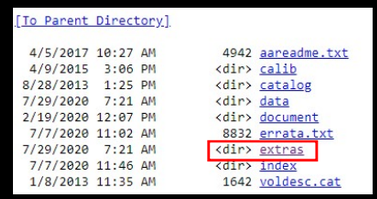




+ more (and new data every 90 days)

APXS Data: Availability

- APXS compositional context is most easily gained through exploring APXS data and associated targets in the Analyst's Notebook (see Zoom tutorial here on Thursday October 29th, 15:00 EDT: Content and Use of PDS Geosciences Node Landed Mission Analyst Notebooks)
  - MER: https://an.rsl.wustl.edu/mer/
  - MSL: https://an.rsl.wustl.edu/msl/

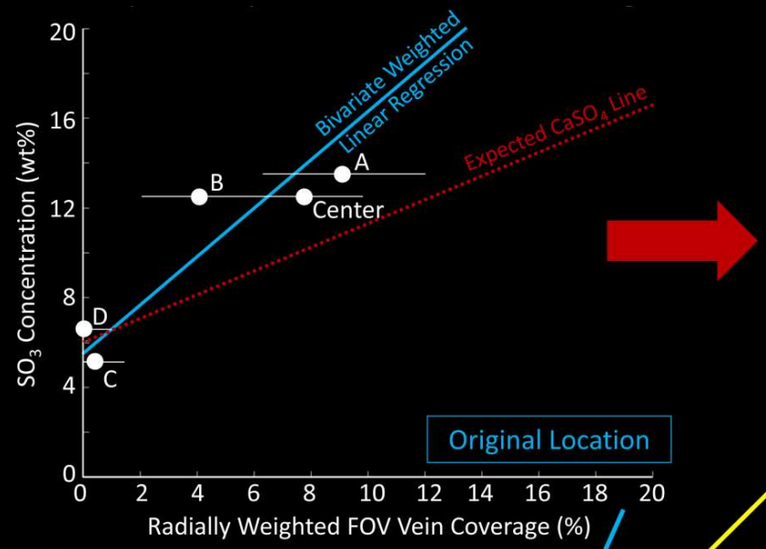
sol	target	start_time	gnorm	sh_tavg	lifetime	Fe_FWHM	Na2O	Na2O_err	MgO	MgO_err	Al2O3	Al2O3_err	SiO2	SiO2_err	P2O5	P2O5_err	SO3	SO3_err	Cl	Cl_err	K2O	K2O_err	CaO	CaO_err	TiO2	TiO2_err	Cr2O3	Cr2O3_err	MnO	MnO_err	FeO	FeO_err	Ni	Ni_err	Zn	Zn_err	Br	Br_err
46	Jake_Matijevic	00046M11:43:31	101.8	-3	00:32:09	204.1	7.11	0.41	3.61	0.33	16.09	0.87	50.7	1.07	0.49	0.07	2.48	0.12	0.87	0.05	2.23	0.12	6.07	0.31	0.49	0.03	0.04	0.01	0.14	0.02	9.47	0.20	30	20	221	15	92	10
47	JM2_APXS_RP2	00047M11:53:23	96	-2	00:12:00	211.6	6.61	0.55	4.57	0.58	14.59	0.77	49.29	1.07	0.6	0.14	3.05	0.17	1.03	0.06	2.01	0.11	6.54	0.34	0.65	0.07	0.09	0.03	0.17	0.06	10.61	0.26	0	0	340	24	93	15
47	JM2_APXS_RP2_OVERNIGHT	00048M00:01:42	90.5	-55	00:30:00	148.6	6.59	0.20	4.60	0.17	14.65	0.38	48.87	0.54	0.85	0.05	2.81	0.08	0.95	0.03	1.89	0.06	6.78	0.08	0.73	0.03	0.04	0.01	0.23	0.02	10.94	0.13	60	20	318	15	93	5
54	Bathurst_Inlet_RP_For_Real	00054M11:51:54	113.1	-4	00:22:14	196.7	2.21	0.27	8.56	0.33	7.85	0.38	43.65	0.64	0.82	0.07	3.05	0.12	0.73	0.04	2.18	0.07	6.28	0.08	1.09	0.09	0.42	0.03	0.83	0.06	22.07	0.26	399	40	1359	44	13	10
54	Bathurst_Inlet_Top_RP	00054M12:42:20	132.3	-2	00:22:15	212.7	2.06	0.14	8.68	0.50	7.92	0.48	43.95	0.96	0.88	0.09	3.31	0.17	0.81	0.05	2.88	0.15	6.45	0.34	1.06	0.07	0.36	0.03	0.46	0.06	21.00	0.46	326	30	1221	65	40	10
58	Scuffed_E	00058M11:36:26	8.2	-1	01:04:19	217.9	1.99	0.41	7.90	1.67	9.02	0.48	43.94	0.96	0.65	0.14	5.97	0.30	0.84	0.08	0.55	0.12	7.45	0.38	0.97	0.21	0.39	0.06	0.39	0.08	19.13	0.39	436	115	544	70	0	5
