

Infrared Spectra of Trans-Neptunian Object Ice Analogs

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Issues Identified

- Data quality issues
- Potential documentation issues

Data Quality Examples

13ch3oh_10k_ir_irradiated.csv

```
# Keywords,  
Product Name,FTIR Spectra  
Product Description,IR Spectrum of 13CH3OH irradiated by GCR proxy at 10K  
Start Time,2023-01-15  
Stop Time,2023-01-16  
Target Name,irradiated 13CH3OH ice at 10K  
Target Type,laboratory analog  
Author List,Zhang C.  
Product Processing Level,Derived  
Science Search Facet,"Physical Properties, Neutrals"  
Product Wavelength Ranges,Infrared  
Observing System Bookmark,Keck Laboratory  
# Column Definitions,  
Wavenumbers,Absorbance  
real,real  
1/cm,Intensity  
-9.99,-9.99  
1/cm,Intensity  
# Data,  
4.99E+02,1.98E-03  
5.01E+02,3.38E-03  
5.03E+02,4.39E-03  
5.05E+02,5.31E-03  
5.07E+02,6.27E-03  
5.09E+02,7.26E-03
```

h2s_40k_ir_unirradiated.csv

```
# Keywords,  
File Name,H2S_40K_IR_unirradiated.csv  
Product Name,FTIR Spectra  
Product Description,IR Spectrum of H2S at 40K  
Start Time,2024-02-07  
Stop Time,N/A  
Target Name,Unirradiated H2S ice at 40K  
Target Type,Laboratory analog  
Author List,Zhang C.  
Product Processing Level,Derived  
Science Search Facet,"Physical Properties, Neutrals"  
Product Wavelength Ranges,Infrared  
Observing System Bookmark,Keck Laboratory  
# Column Definitions,  
Wavenumbers,Absorbance  
real,real  
1/cm,Intensity  
-9.99,-9.99  
1/cm,Intensity  
# Data,  
600,-0.00848  
602,-0.0082  
604,-0.00901  
606,-0.00945  
607,-0.00909  
609,-0.00902
```

what do these
numbers represent?

Data Quality Examples

13ch3oh_10k_ir_irradiated.csv

```
5.95E+03,-2.74E-04
5.95E+03,-2.51E-04
5.95E+03,-2.22E-04
5.95E+03,-1.47E-04
5.96E+03,-1.85E-04
5.96E+03,-2.10E-04
5.96E+03,-1.22E-04
5.96E+03,-1.30E-04
5.96E+03,-7.38E-05
5.96E+03,6.48E-05
5.97E+03,-5.04E-05
5.97E+03,-1.19E-04
5.97E+03,-1.72E-05
5.97E+03,1.36E-05
5.97E+03,-1.68E-05
5.98E+03,-6.32E-05
5.98E+03,-3.59E-05
5.98E+03,7.61E-05
5.98E+03,1.20E-04
5.98E+03,6.11E-05
5.99E+03,6.85E-05
5.99E+03,1.46E-04
5.99E+03,9.27E-05
5.99E+03,7.25E-05
5.99E+03,7.25E-05
6.00E+03,1.09E-04
6.00E+03,2.59E-04
6.00E+03,3.40E-04
```

non-unique x values
(excessive rounding?)

h2s_40k_ir_unirradiated.csv

```
5950,0.0136
5950,0.0137
5950,0.0137
5950,0.0137
5960,0.0138
5960,0.0138
5960,0.0139
5960,0.0139
5960,0.0139
5960,0.013
5970,0.0139
5970,0.0139
5970,0.0142
5970,0.0143
5970,0.0141
5980,0.014
5980,0.0141
5980,0.0142
5980,0.0143
5980,0.0143
5990,0.0143
5990,0.0142
5990,0.0142
5990,0.0143
5990,0.0144
6000,0.0144
6000,0.0145
6000,0.0145
```

inconsistent numerical
data formats

Data Quality Examples

13ch4_10k_ir_irradiated.csv

4769.17,6.82E-06
4771.1,4.40E-06
4773.03,-1.84E-05
4774.96,-8.43E-05
4776.89,-2.89E-05
4778.82,2.25E-05
4780.74,4.23E-05
4782.67,5.10E-05
4784.6,7.18E-05
4786.53,8.21E-05
4788.46,7.12E-05
4790.39,1.34E-05
4792.31,-4.58E-06
4794.24,-7.86E-05
4796.17,-1.17E-04
4798.1,-2.00E-05
4800.03,2.98E-05
4801.96,2.02E-05
4803.89,5.74E-05
4805.81,9.18E-06
4807.74,2.58E-05
4809.67,6.55E-05
4811.6,-1.71E-05
4813.53,-7.05E-05
4815.46,-1.84E-04
4817.39,-1.65E-04
4819.31,-2.80E-05
4821.24,7.75E-05

this example has a
reasonable number
of decimals

13co2_40k_ir_unirradiated.csv

5949.32,0.006488446
5951.248,0.006485164
5953.177,0.006481007
5955.105,0.006504893
5957.034,0.006550841
5958.962,0.006543167
5960.891,0.006529
5962.819,0.006580763
5964.748,0.006690111
5966.676,0.006702516
5968.604,0.006643035
5970.533,0.00659553
5972.461,0.006571174
5974.39,0.006576758
5976.318,0.006606717
5978.247,0.006637294
5980.175,0.006720703
5982.104,0.006717052
5984.032,0.006646566
5985.96,0.006682608
5987.889,0.00674719
5989.817,0.00683172
5991.746,0.006891541
5993.674,0.006896853
5995.603,0.006893612
5997.531,0.00689663
5999.46,0.006909631

