IR spectra of silica (SiO_2) polymorphs

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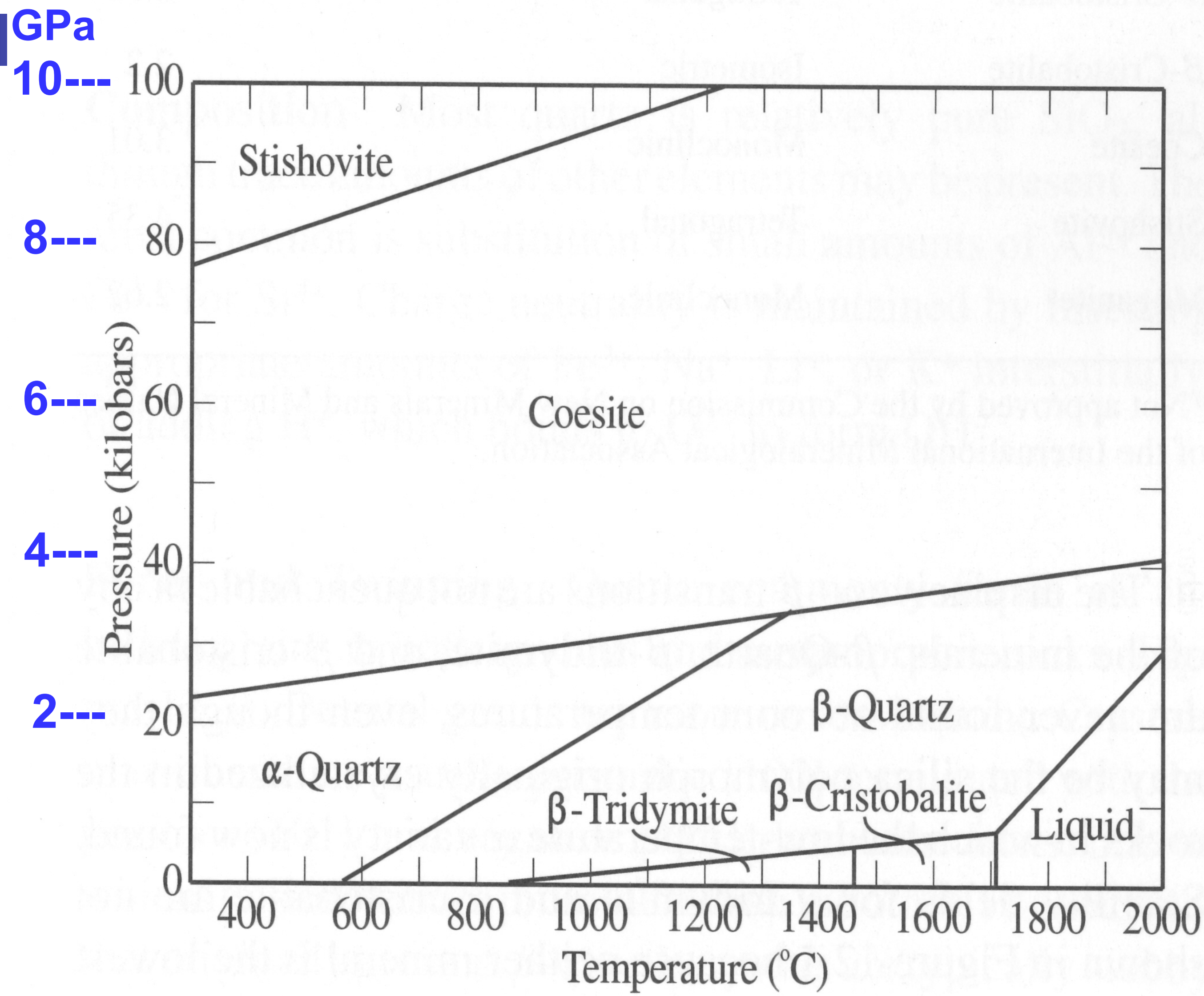
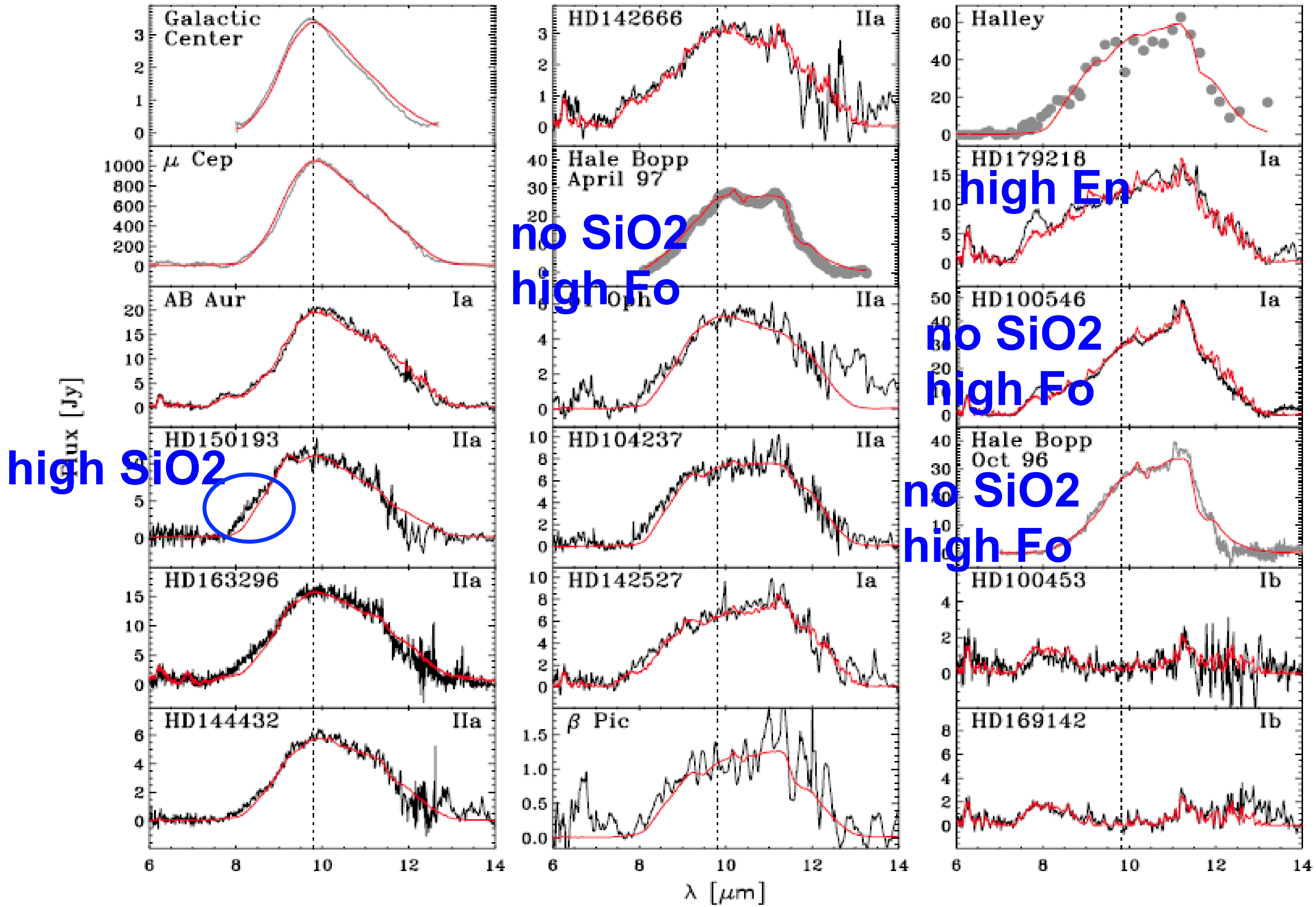


Silica SiO_2

not exactly used in observation

quartz, amorphous SiO_2, annealed SiO_2 (cristobalite)



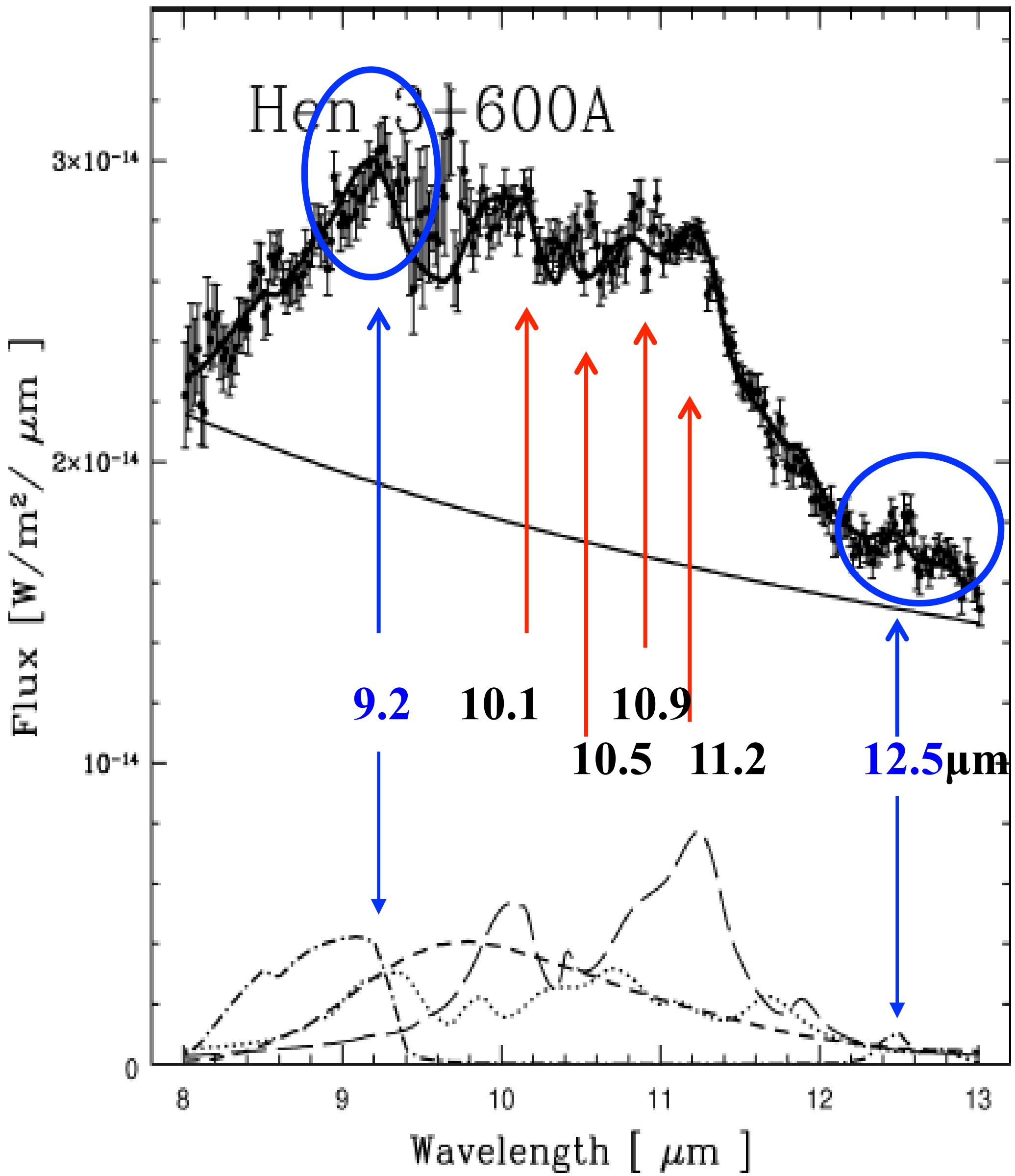
(1)broad shoulder at 8.6um - SiO2 (quartz)