58	Unscuffed_A	00058M12:48:47	8.2	4	00:19:01	264.9	2.14	1.64	7.79	1.58	8.84	1.25	43.54	1.82	0.00	0.82	6.93	1.23	1.05	0.23	0.76	0.16	7.11	0.71	0.44	0.47	0.30	0.17	0.5	0.18	19.58	1.44	649	299	649	179	0	0
86	Et_Then	00086M11:52:32	5.4	3	00:22:18	259.5	2.91	0.95	4.71	1.50	8.96	0.58	45.42	0.96	0.55	0.44	4.23	0.45	0.98	0.18	1.63	0.67	4.41	0.25	0.61	0.29	0.30	0.14	0.44	0.40	24.67	0.52	288	270	353	149	0	5
89	PortageRP	00089M05:23:06	27.2	-62	03:14:02	144.9	2.70	0.14	8.69	0.25	9.37	0.19	42.97	0.54	0.95	0.07	5.47	0.10	0.69	0.03	0.49	0.02	7.26	0.08	1.19	0.05	0.49	0.03	0.42	0.04	19.18	0.20	456	30	326	15	34	10
91	Et_Then_overnight	00091M01:03:40	6.7	-61	02:00:43	141.6	2.95	0.95	4.19	1.33	8.41	0.29	45.06	0.75	0.99	0.42	4.06	0.17	0.79	0.06	1.57	0.64	4.27	0.11	0.73	0.31	0.08	0.05	0.39	0.02	26.33	0.33	225	89	485	54	49	15
102	rocknest3_rp	00102M11:46:35	105.7	0	00:22:18	227.0	4.02	0.41	5.32	0.50	10.52	0.58	45.97	0.96	1.08	0.14	4.06	0.22	0.88	0.05	1.86	0.10	6.05	0.31	0.96	0.05	0.24	0.03	0.46	0.04	18.39	0.39	368	35	891	44	65	10
117	Bell_Island_target9_day	00117M12:00:02	84.6	-5	00:22:18	195.5	3.17	0.14	8.01	0.17	8.99	0.19	42.72	0.43	0.80	0.07	7.40	0.15	1.22	0.05	1.05	0.04	6.84	0.08	0.81	0.03	0.46	0.03	0.48	0.06	17.93	0.20	286	35	662	30	92	10
117	Bell_Island_target9_night	00117M21:01:49	81.8	-40	00:16:01	151.1	3.01	0.14	8.18	0.17	9.08	0.19	42.77	0.43	1.00	0.07	7.09	0.17	1.21	0.05	1.01	0.04	6.79	0.10	0.81	0.05	0.50	0.03	0.48	0.06	17.89	0.20	291	40	625	35	86	15
129	Costello	00129M12:39:12	113	5	00:44:19	273.8	2.19	0.48	8.72	0.50	8.35	0.48	42.28	0.86	0.51	0.33	6.25	0.65	1.36	0.14	0.46	0.05	6.58	0.67	1.04	0.12	0.48	0.06	0.41	0.06	21.12	1.50	505	60	828	85	168	20
129	Flaherty	00129M17:10:42	107.8	-23	06:01:01	149.6	2.59	0.14	8.67	0.25	8.20	0.19	41.36	0.43	0.93	0.07	6.42	0.08	1.18	0.02	0.42	0.02	6.63	0.07	0.95	0.03	0.49	0.01	0.36	0.02	21.60	0.26	441	24	795	24	324	10
132	Gillespie_Lake_1	00132M11:32:14	69.4	-2	00:44:18	213.3	2.58	0.34	9.18	0.50	9.11	0.48	45.60	0.96	0.88	0.12	2.88	0.15	1.10	0.06	0.51	0.04	6.45	0.34	1.12	0.07	0.52	0.03	0.35	0.06	19.59	0.46	320	35	590	30	93	10

