

*GRL*

Supporting Information for

## **Recovery of Phosphine in Venus' Atmosphere from SOFIA Observations**

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## **Contents of this file**

Text S1

## **Introduction**

Text S1 contains the shell script used to process the *SOFIA/GREAT* data. Comment lines describe the methods used and include a link to download the software, which is supported by the East Asian Observatory. The script was run in a Linux environment. To run the script, copy the text into a file such as phosphine.sh and then run the command  
>> source phosphine.sh.

## **Text S1.**

```

#!/bin/bash
alias echo "echo > /dev/null"

# command set to generate stacked PH3 J=4-3 spectrum
# from SOFIA/GREAT observations of Nov 2021 - uses Level 1 data
# leading digits of observation numbers are omitted in file-naming

# Level 1 archival ON and OFF spectra were pre-processed, as follows
# for example: in /2021-11-13_GR_F791/r1/040402_..._4G2_PX00_S.fits
# there are 16 files, 8 ON and 8 OFF Venus, identifiable in the headers
# the file formats were first converted to NDF, using e.g.:
#   fits2ndf 040402_001_4G2_PX00_S.fits 040402_001_4G2_PX00_S.sdf
# then to make e.g. the ON average, list the 8 filenames within in="...", in this command:
#   makemos method=mean weights=! in="..." out=402-ON
# to make a cut of only the central 6000 channels, around the PH3 lines, e.g:
#   ndfcopy 402-ON'(5191:11191)' out=402-ON-cut
# (channels are +0.244141 MHz and centre channel is 8191)
# then to find/subtract a smooth trend of background signals, for example:
#   mfittrend fittype=poly order=4 subtract=false 402-ON-cut out=402-ON-base
#   mfittrend fittype=poly order=4 subtract=true 402-ON-cut out=402-ON-resid
# necessary output files: 402-ON-cut, 402-ON-base, 402-OFF-base, 402-OFF-resid (for example)

# start packages (download at https://starlink.eao.hawaii.edu/starlink)
kappa
ccdpack

# OBS 040091

# set PH3 line regions temporarily to bad values
chpix in=91-ON-cut out=temp1 section=""7600:7740"" newval=""Bad""
chpix in=temp1 out=temp2 section=""7768:7908"" newval=""Bad""
chpix in=temp2 out=temp3 section=""8273:8413"" newval=""Bad""
chpix in=temp3 out=91blank section=""9117:9257"" newval=""Bad""

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK (on standard deviation)
maths exp=""ia-(pa*ib+ic)" ia=91blank ib=91-OFF-resid ic=91-ON-base out=91diff pa=1.056780 | stats 91diff | grep dev

# apply the scaling factor and make residual spectrum (ON-OFF*)
maths exp=""ia-(pa*ib+ic)" ia=91-ON-cut ib=91-OFF-resid ic=91-ON-base pa=1.056780 out=91diffnoblanks

# make linear interpolations across each line component
mfittrend subtract=false order=1 ranges=""7570,7770"" in=91diff out=temp
ndfcopy temp'(7570:7770)' 91inter1
mfittrend subtract=false order=1 ranges=""7738,7938"" in=91diff out=temp
ndfcopy temp'(7738:7938)' 91inter2
mfittrend subtract=false order=1 ranges=""8243,8443"" in=91diff out=temp
ndfcopy temp'(8243:8443)' 91inter3
mfittrend subtract=false order=1 ranges=""9087,9287"" in=91diff out=temp
ndfcopy temp'(9087:9287)' 91inter4

# re-combine so the interpolated sections over-write the bad values
makemos method=median weights=! in=""91diff,91inter1,91inter2,91inter3,91inter4"" out=91interpolated

# run the Fourier transform step
# the output is a model spectral baseline
# the Hermitian is cut to retain values above/below 1000 counts <- USER CHOICE

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# 1000 counts is approx. 3 sigma in the Hermitian for all the observations
