# 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







#### Webinars

To enter a tutorial session, click on "Let's talk" at

the **PDS Exhibitor Booth** at the DPS web site.

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



MER Contact Science Target List: https://pds-geosciences.wustl.edu/mer/urn-nasa-pds-mer\_cs\_target\_list/



MER Contact Science Target List: https://pds-geosciences.wustl.edu/mer/urn-nasa-pds-mer\_cs\_target\_list/

+0 00

#### Mission Overview: Curiosity





# Unique APXS Measurements: ~950

MSL APXS Data Supplement (to sol 2301): <u>https://pds-geosciences.wustl.edu/msl/urn-nasa-pds-msl\_apxs\_supplement\_sols\_0\_2301/</u>



1997 – Mars Pathfinder (Sojourner)





2004 – MER (Spirit, Opportunity)





2012 – MSL (*Curiosity*)







MER





Specifications

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

Contact Sensor Plate 10 mCi Beryllium-covered <sup>244</sup>Cm (x3) SDD X-ray Detector 10 mCi Ti-foil-covered <sup>244</sup>Cm (x3)





specifications												
18 mm (Contact)												
15 mm ø												
0.7 – 25 keV												
140 eV (FWHM)												
-130°C to -5°C												
5 W (+3 w/Peltier)												

Spacifications





Fe

Ti

Energy (keV)

Λ

Atmosphere and Detector

Window Attenuation

Si

 $K_{\alpha} cps/wt\%$ 











## 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 standoffdependent 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



#### **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



#### APXS Data Considerations: Heterogeneities



### 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<sub>2</sub>O, MgO, Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, P<sub>2</sub>O<sub>5</sub>, SO<sub>3</sub>, Cl, K<sub>2</sub>O, CaO, TiO<sub>2</sub>, Cr<sub>2</sub>O<sub>3</sub>, 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

MSLAPXS Concentration Data Availability (PDS3)

• Curiosity:

https://pds-geosciences.wustl.edu/msl/msl-m-apxs-4\_5-rdr-v1/mslapx\_1xxx/extras/



#### APXS Data: Availability

+ NASA Homepage

+ NASA en Español



NADA

NATIONAL AERONAUTICS

AND SPACE ADM	MINISTRATION + Contact N	ASA
210 00	PDS Geosciences Node Washington University in St. Louis	
HOME DATA AND	SERVICES TOOLS ABOUT US CONTACT US	SITE MAP
Services Services Analyst's Notebook Orbital Data Explorers Spectral Library Virtual Astronaut FTP Access Workshops Geosciences Node Data Mars Venus Mercury Moon Earth Asteroids Radio Science Gravity Models AII Geosciences Data Holdings Help FTP access Help for Data Reviewers Help for Data Reviewers Help for Data Reviewers Help for Poposers About PDS4 About PDS4 About PDS4 Schedueld Maintenance This site may be down on Thursdays between 7:00 and	Down         Does         Does         Contract dos           Mars Exploration Rover Oxide Abundance Data         September 19, 2016. PDS release 49 includes APXS Oxide Abundance data for 0 through 4000, updating the previous delivery from 2012.         This data set contains oxide abundance data derived from the APXS Reduced Dat products acquired by the Alpha Particle X-ray Spectrometers on both MER rovers. provided by Raif Gellert, University of Guelph, and Rudolph Rieder. Max Planck Ins archived by the PDS Geosciences Node.           Download the Archive         mer_apxs_oxide.zip is a zip-compressed 315 KB file containing the complete arc           Direct Access to Archive Contents Online         Root Directory - Start here for access to the entire volume.           AREADME.TXT - Introduction to the archive. WOLDESC.CAT - Description of the volume contents as a PDS catalog obj         DATA Directory - This archive consists of two tables, one for each rover. E is accompanied by a PDS label that defines the table columns. The tables comma-separated-value (CSV) format, viewable in any text editor and suit loading into a spreadsheet program such as Microsoft Excel.           CATALOG Directory - Files in the CATALOG directory are text files contain documentation formatted for reading by humans and by software. The files information about the data set, the instrumentation, references, and personnel involved in archiving the data.set the file CATINFO.TXT for det These files are called catalog files because they are entered into the PDS online searching.	pportunity sols a Record (RDR) The data were titute, and hive. ect. ach table are in able for ning contain ails. Catalog for
Thursdays between / Jou and 9:30 pm Central Time for maintenance.	online searching.  APXS_OXIDE_DS.CAT - MER Oxide Abundance data set descripti ARE1_APXS_INST.CAT_MER2_APXS_INST.CAT_APXS_Instrum descriptions.  MER1_INSTHOST.CAT_MER2_APXS_INST.CAT_APXS_Instrum description.  PERSON.CAT - MER mission description.  PERSON.CAT - References mentioned in the above catalog files.  DOCUMENT Directory - The DOCUMENT directory has notes from the AF Payload Element Lead. These notes contain important caveats regardin of the data. Read these notes contain important caveats regardin of the data. Read these notes contain important caveats regardin of the data. Read these notes contain important caveats regardin of the data. Read these notes contain sing and the and the above contains an material that may be useful but is not required for the understanding of the this archive, the EXTRAS directory contains the original Excel spreadsheet submitted to PDS, which became the basis for the tables in the DATA direc APXS_PDS_541_720_OXIDES_MERAB.XLS-Excel spreadsheet APXS_PDS_541_720_OXIDES_MERAB.XLS-Excel spreadsheet APXS_OXDES_A_1400_2071_B_700_2670_XLS - Excel spreadsheet APXS_OXDES_MERAB SOL4000.XLS - Excel spreadsheet APXS_OXDES_MERAB SOL4000.XLS - Excel spreadsheet	on. ent riptions. <u>19 the use</u> <u>te data.</u> cillary archive. In is as toty TXT.