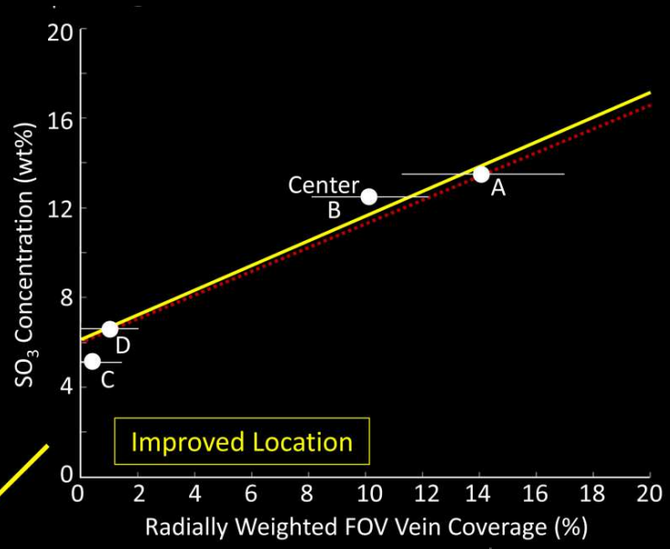
APXS Analytical Techniques: Deconvolution & Emulation

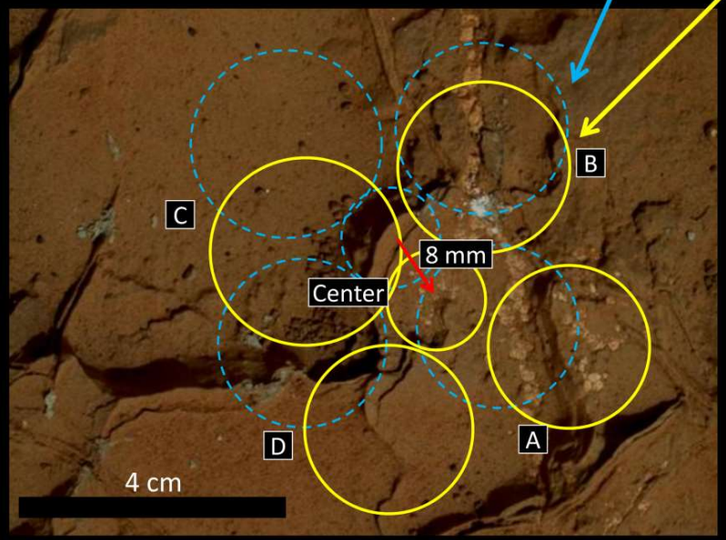
- APXS data is integral to elucidating geochemical trends on the surface of Mars
- The additional complement of data from other instruments on the rover enables one to assess whether past conditions on Mars were once habitable through a detailed characterization of Mars' paleoclimate

- New techniques are advancing the scientific return of data acquired by the APXS
  - Computational deconvolution techniques have increased the spatial resolution upon which the APXS can provide quantitative chemistry, essential for determining the chemical composition of diagenetic features
  - Artificial Intelligence has effectively created a "lab APXS" within a computer, enabling detailed studies of acquired and theoretical APXS data

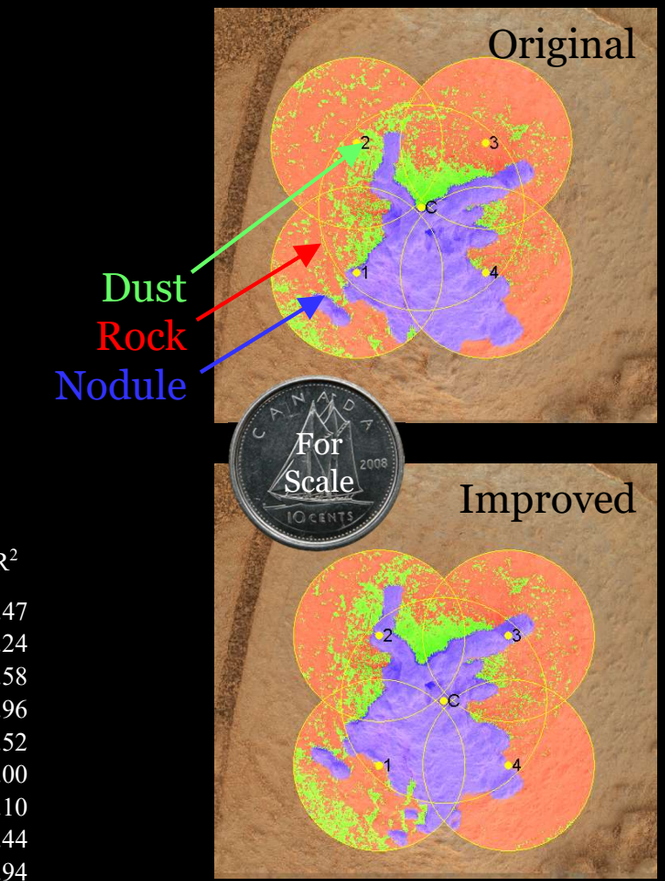
APXS Analytical Techniques: Deconvolution