# the cut is implemented with thresholds 0.001 in (1/spectrum)
# new values in (1/spectrum) are arbitrary high values (-> ~zero in spectrum)
fourier in=91interpolated hermout=91herm
maths exp=1/ia ia=91herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp="1/ia" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=91mod

# subtract the model baseline
# then make the line/continuum spectrum
sub 91diffnoblanks 91mod out=91-adjFT-4G2
maths exp="ia/(ib-ic)" ia=91-adjFT-4G2 ib=91-ON-base ic=91-OFF-base out=91div

# OBS 040093

# all the same steps are repeated
chpix in=93-ON-cut out=temp1 section="7600:7740" newval="Bad"
chpix in=temp1 out=temp2 section="7768:7908" newval="Bad"
chpix in=temp2 out=temp3 section="8273:8413" newval="Bad"
chpix in=temp3 out=93blank section="9117:9257" newval="Bad"

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK
maths exp="ia-(pa*ib+ic)" ia=93blank ib=93-OFF-resid ic=93-ON-base out=93diff pa=1.056202 | stats 93diff | grep dev

maths exp="ia-(pa*ib+ic)" ia=93-ON-cut ib=93-OFF-resid ic=93-ON-base pa=1.056202 out=93diffnoblanks

mfittrend subtract=false order=1 ranges="7570:7770" in=93diff out=temp
ndfcopy temp'(7570:7770)' 93inter1
mfittrend subtract=false order=1 ranges="7738:7938" in=93diff out=temp
ndfcopy temp'(7738:7938)' 93inter2
mfittrend subtract=false order=1 ranges="8243:8443" in=93diff out=temp
ndfcopy temp'(8243:8443)' 93inter3
mfittrend subtract=false order=1 ranges="9087:9287" in=93diff out=temp
ndfcopy temp'(9087:9287)' 93inter4

makemos method=median weights=! in="93diff,93inter1,93inter2,93inter3,93inter4" out=93interpolated

fourier in=93interpolated hermout=93herm
maths exp=1/ia ia=93herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp="1/ia" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=93mod

sub 93diffnoblanks 93mod out=93-adjFT-4G2
maths exp="ia/(ib-ic)" ia=93-adjFT-4G2 ib=93-ON-base ic=93-OFF-base out=93div

# OBS 040095

# all the same steps are repeated
chpix in=95-ON-cut out=temp1 section="7600:7740" newval="Bad"
chpix in=temp1 out=temp2 section="7768:7908" newval="Bad"
chpix in=temp2 out=temp3 section="8273:8413" newval="Bad"
chpix in=temp3 out=95blank section="9117:9257" newval="Bad"

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK
maths exp="ia-(pa*ib+ic)" ia=95blank ib=95-OFF-resid ic=95-ON-base out=95diff pa=1.055950 | stats 95diff | grep dev

maths exp="ia-(pa*ib+ic)" ia=95-ON-cut ib=95-OFF-resid ic=95-ON-base pa=1.055950 out=95diffnoblanks

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mfittrend subtract=false order=1 ranges=""7570,7770"" in=95diff out=temp
ndfcopy temp'(7570:7770)' 95inter1
mfittrend subtract=false order=1 ranges=""7738,7938"" in=95diff out=temp
ndfcopy temp'(7738:7938)' 95inter2
mfittrend subtract=false order=1 ranges=""8243,8443"" in=95diff out=temp
ndfcopy temp'(8243:8443)' 95inter3
mfittrend subtract=false order=1 ranges=""9087,9287"" in=95diff out=temp
ndfcopy temp'(9087:9287)' 95inter4

makemos method=median weights=! in=""95diff,95inter1,95inter2,95inter3,95inter4"" out=95interpolated

fourier in=95interpolated hermout=95herm
maths exp=1/ia ia=95herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp=""1/ia"" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=95mod

sub 95diffnoblanks 95mod out=95-adjFT-4G2
maths exp=""ia/(ib-ic)"" ia=95-adjFT-4G2 ib=95-ON-base ic=95-OFF-base out=95div