(2)broad peak at 9.8 um - amorphous olivine

(3)peak at 11.3 um - forsterite

young stars

Bouwman et al. 2001



T Tauri star
Hen 3-600A

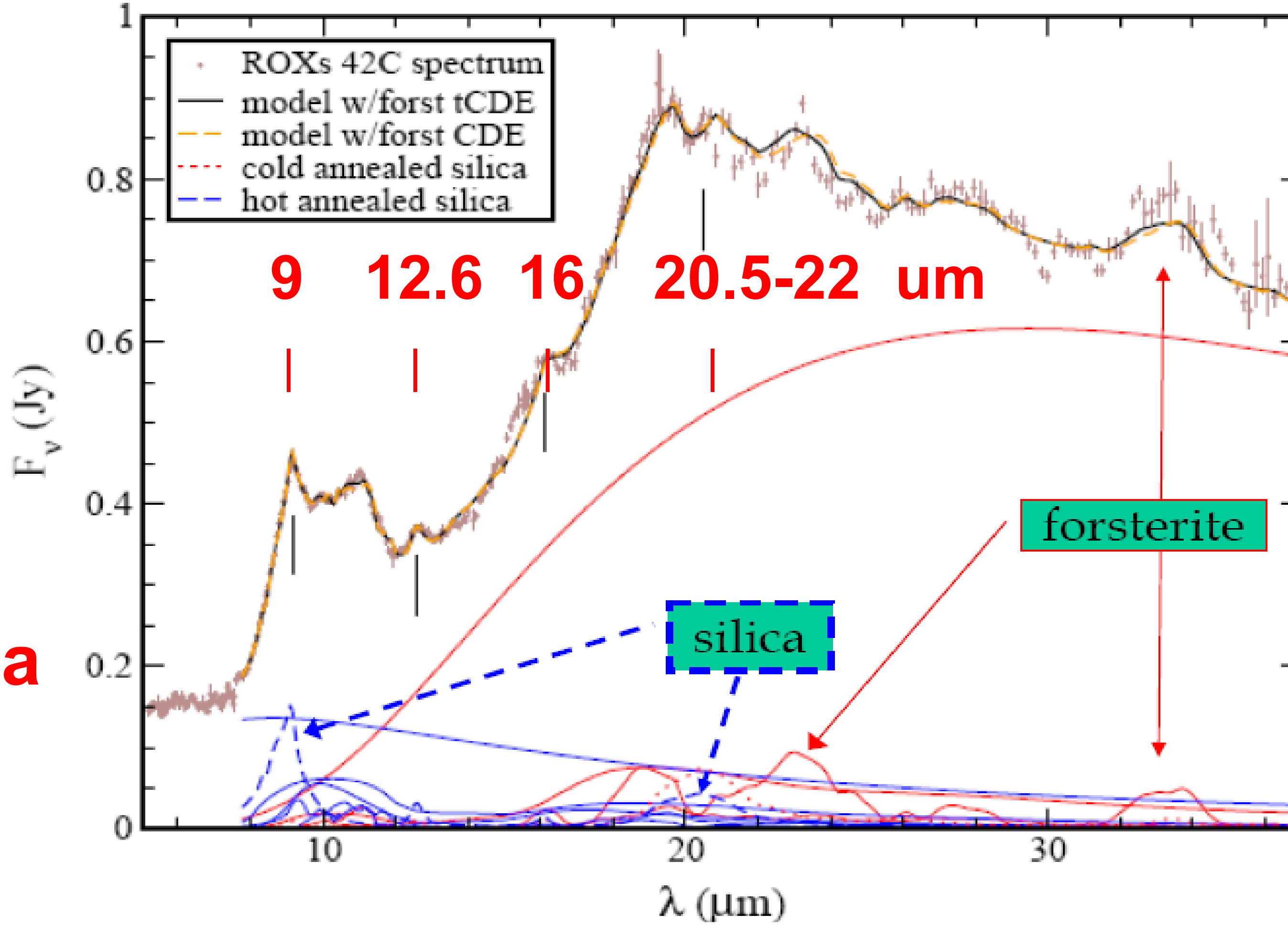
(protoplanetary disk of about solar mass)

Honda et al.
APJ 585, L59 (2003)

forsterite
orthoenstatite
glassy olivine
Silica (quartz)

Protoplanetary disk T Tauri

Sargent et al.
2009, APJ, 690, 1193



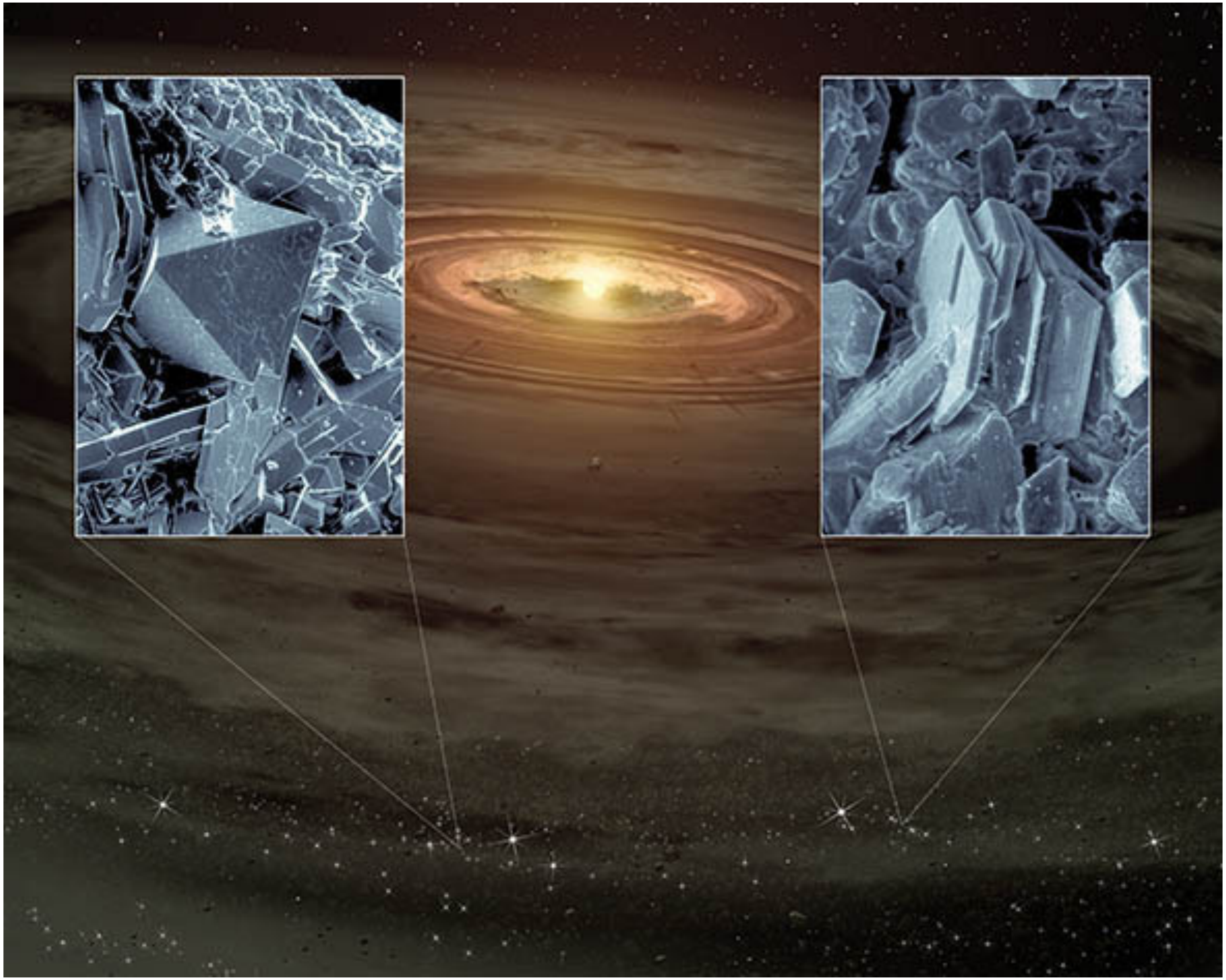
annealed silica
SiO_2

Model fitting
warm dust (1051 K) + cold dust 191 K (K)

annealed silica   + amorphous Silicate   + crystalline silicates (En90, Fo)
9, 12.6, 20.5-22   +   9.8   +   11.2,   16,   23,   33 um
16 um
Size   small and large (>10 um)

Quartz-like Crystals Found in Planetary Disks

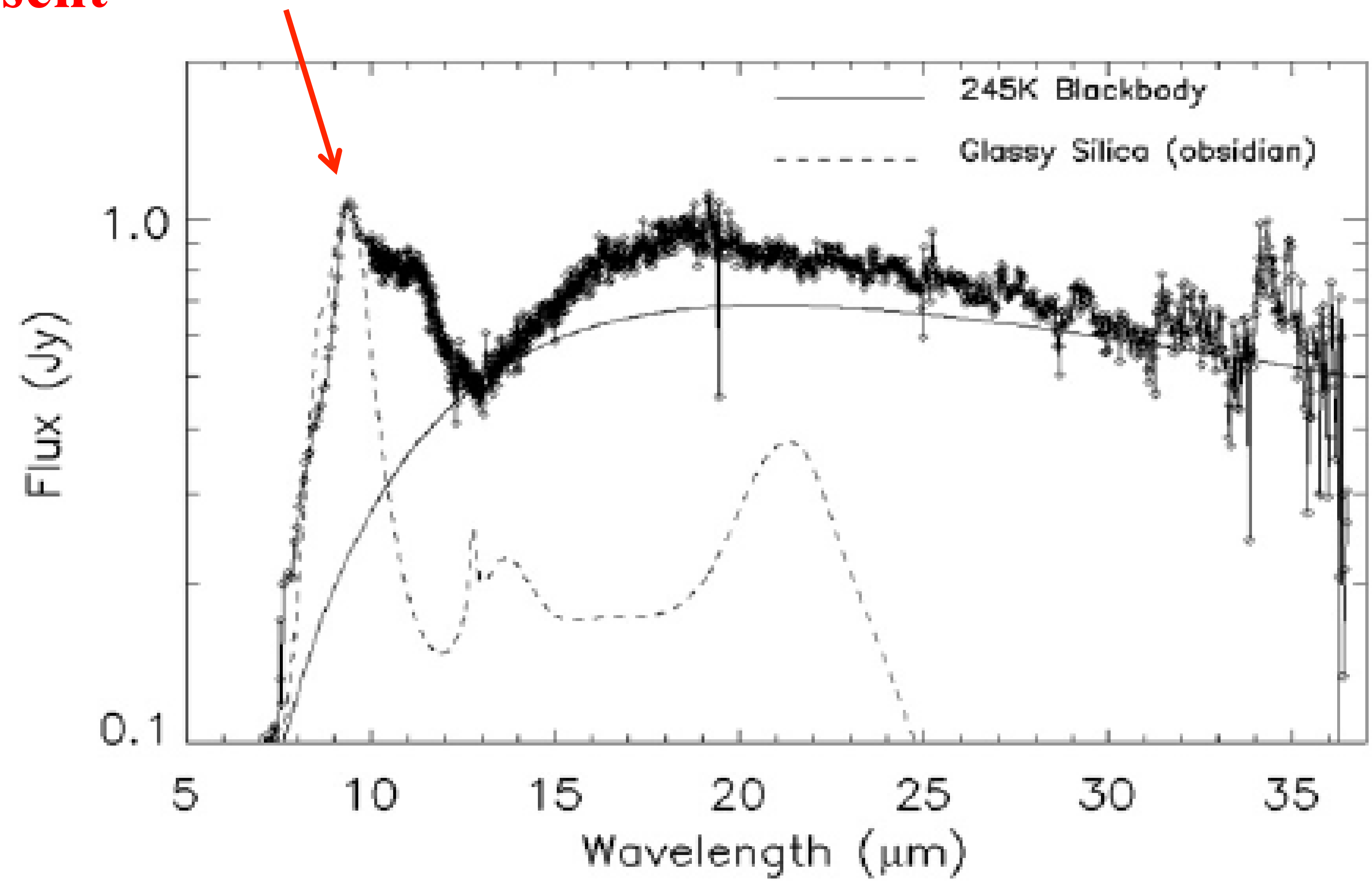
cristobalite



tridymite

(cristobalite is on the left, and tridymite on the right). NASA JPL Spitzer

9.3 μm feature matching amorphous silica (obsidian, tektite) , 12.6 μm absent



HD172555 - debris disk Lisse et al. APJ 701, 2019 (2009)