	Dusty Rock		Vein		R^2
	Conc. (wt%)	Error (wt%)	Conc. (wt%)	Error (wt%)	
Na_2O	2.75	0.10	0.00	0.07	0.47
MgO	9.58	0.12	0.00	0.06	0.24
Al_2O_3	8.65	0.12	0.00	0.07	0.58
SiO_2	43.08	0.18	0.00	0.07	0.96
P_2O_5	1.01	0.04	0.00	0.07	0.52
SO_3	5.38	0.11	**65.04**	0.61	1.00
Cl	1.54	0.02	0.00	0.01	0.10
K2O	0.55	0.01	0.00	0.01	0.44
CaO	5.54	0.07	**34.96**	0.61	0.94
TiO_2	0.90	0.03	0.00	0.07	0.41
Cr_2O_3	0.40	0.01	0.00	0.13	0.00
MnO	0.31	0.01	0.00	0.01	0.95
FeO	20.12	0.11	0.00	0.06	0.59
Ni (ppm)	817	30	0	40	0.07
Zn (ppm)	827	20	0	15	0.82
Br (ppm)	240	5	0	5	0.02



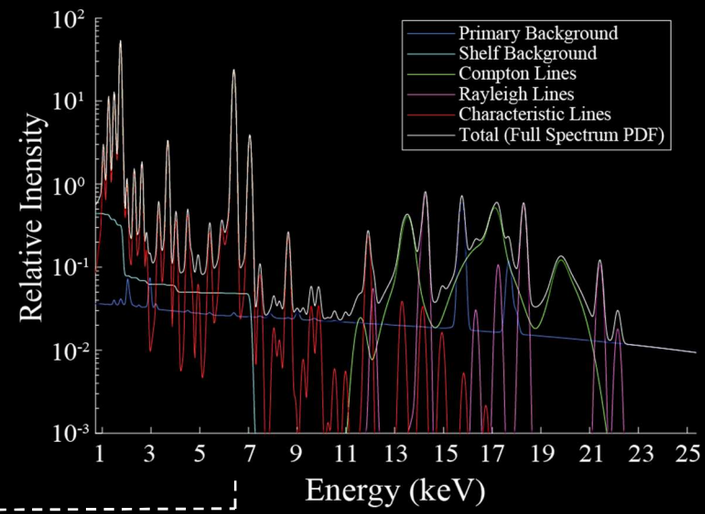
APXS Analytical Techniques: Emulation

Calibration Data

Mars Data (Pt. I)

ACES Simulation Routine

Output Spectrum (PDF)