# OBS 040220

# all the same steps are repeated
chpix in=220-ON-cut out=temp1 section=""7595:7735"" newval=""Bad""
chpix in=temp1 out=temp2 section=""7763:7903"" newval=""Bad""
chpix in=temp2 out=temp3 section=""8268:8408"" newval=""Bad""
chpix in=temp3 out=220blank section=""9112:9252"" newval=""Bad""

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK
maths exp=""ia-(pa*ib+ic)"" ia=220blank ib=220-OFF-resid ic=220-ON-base out=220diff pa=1.043051 | stats 220diff | grep dev

maths exp=""ia-(pa*ib+ic)"" ia=220-ON-cut ib=220-OFF-resid ic=220-ON-base pa=1.043051 out=220diffnoblanks

mfittrend subtract=false order=1 ranges=""7565,7765"" in=220diff out=temp
ndfcopy temp'(7565:7765)' 220inter1
mfittrend subtract=false order=1 ranges=""7733,7933"" in=220diff out=temp
ndfcopy temp'(7733:7933)' 220inter2
mfittrend subtract=false order=1 ranges=""8238,8438"" in=220diff out=temp
ndfcopy temp'(8238:8438)' 220inter3
mfittrend subtract=false order=1 ranges=""9082,9282"" in=220diff out=temp
ndfcopy temp'(9082:9282)' 220inter4

makemos method=median weights=! in=""220diff,220inter1,220inter2,220inter3,220inter4"" out=220interpolated

fourier in=220interpolated hermout=220herm
maths exp=1/ia ia=220herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp=""1/ia"" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=220mod

sub 220diffnoblanks 220mod out=220-adjFT-4G2
maths exp=""ia/(ib-ic)"" ia=220-adjFT-4G2 ib=220-ON-base ic=220-OFF-base out=220div

# OBS 040235

# all the same steps are repeated
chpix in=235-ON-cut out=temp1 section=""7595:7735"" newval=""Bad""

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chpix in=temp1 out=temp2 section=""7763:7903"" newval=""Bad""
chpix in=temp2 out=temp3 section=""8268:8408"" newval=""Bad""
chpix in=temp3 out=235blank section=""9112:9252"" newval=""Bad""

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK
maths exp=""ia-(pa*ib+ic)" ia=235blank ib=235-OFF-resid ic=235-ON-base out=235diff pa=1.049978 | stats 235diff | grep dev

maths exp=""ia-(pa*ib+ic)" ia=235-ON-cut ib=235-OFF-resid ic=235-ON-base pa=1.049978 out=235diffnoblanks

mfittrend subtract=false order=1 ranges=""7565,7765"" in=235diff out=temp
ndfcopy temp'(7565:7765)' 235inter1
mfittrend subtract=false order=1 ranges=""7733,7933"" in=235diff out=temp
ndfcopy temp'(7733:7933)' 235inter2
mfittrend subtract=false order=1 ranges=""8238,8438"" in=235diff out=temp
ndfcopy temp'(8238:8438)' 235inter3
mfittrend subtract=false order=1 ranges=""9082,9282"" in=235diff out=temp
ndfcopy temp'(9082:9282)' 235inter4

makemos method=median weights=! in=""235diff,235inter1,235inter2,235inter3,235inter4"" out=235interpolated

fourier in=235interpolated hermout=235herm
maths exp=1/ia ia=235herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp=""1/ia" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=235mod

sub 235diffnoblanks 235mod out=235-adjFT-4G2
maths exp=""ia/(ib-ic)" ia=235-adjFT-4G2 ib=235-ON-base ic=235-OFF-base out=235div

# OBS 040402

# all the same steps are repeated
chpix in=402-ON-cut out=temp1 section=""7584:7724"" newval=""Bad""
chpix in=temp1 out=temp2 section=""7752:7892"" newval=""Bad""
chpix in=temp2 out=temp3 section=""8257:8397"" newval=""Bad""
chpix in=temp3 out=402blank section=""9101:9241"" newval=""Bad""

# find + show the residual of (ON - OFF x pa) where pa is scaling factor <- USER CHECK
maths exp=""ia-(pa*ib+ic)" ia=402blank ib=402-OFF-resid ic=402-ON-base out=402diff pa=1.031155 | stats 402diff | grep dev