HD 15407 - debris disk

Peak at
9 μm
20-21 μm
16 μm

Amorphous silicate (px)
9.3-9.7 μm
17-18 μm

Fused quartz SiO2
9 μm
20-21 μm

Fujiwara et al. (GFW2009)

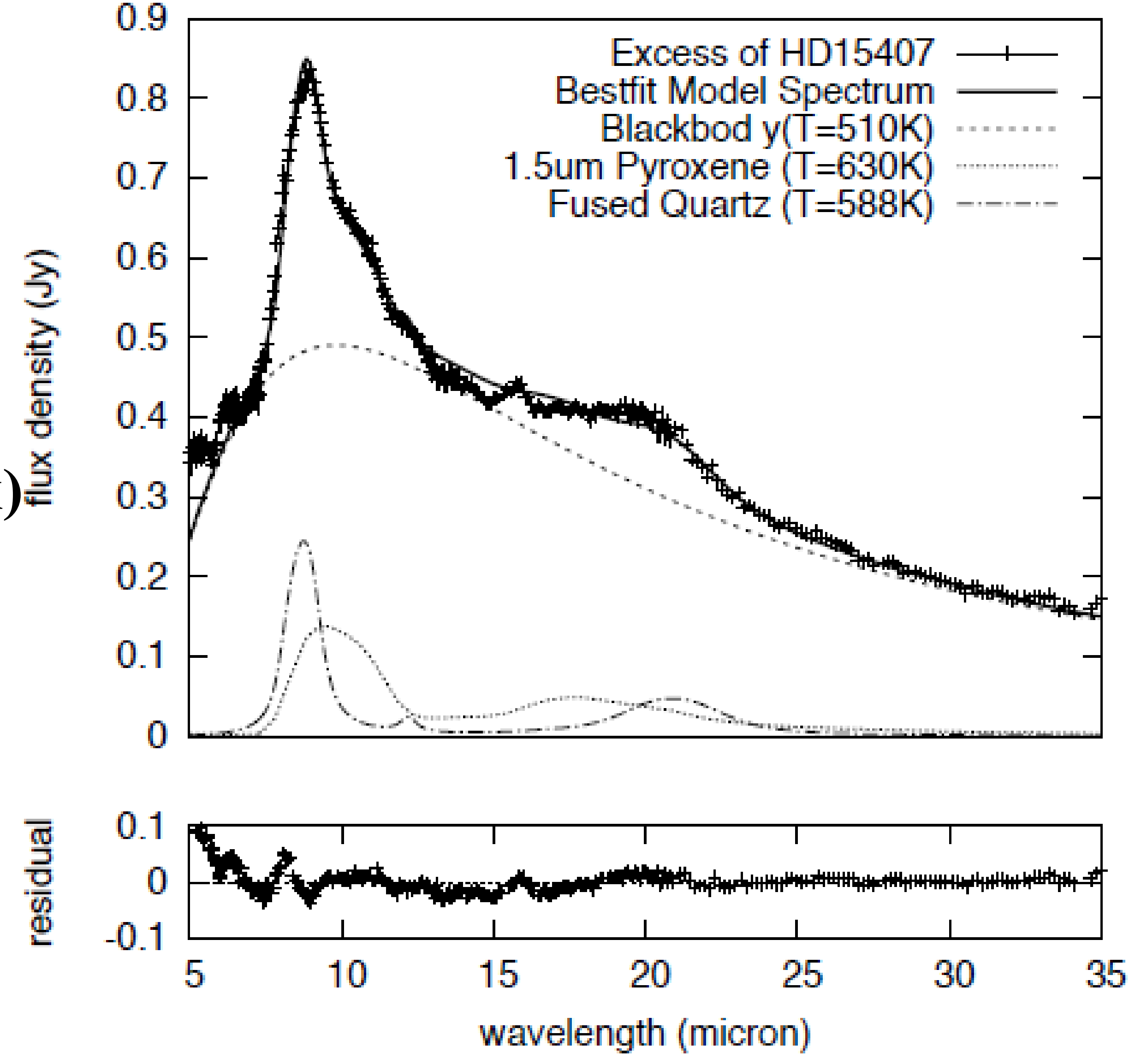
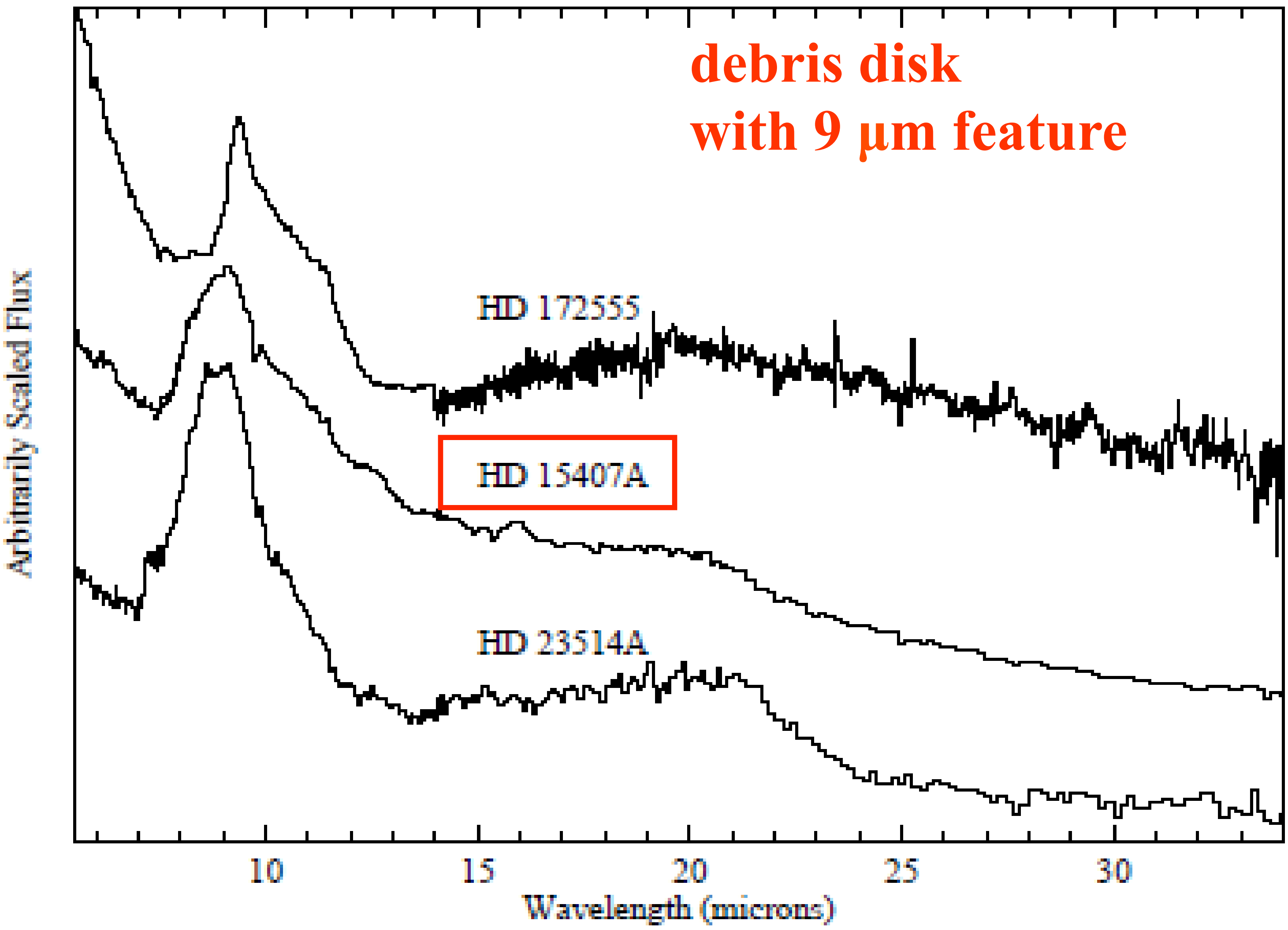
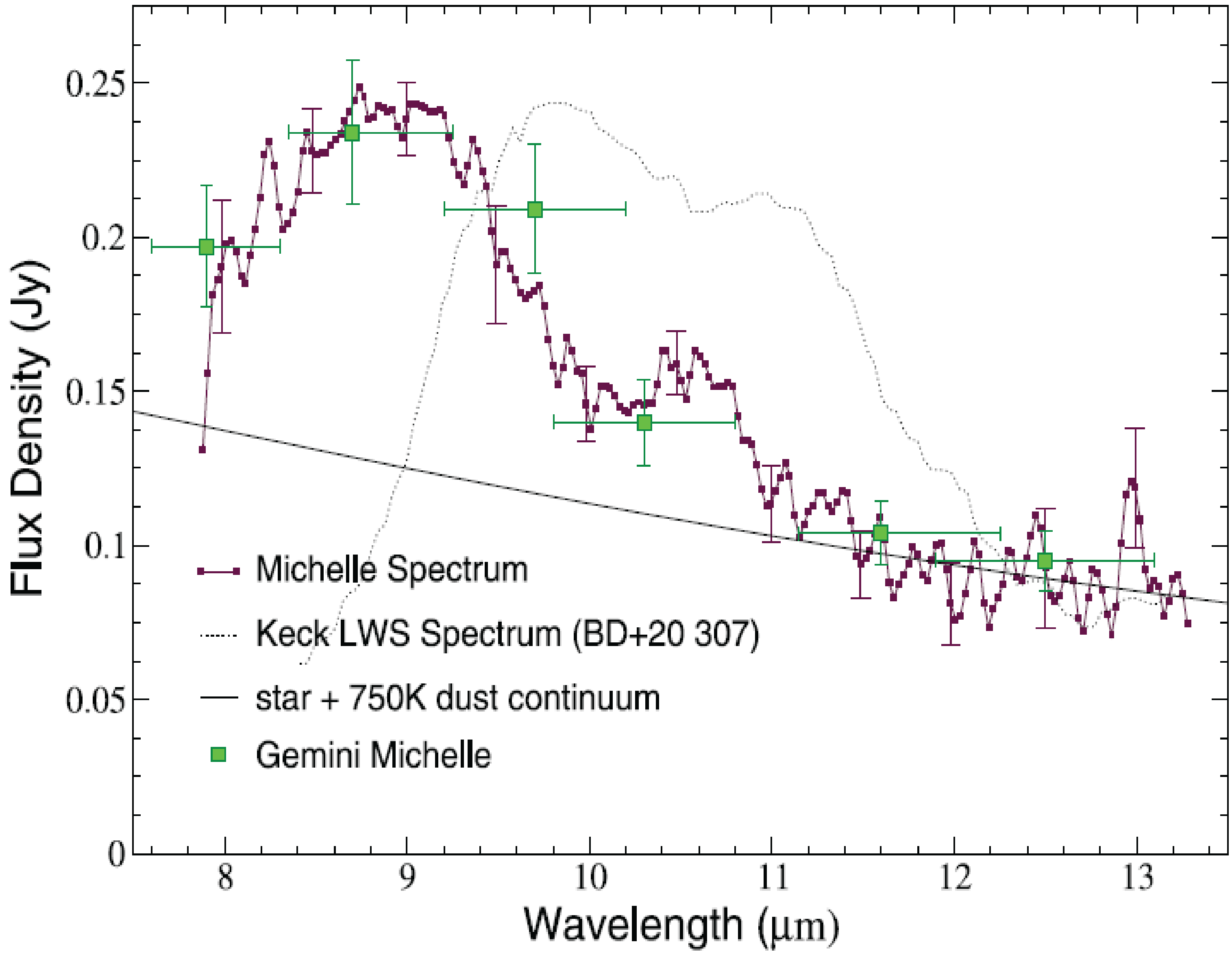


Fig. 1.— *Top*: The IRS spectrum of HD 15407 and the results of SED fitting with a model. *Bottom*: The residuals subtracted by the best-fit spectrum model.