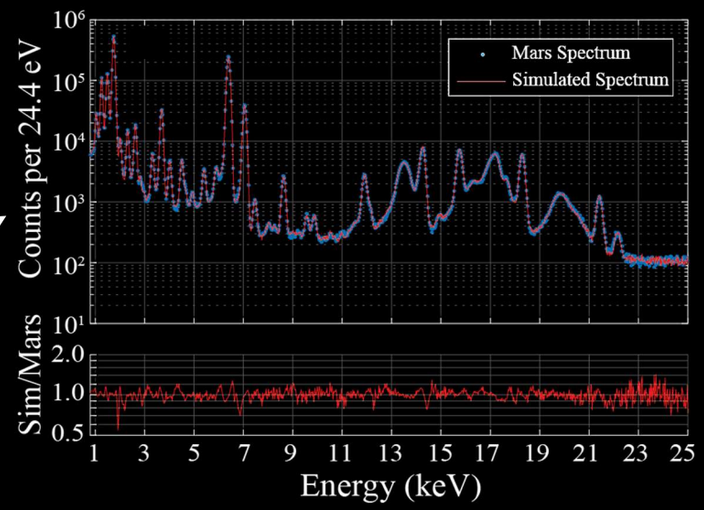


Input
Composition(s)
Standoff
Duration
Sol
Temperature

Learning

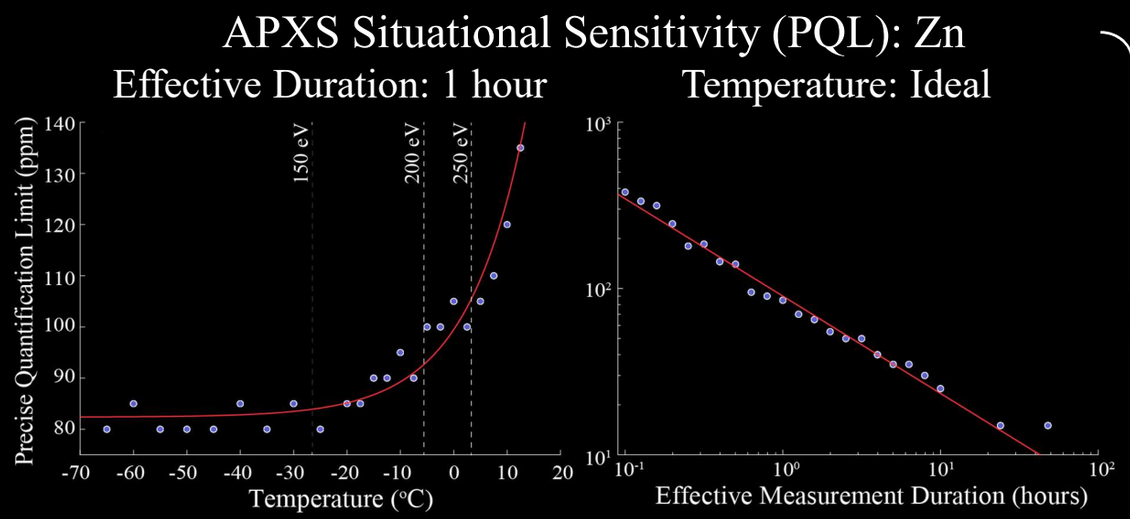
Validation/Utilization

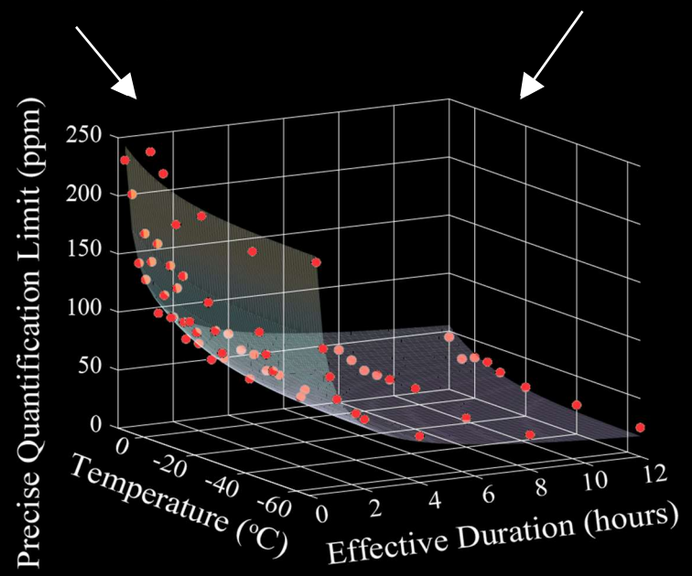
Mars Data (Pt. II)



More info: VanBommel et al., 2019, NIM:B, 441, 79-87.