maths exp=""ia-(pa*ib+ic)" ia=402-ON-cut ib=402-OFF-resid ic=402-ON-base pa=1.031155 out=402diffnoblanks

mfittrend subtract=false order=1 ranges=""7554,7754"" in=402diff out=temp
ndfcopy temp'(7554:7754)' 402inter1
mfittrend subtract=false order=1 ranges=""7722,7922"" in=402diff out=temp
ndfcopy temp'(7722:7922)' 402inter2
mfittrend subtract=false order=1 ranges=""8227,8427"" in=402diff out=temp
ndfcopy temp'(8227:8427)' 402inter3
mfittrend subtract=false order=1 ranges=""9071,9271"" in=402diff out=temp
ndfcopy temp'(9071:9271)' 402inter4

makemos method=median weights=! in=""402diff,402inter1,402inter2,402inter3,402inter4"" out=402interpolated

fourier in=402interpolated hermout=402herm
maths exp=1/ia ia=402herm out=inv
thresh inv out=thr thrlo=-1e-3 newlo=-1e8 thrhi=1e-3 newhi=1e8
maths exp=""1/ia" ia=thr out=inv2
fourier inverse=true hermin=inv2 out=402mod

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sub 402diffnoblanks 402mod out=402-adjFT-4G2
maths exp="ia/(ib-ic)" ia=402-adjFT-4G2 ib=402-ON-base ic=402-OFF-base out=402div

# now slide the spectra in channel number to correct to Venus velocity frame
# original frame set was LSR and velocities were given by VFRAME
# use settings from Level 1 headers, noting VFRAME + LSR did not put PH3 at band-centre

# use if prior runs gave similar names for outputs
rm slid*

# slide files with per-flight corrections
slide in=91div out=slid91 abs=-8343
slide in=93div out=slid93 abs=-8343
slide in=95div out=slid95 abs=-8343
slide in=220div out=slid220 abs=-8338
slide in=235div out=slid235 abs=-8338
slide in=402div out=slid402 abs=-8327

# co-add the spectra using weights derived from their standard deviations
# unresolved command-line syntax problem <- INPUT WEIGHTS INTERACTIVELY
# file order (numerical) is 220, 235, 402, 91, 93, 95
# respective inputs for weights: 0.6 (value already within the command) then input 0.6, 0.3, 1, 1, 1
makemos weights=0.6 method=mean usevar=false genvar=true in="slid*" out=aligned

# alternative command to co-add with equal weights
# makemos weights=! method=mean usevar=false genvar=true in="slid*" out=aligned

# make a smaller section (for visual inspection)
ndfcopy in=aligned'(-3052:2764)' out=aligned-trunc

# copy the sections with the 4 (resolved) PH3 components to new files
# the file names refer to frequency offset from the 1067.00003 GHz component
ndfcopy aligned-trunc'(-1123:-223)' out=Comp-164
ndfcopy aligned-trunc'(-955:-55)' out=Comp-123
ndfcopy aligned-trunc'(-450:450)' out=Comp0
ndfcopy aligned-trunc'(394:1294)' out=Comp+206

# slide the 4 components to align in Venus-frame centred on 1067.00003 GHz component
slide Comp-164 out=Comp-164-onzero abs=673
slide Comp-123 out=Comp-123-onzero abs=505
slide Comp0 out=Comp-0-onzero abs=0
slide Comp+206 out=Comp+206-onzero abs=-844

# in the first two sections, set to bad the duplicates of the nearby adjacent component
# for the other sections, just blank one channel, to maintain filename uniformity
chpix in=Comp-164-onzero out=Comp-164-onzero-chpix section=""68:268"" newval=""Bad""
chpix in=Comp-123-onzero out=Comp-123-onzero-chpix section=""-268:-68"" newval=""Bad""
chpix in=Comp-0-onzero out=Comp-0-onzero-chpix section=""-500:-499"" newval=""Bad""
chpix in=Comp+206-onzero out=Comp+206-onzero-chpix section=""499:500"" newval=""Bad""

# co-add the 4 components + write to output file <- USER CHOICE
makemos weights=! method=mean usevar=false genvar=true in="*onzero-chpix.sdf"

```