Melis et al. 2010 APJ717, L57



HD 23514 - debris disk
9μm feature

Rhee et al. 2008 APJ675, 777

A shocked lunar meteorite Asuka-881757

Ohtani et al.

PNAS Early Edition, 2010

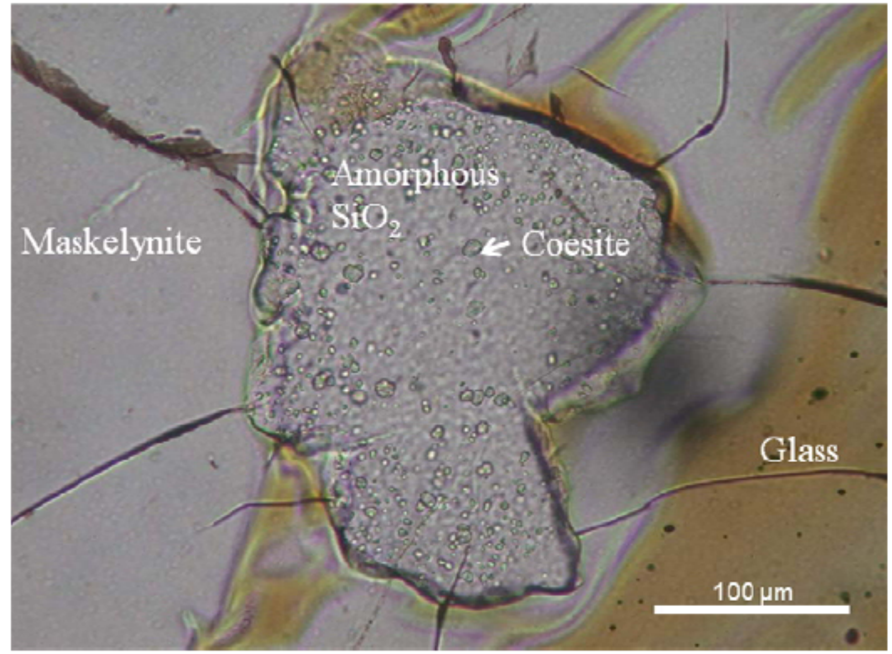


Figure 1. Optical microscopic image of coesite.

coesite **stishovite**

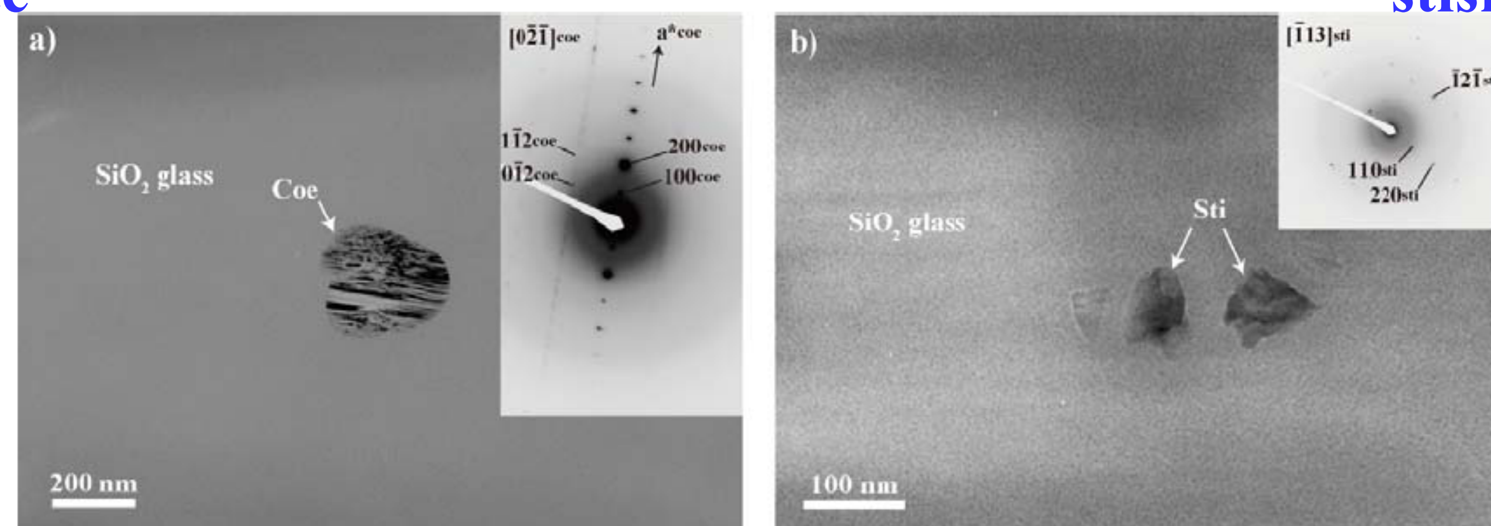


Figure 2. TEM images of a) coesite and b) stishovite.

Sample _silica (SiO_2) polymorphs

→ IR measurements (mir&fir) (KBr&PE) (Nicolet 670)

fused quartz (FQ)

(Koike et al. 1994)

quartz (natural) (fine powder with ball mill)

cristobalite

annealing at high temperature

coesite (by Ohtaka, Osaka University)

FQ 6 GPa、 1300 ℃ 30min

stishovite (by Tani) (2000)

quartz (natural) 13 GPa, 1200 ℃, ?min

Annealing at 1220 K (947 ℃) 4.5 – 5 h

commercial SiO_2 (10-50 nm) (fused quartz)

→ cristobalite, tridymite

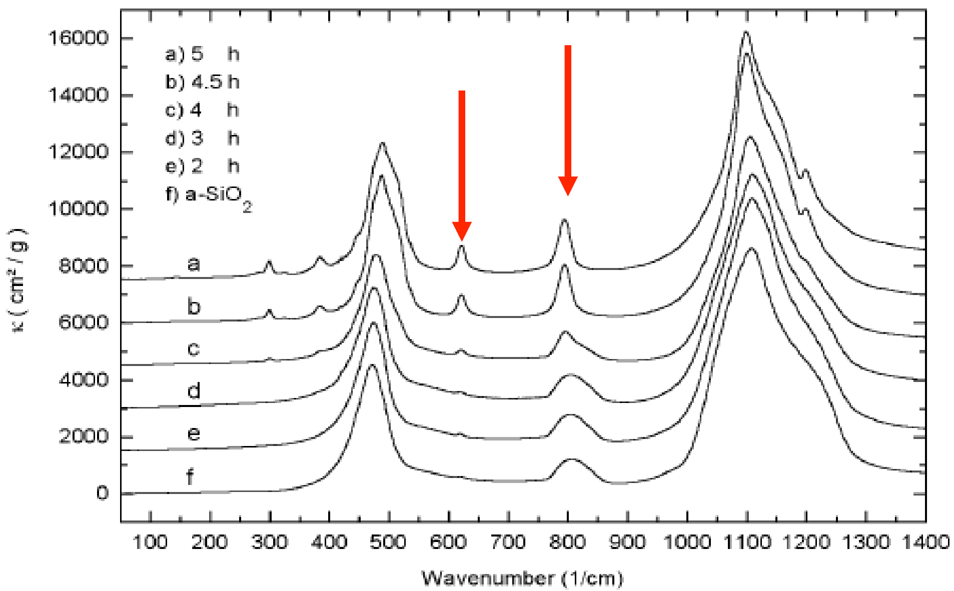


Fig. 12. Evolution of the MIR spectrum of silica that has been annealed at 1220 K. The annealing times are indicated. For clarity, the spectra have been shifted vertically: a, b, c, d, e by +7500, +6000, +4500, +3000, +2500 cm^2/g, respectively. τ has been approximated to 4.5 $\pm$0.5 h.

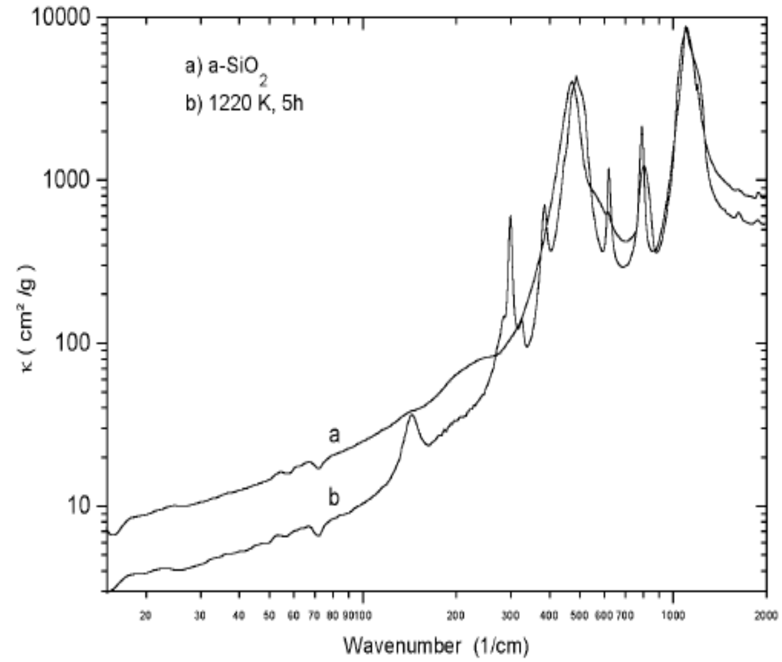


Fig. 13. Comparison of the IR spectrum of amorphous (a) with that of annealed silica (b) (T= 1220 K, 5 h).

astronomers

annealed silica

Fabian et al. 2000 (A&A,364, 282)

Fused quartz annealed at 800 – 1200 ℃

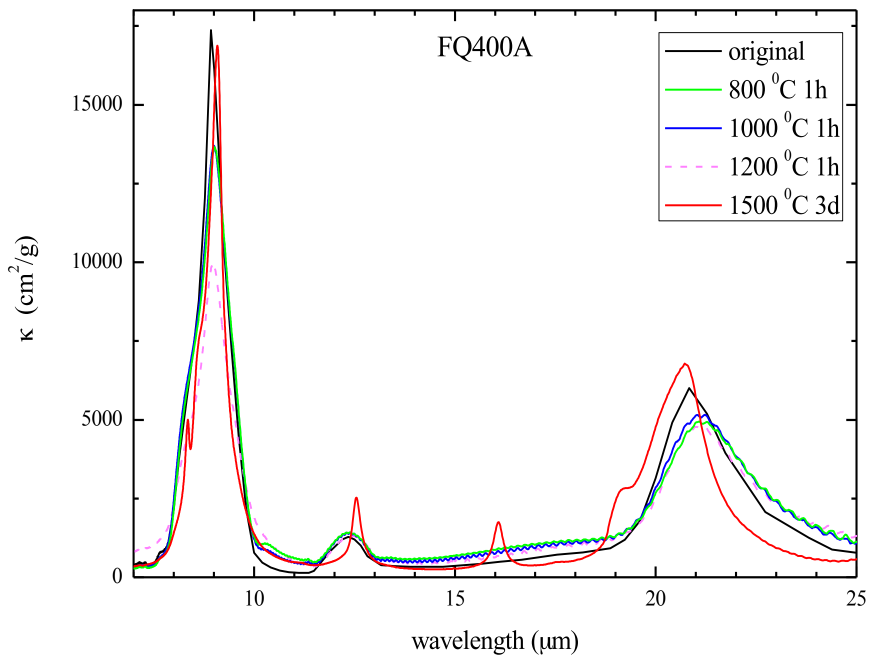
difficult to transform to cristobalite ?