APXS Analytical Techniques: Emulation



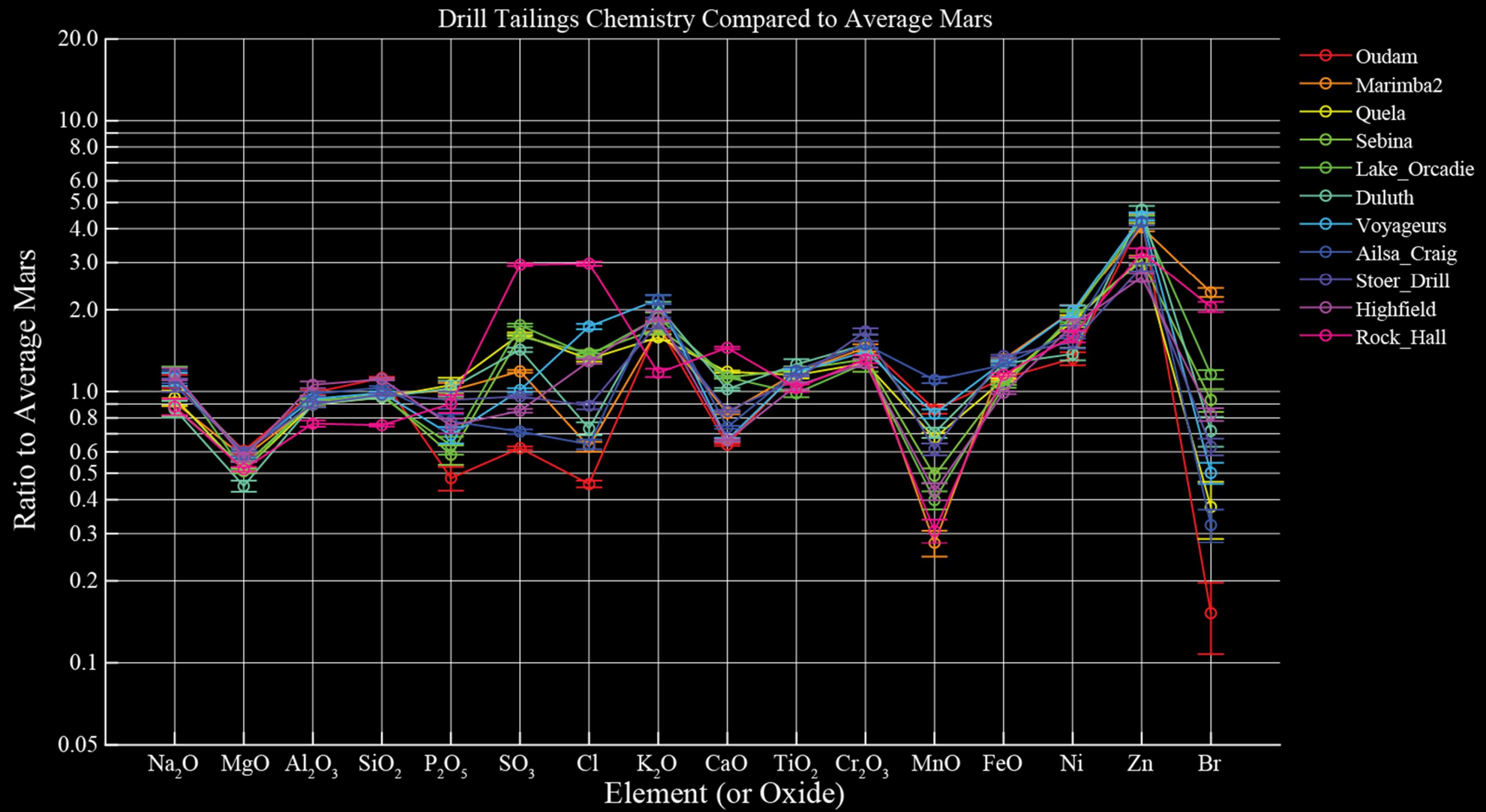


Element	PQL (ppm) by Measurement Condition		
	Touch-and-Go	Evening	Overnight
Ni	365	115	55
Cu	220	75	30
Zn	190	55	30
Ga	135	45	25
Ge	150	45	25
Br	85	25	15