#### [To Parent Directory]

4/5/2017	10:27	AM	4942	aareadme.txt
4/9/2015	3:06	PM	<dir></dir>	calib
8/28/2013	1:25	PM	<dir></dir>	catalog
7/29/2020	7:21	AM	<dir></dir>	data
2/19/2020	12:07	PM	<dir></dir>	<u>document</u>
7/7/2020	11:02	AM	8832	errata.txt
7/29/2020	7:21	AM	<dir></dir>	extras
7/7/2020	11:46	AM	<dir></dir>	<u>index</u>
1/8/2013	11:35	AM	1642	voldesc.cat

3/11/2019	10:53	AM	2821	extrinfo.txt
2/25/2013	5:07	PM	2572	msl_apxs_activities_sol0000_0089.csv
5/31/2013	12:48	PM	2740	msl apxs activities sol0090 0179.cs
8/9/2013	1:54	PM	1187	msl_apxs_activities_sol0180_0269.csv
12/6/2013	9:07	PM	1683	msl apxs activities sol0270 0359.csv
2/27/2014	2:19	PM	1820	msl_apxs_activities_sol0360_0449.csv
6/12/2014	12:13	PM	2865	msl apxs activities sol0450 0583.csv
10/28/2014	8:27	AM	2888	msl_apxs_activities_sol0584_0707.csv
2/17/2015	2:39	PM	2301	msl apxs activities sol0708 0804.csv
7/6/2015	2:24	PM	6974	msl_apxs_activities_sol0805_0938.csv
10/30/2015	12:30	PM	2214	msl apxs activities sol0939 1062.cs
2/16/2016	12:37	PM	3650	msl_apxs_activities_sol1063_1159.csv
6/28/2016	2.21	PM	5572	msl anys activities sol1160 1203 csv

#### + more (and new data every 90 days)



**MSL** 

#### 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 29<sup>th</sup>, 15:00 EDT: Content and Use of PDS Geosciences Node Landed Mission Analyst Notebooks)
  - MER: <u>https://an.rsl.wustl.edu/mer/</u>
  - MSL: <u>https://an.rsl.wustl.edu/msl/</u>

sol	target	start_time	gnorm	sh_tav	g lifetime	Fe_FWHN	/I Na2O N	la2O_er	r MgO N	/lgO_err	r Al2O3 Al	203_err	SiO2	iO2_er	P2O5 P	205_err	SO3 S	503_eri	Cl Cl_err K2O	K2O_er	r CaO	CaO_er	r TiO2 1	iO2_err	Cr2O3 Cr	203_er	r MnO M	nO_er	r FeO	FeO_err	Ni N	Ni_err	Zn Z	n_err	Br B	r_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



### **APXS** Analytical Techniques: Emulation



### **APXS** Analytical Techniques: Emulation



Element	PQL (ppm) by Measurement Condition										
Element	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



#### APXS Analytical Techniques: PCA



25 0

### 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



#### Webinars

To enter a tutorial session, click on "Let's talk" at

the **PDS Exhibitor Booth** at the DPS web site.

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*