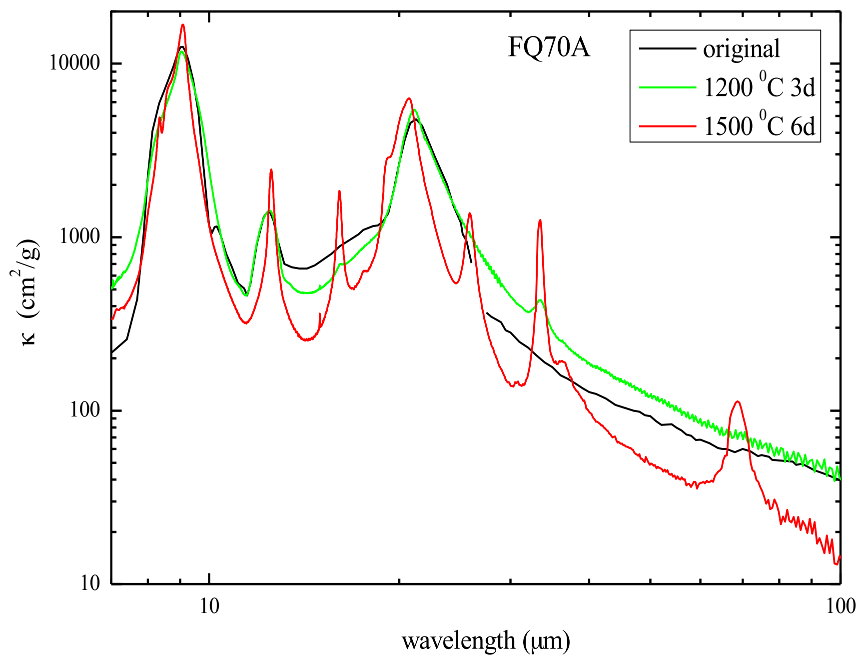
(powder (fused quartz) 947 ℃ 4.5-5h → cristobalite ??????)
(Fabian et al. 2000)

800 ℃ 1h, 1000 ℃ 1h, 5h, 7h 1100 ℃ 48h
1150 ℃ 8d 1200 ℃ 1h, 3d

no change of infrared spectra

Fused quartz annealed at 1500 ℃ 3d, 6d cristobalite





Synthesize of cristobalite > 1400 ℃

vitreous silica (fused quartz) 1400 ℃ ?h → cristobalite
Simon et al. 1953

0.4mm thick fused plate 1452 ℃ 16h → α-cristobalite
Plendl et al. 1967

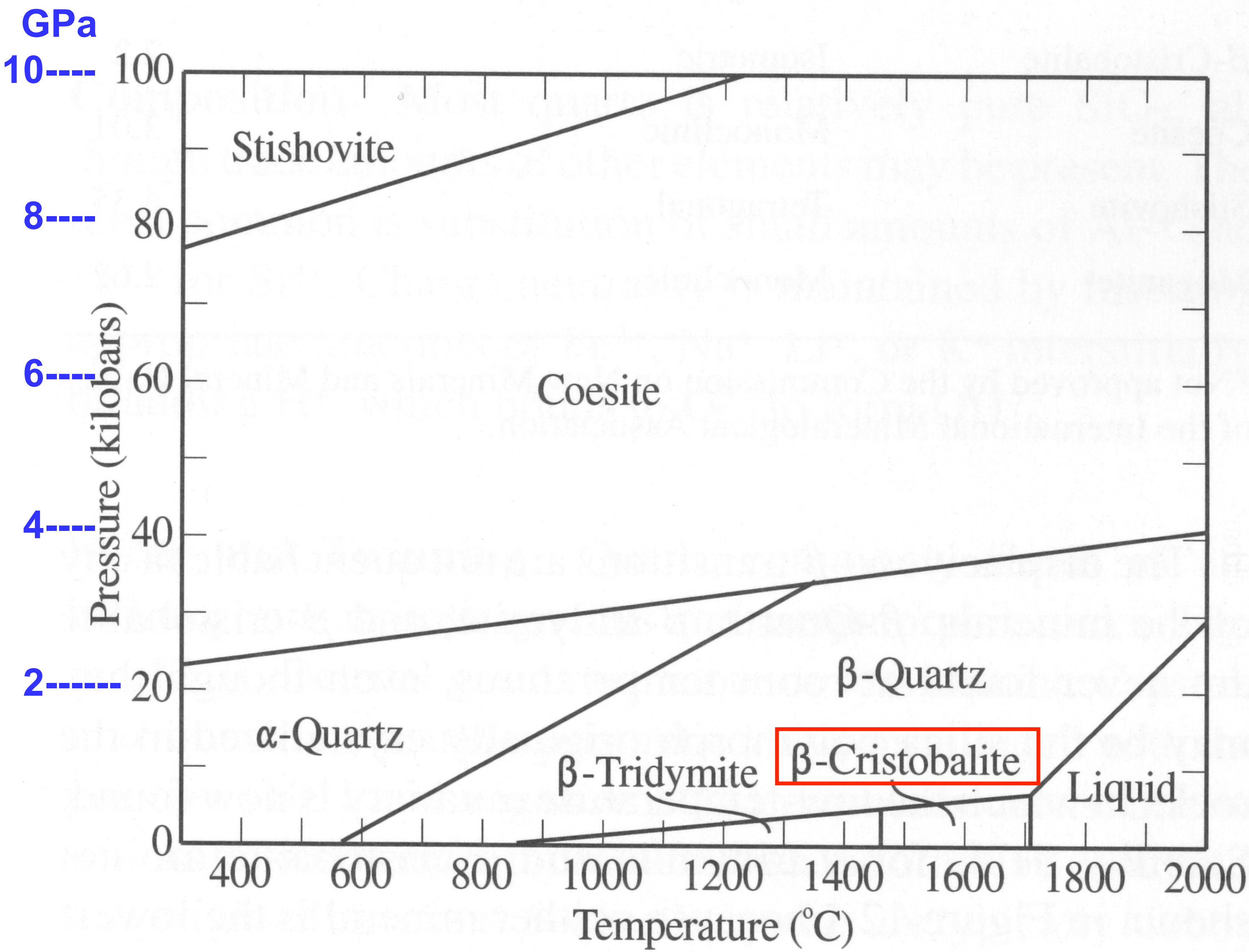
2mm thick slab of vitreous SiO2 1540 ℃ 17h → α -cristobalite
Bates 1972

silica SiO2 1480 ℃ 8h → α -cristobalite
Ocana et al. 1987

Silica glass 1500 ℃3d → α- cristobalite
Swainson et al. 2003

(powder (fused quartz) 947 ℃ 4.5-5h → cristobalite ??????)
(Fabian et al. 2000)

some impurity effects?



GPa
10----
8----
6----
4----
2------
100
80
60
40
20
0
Pressure (kilobars)
Stishovite
Coesite
α-Quartz
β-Quartz
β-Tridymite
β-Cristobalite
Liquid
400
600
800
1000
1200
1400
1600
1800
2000
Temperature (°C)

annealed fused Quartz at 1500 ℃ → change of IR spectra

Fabian et al. 2000

powder (fused quartz) 947 ℃ 4.5-5h → cristobalite, tridymite

easily transformed ?

even at 1200 ℃ not transformed, another effects (impurity) ???

cristobalite

● **Annealing of fused quartz (70A & 400A)**

fused quartz 70 A → 1500 ℃ 6 days cristobalite

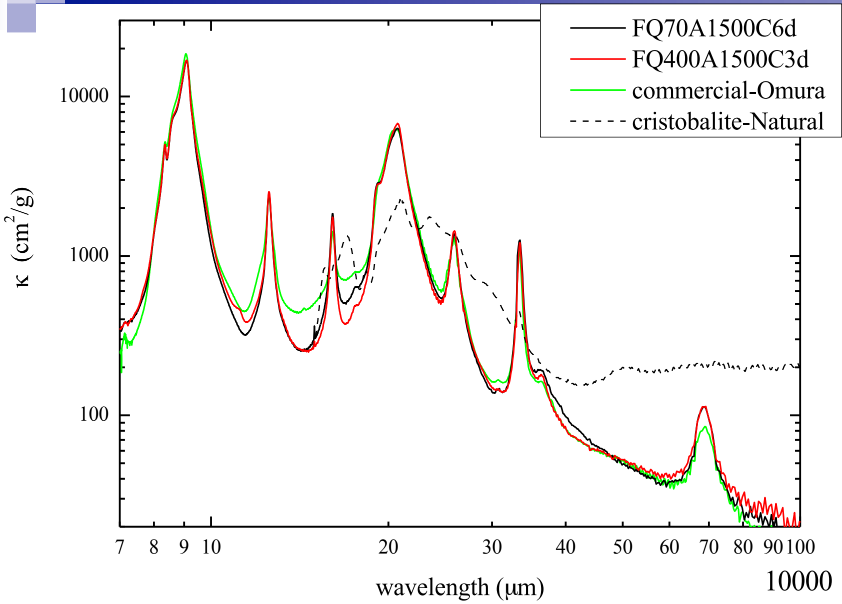
fused quartz 400A → 1500 ℃ 3days cristobalite