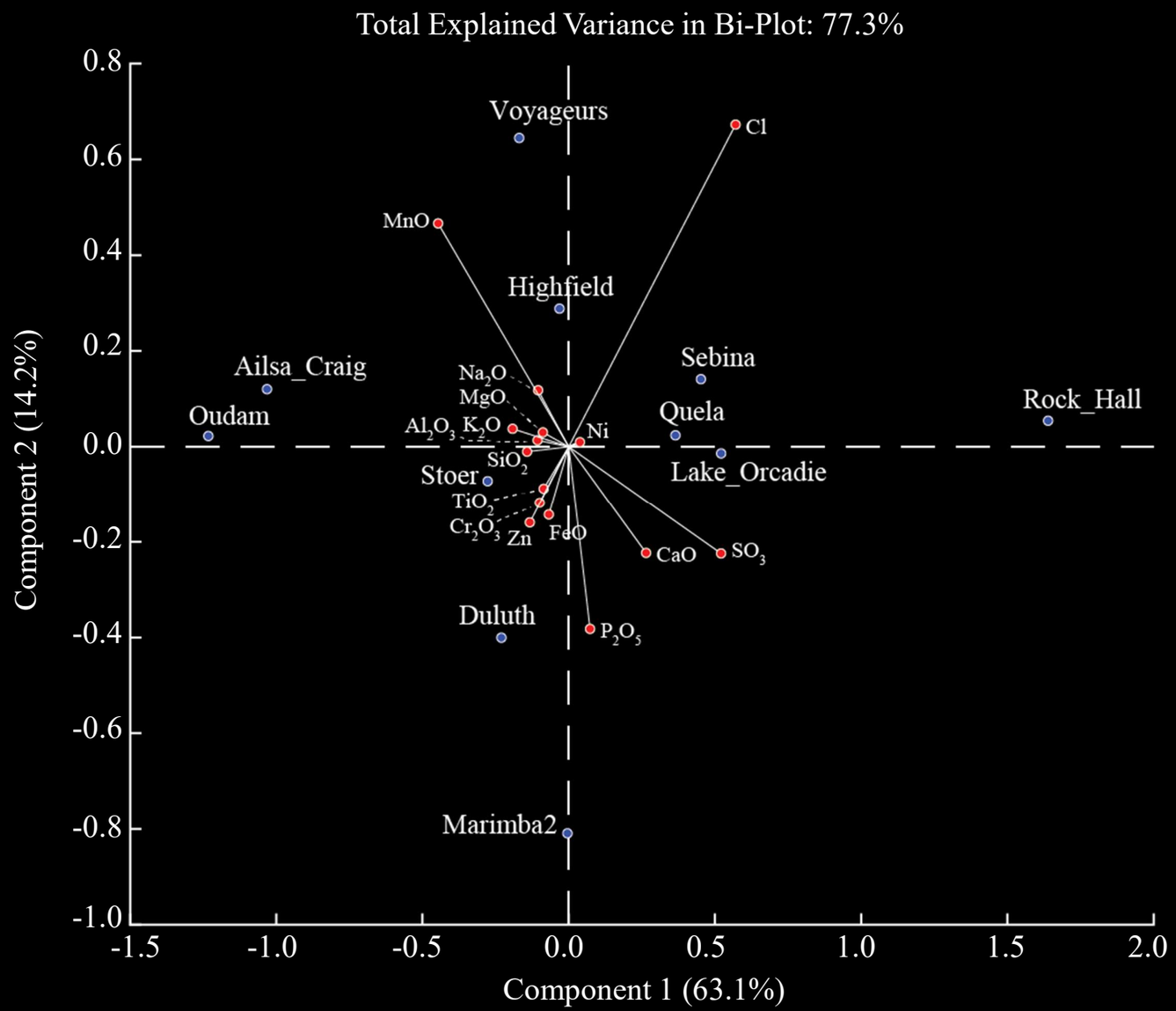
- APXS emulation is also being used to conduct performance testing for possible application on lunar missions, without the need for special laboratory equipment and lunar samples

More info: VanBommel et al., 2019, Acta Astronaut., 165, 32-42.