but this is probably
excessive for the
absorbance

Data Quality Examples

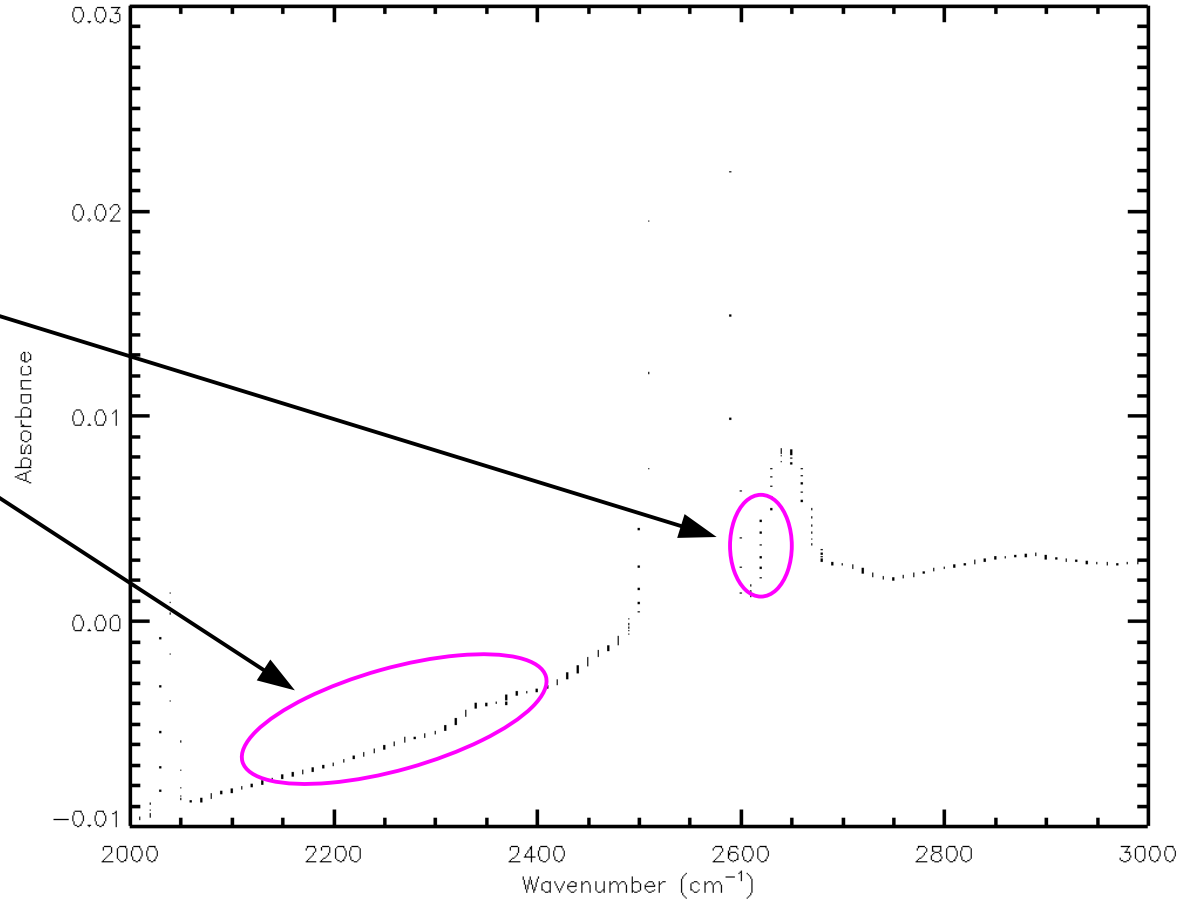
13co2_10k_ir_unirradiated.csv

```
# Keywords,  
File Name,13C02_10K_IR_unirradiated.csv  
Product Name,FTIR Spectra  
Product Description,IR Spectrum of 13C02 irradiated by GCR proxy at 10K  
Start Time,2024-01-04  
Stop Time,N/A  
Target Name,Unirradiated 13C02 ice at 10K  
Target Type,Laboratory analog  
Author List,Zhang C.  
Product Processing Level,Derived  
Science Search Facet,"Physical Properties, Neutrals"  
Product Wavelength Ranges,Infrared  
Observing System Bookmark,Keck Laboratory  
# Column Definitions,  
Wavenumbers,Absorbance  
real,real  
1/cm,Intensity  
-9.99,-9.99  
1/cm,Intensity  
# Data,  
649.8933,0.0287  
651.8218,0.0318  
653.7502,0.043  
655.6787,0.0701  
657.6072,0.0872  
659.5356,0.0512
```

file name says
unirradiated but
1 keyword says
irradiated and 1
says unirradiated

Data Quality Examples

- Non-unique x values
- Negative absorbance values



Potential Documentation Issues

- Numerous details are only provided via the published papers, not in structured files
- No per file information about sample
 - thickness
 - phase/crystallinity
 - radiation dose
 - signal precision
 - spectral resolution
 - saturation
 - continuum removal
 - spectrometer settings
 - etc.