• **commercial**

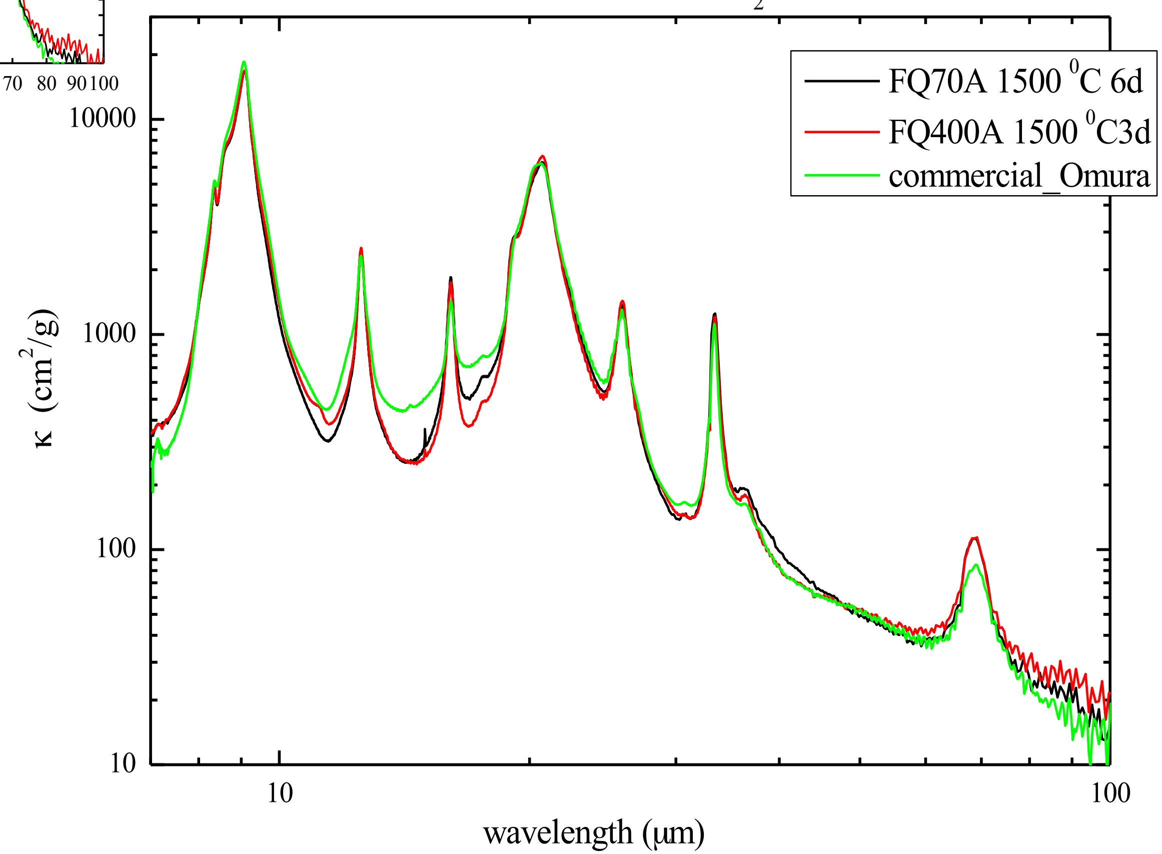
cristobalite Omura (Omura Ceratec Inc.)

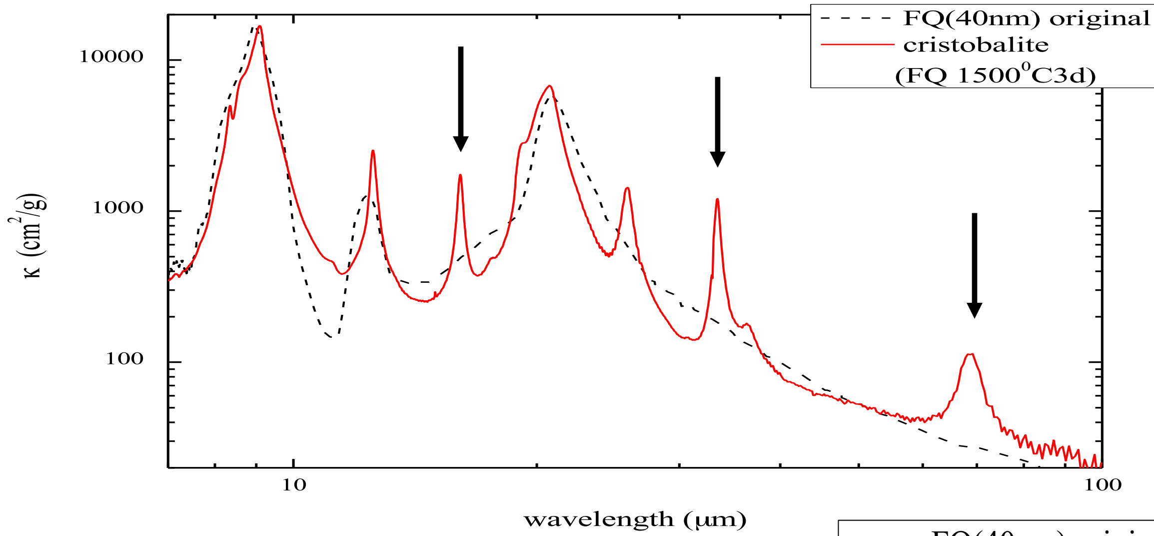
● **natural**

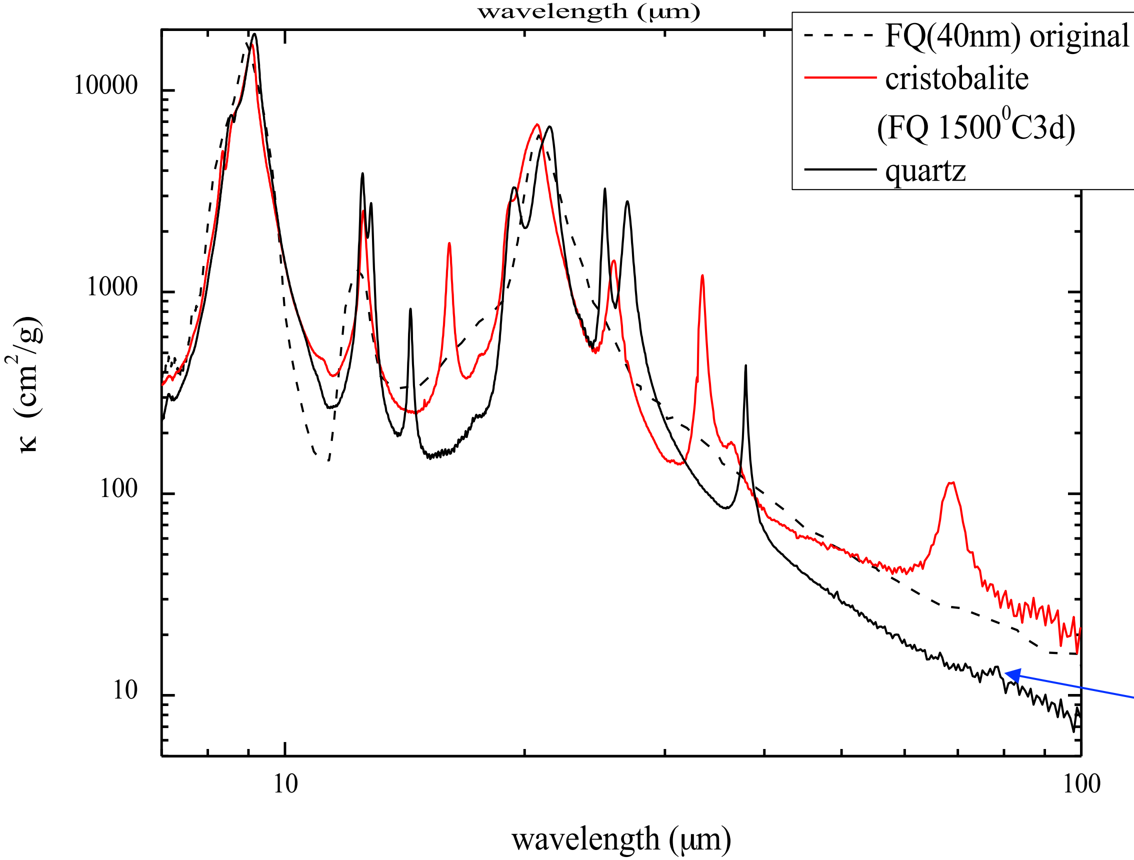
Cougar, Siskiyou Co., California, USA



cristobalite SiO_2







Bulk quartz

Russell et al. 1967

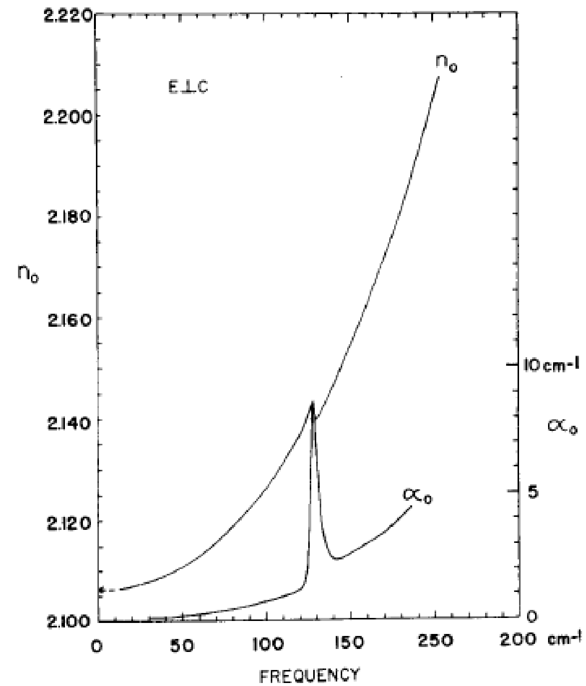
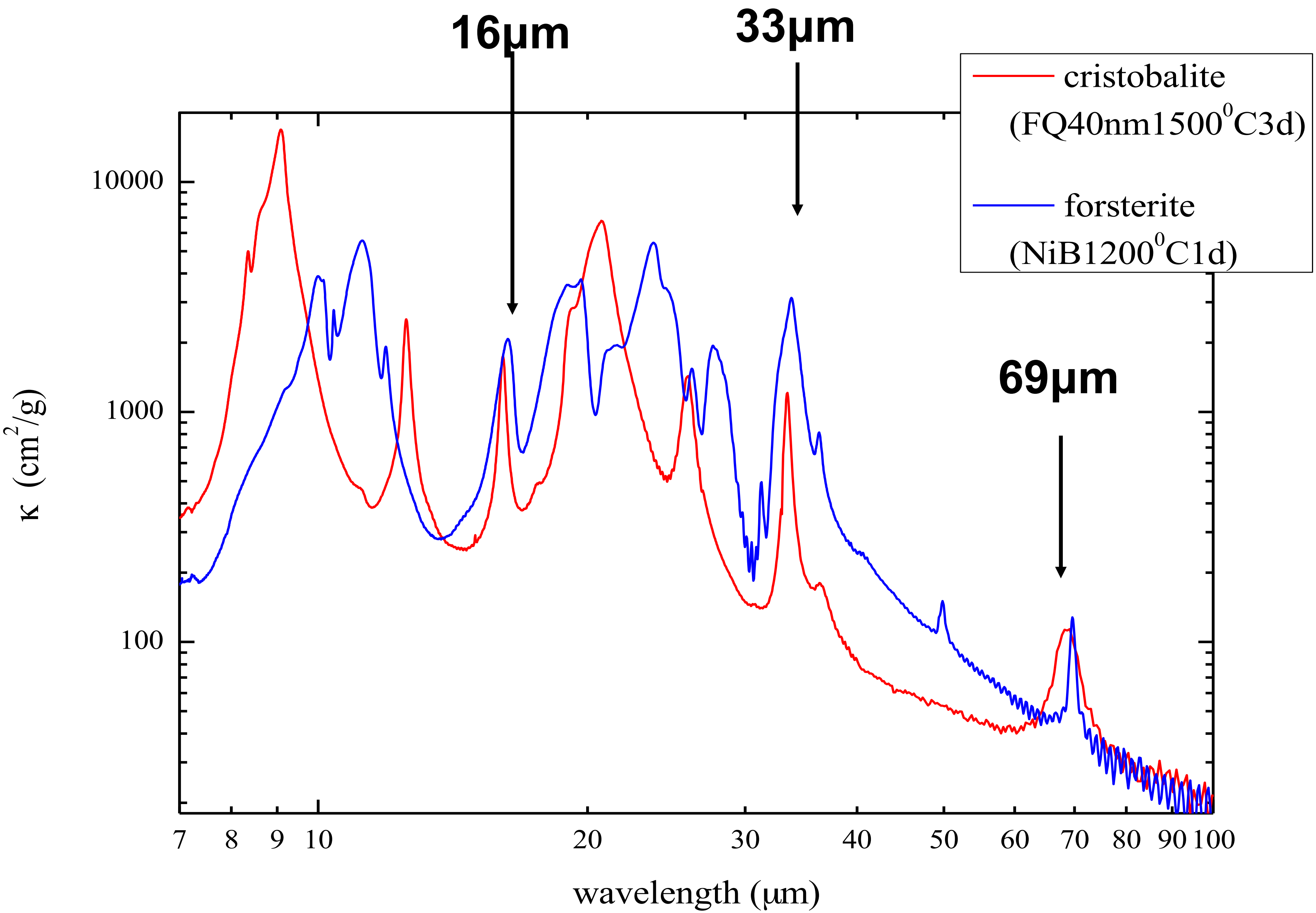