APXS Analytical Techniques: PCA

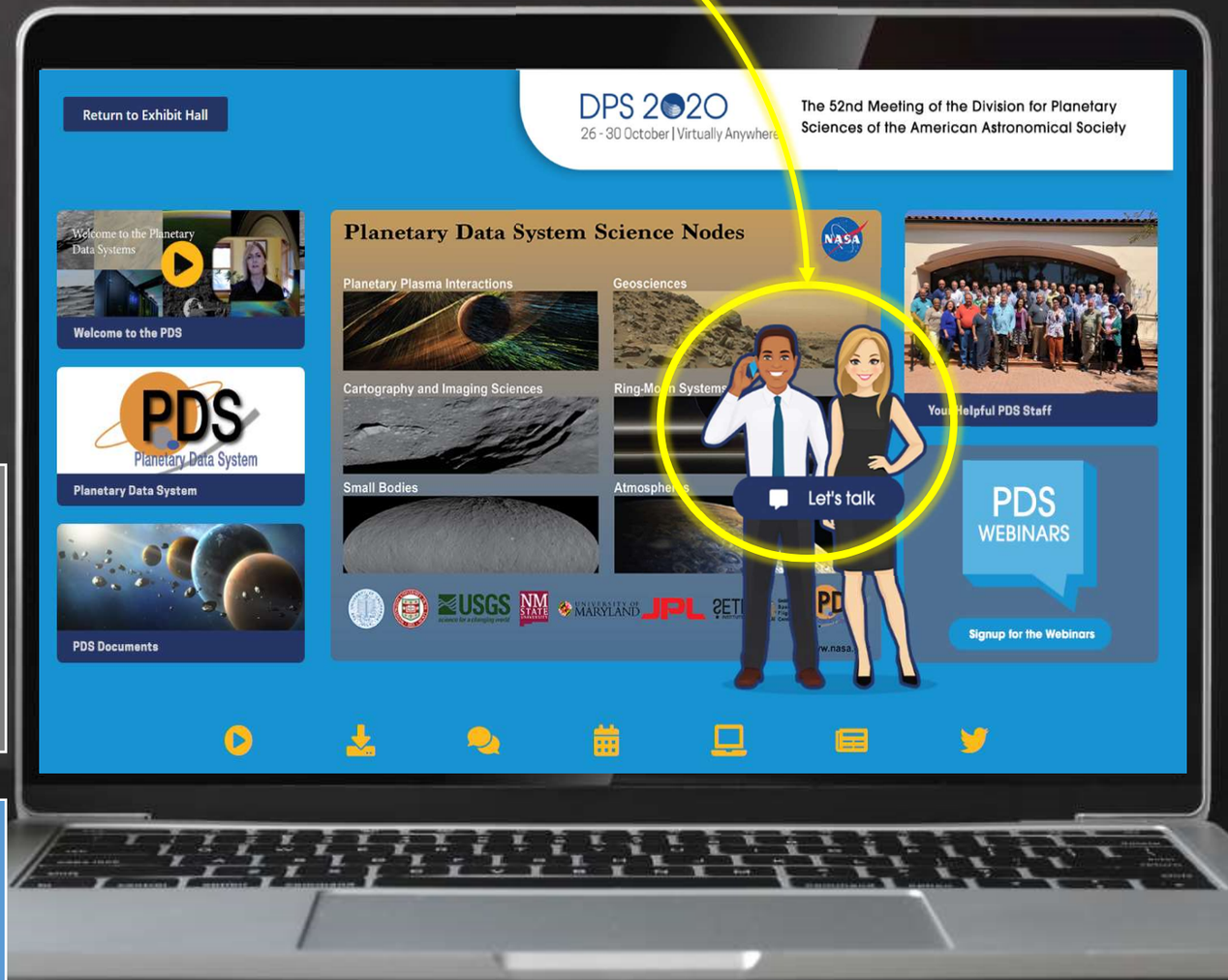


APXS Analytical Techniques: PCA



- PCA analysis follows work by J. Aitchison and corrects for closed-number artifacts
- Quick and convenient way to review multivariate data

To enter a tutorial session, click on “Let’s talk” at the **PDS Exhibitor Booth** at the DPS web site.



Webinars

Introduction to PDS Geosciences Node Data Sets and Analysis Tools
Monday, October 26
12:00 to 12:30 PM EDT

Introduction to PDS Geosciences Node Orbital Data Explorers and Landed Mission Analyst Notebooks
Wednesday, October 28
2:00 to 2:30 PM EDT

Tutorials

MRO CRISM Hyperspectral Data Sets and Analysis Tools
Monday, October 26
2:30 to 3:30 PM EDT

Mars Rover In Situ X-ray Compositional Data Sets and Analysis Tools
Tuesday, October 27
3:00 to 4:00 PM EDT

Content and Use of PDS Geosciences Node Orbital Data Explorers
Wednesday, October 28
4:00 to 5:00 PM EDT

Content and Use of PDS Geosciences Node Landed Mission Analyst Notebooks
Thursday, October 29
3:00 to 4:00 PM EDT