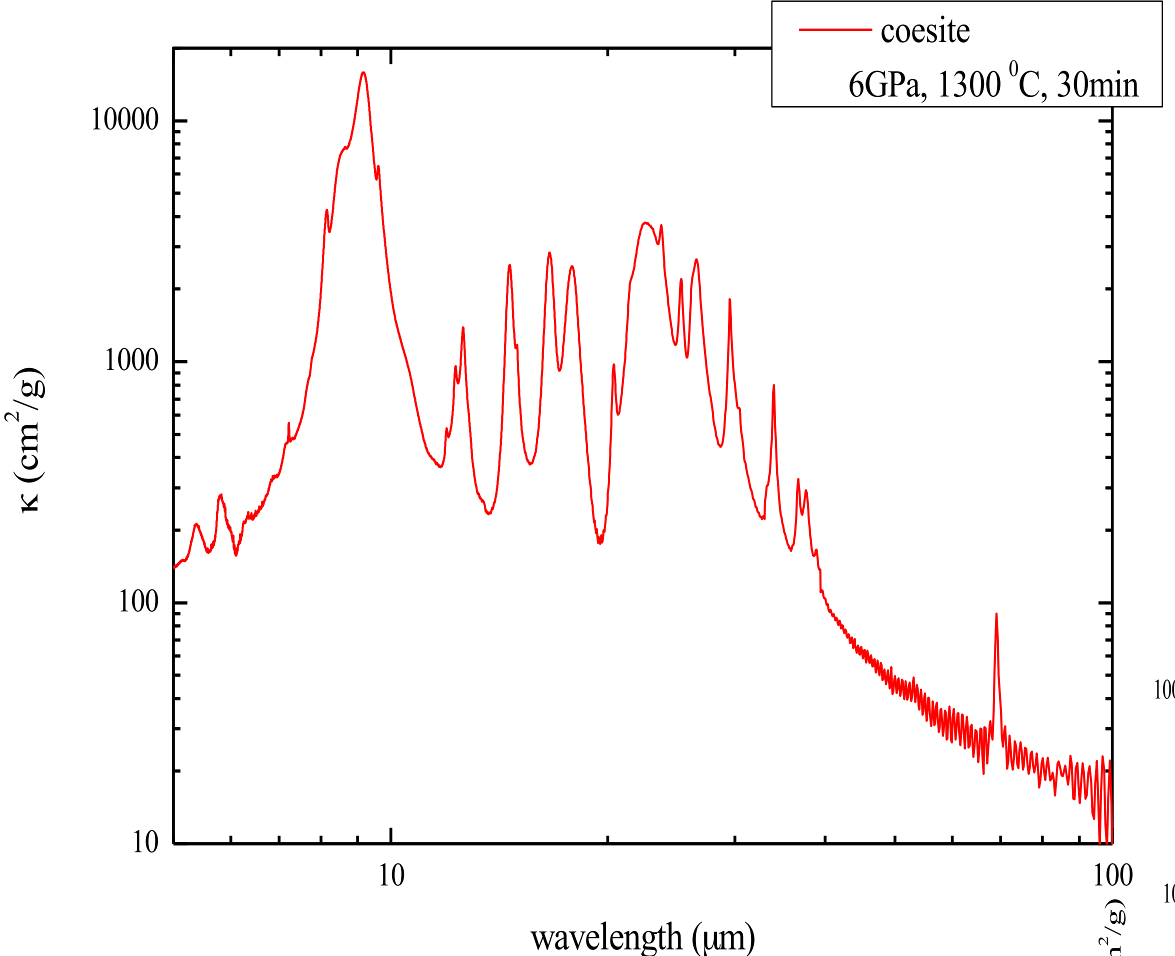
FIG. 2. Ordinary-ray refractive-indices and absorption coefficient of quartz.

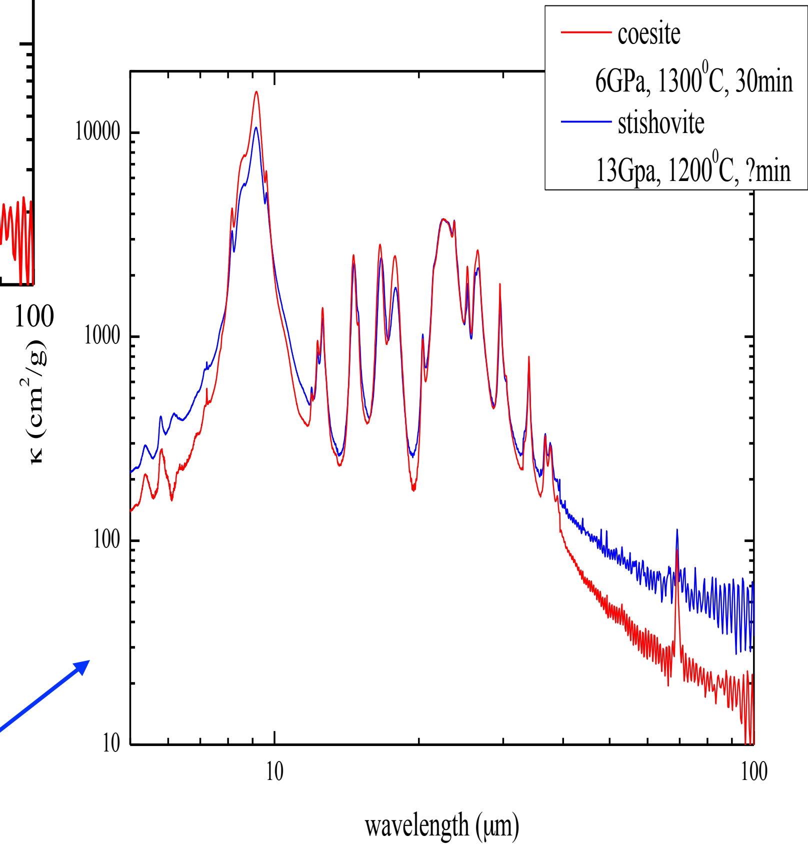
78.12 µm peak

weak peak at 78.3µm

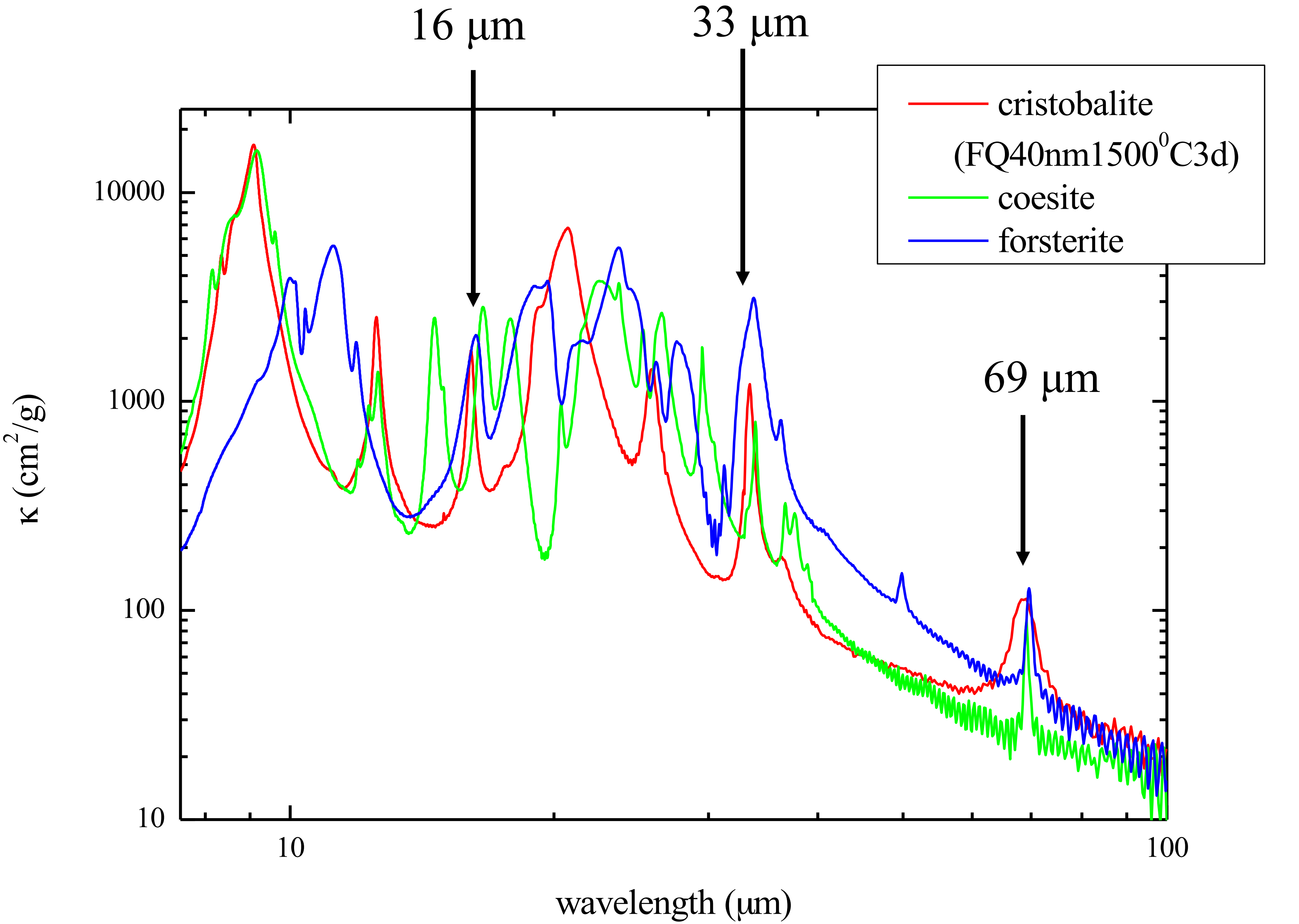
Cristobalite & forsterite



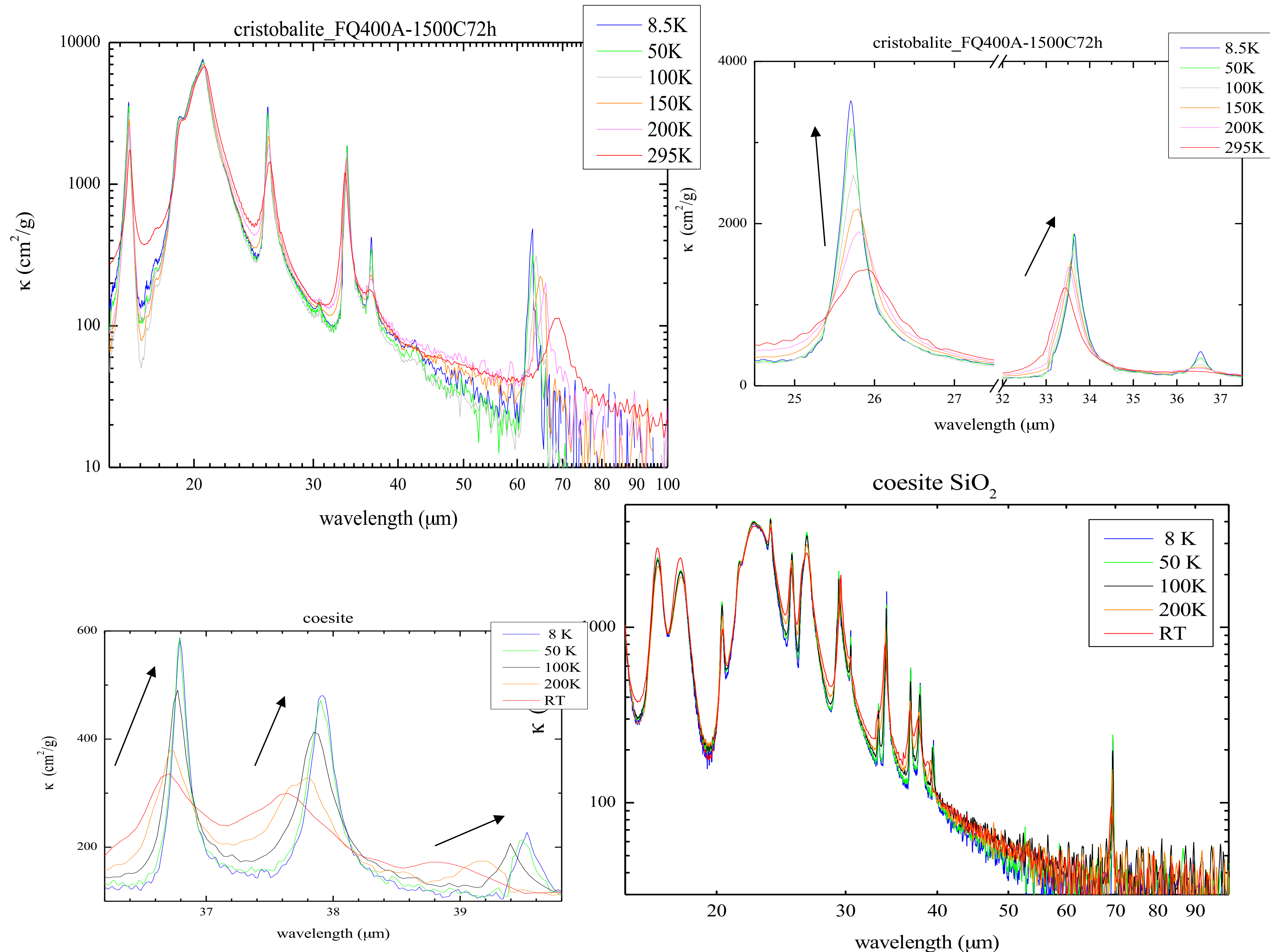

coesite
6GPa, 1300 0C, 30min
κ (cm2/g)
10000
1000
100
10
10
100
wavelength (μm)


coesite
6GPa, 1300 0C, 30min
stishovite
13Gpa, 1200 0C, ?min
κ (cm2/g)
10000
1000
100
10
10
100
wavelength (μm)

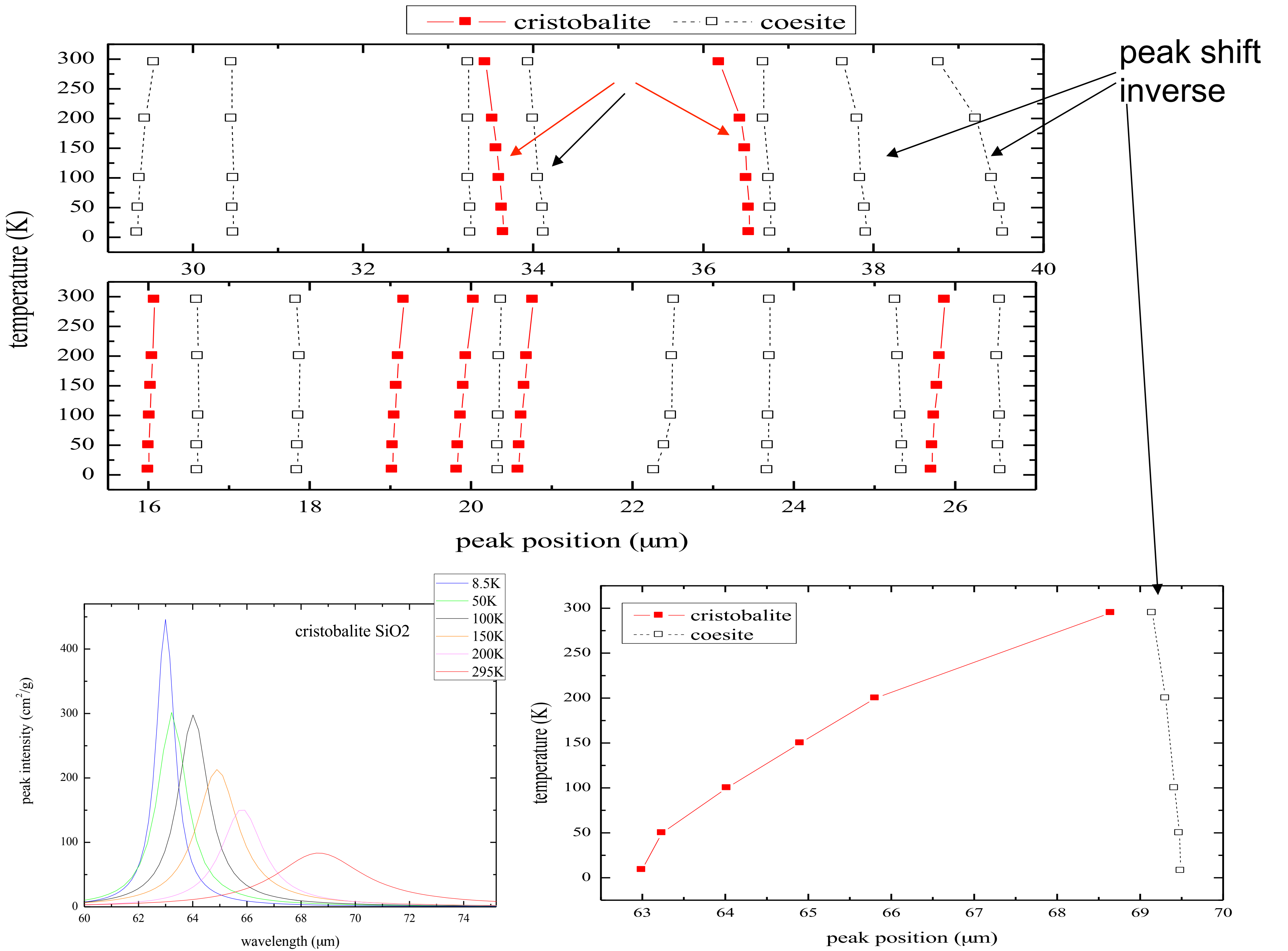
Stishovite ??



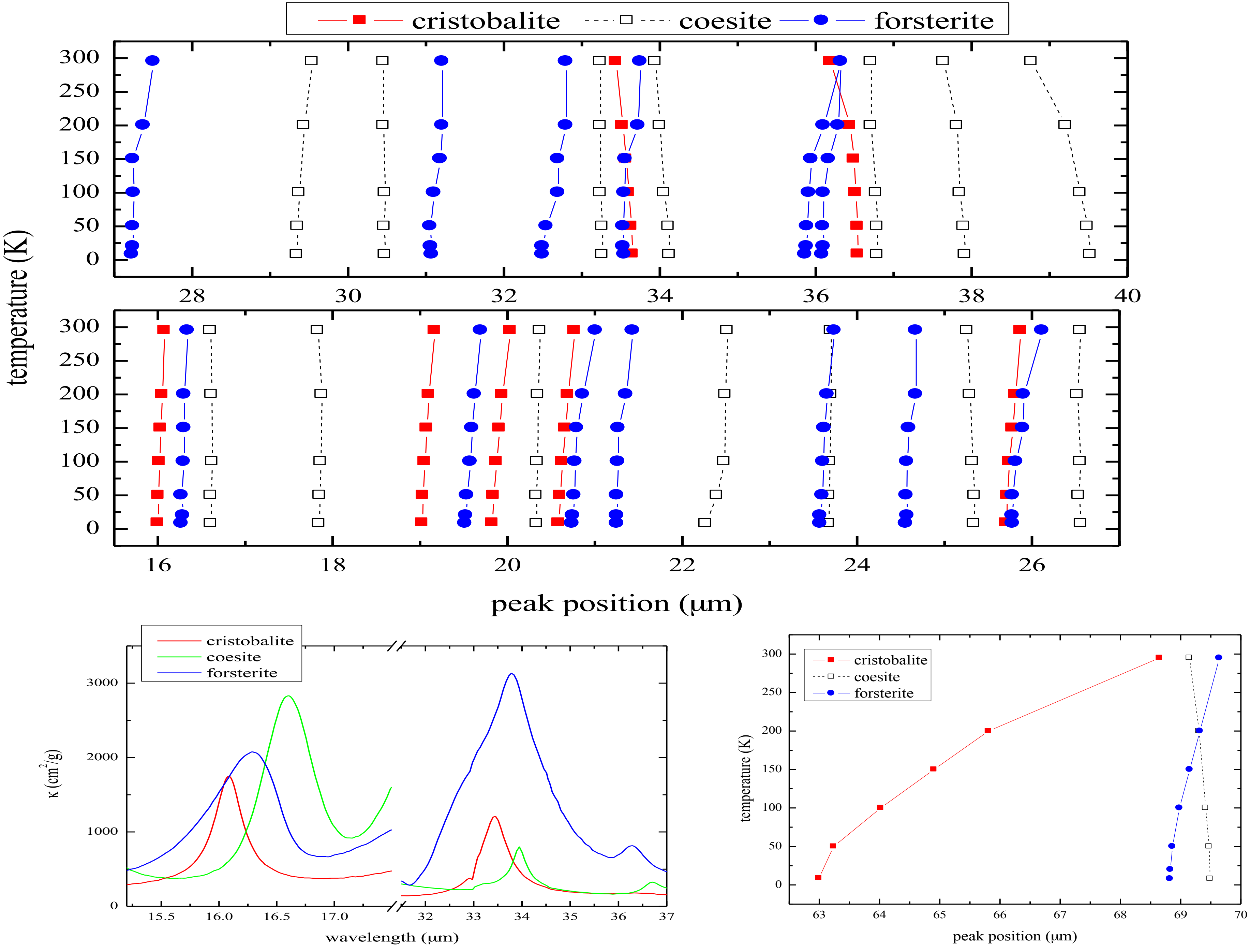
16 μm
33 μm
69 μm
cristobalite
(FQ40nm1500⁰C3d)
coesite
forsterite
κ (cm²/g)
10000
1000
100
10
10
100
wavelength (μm)

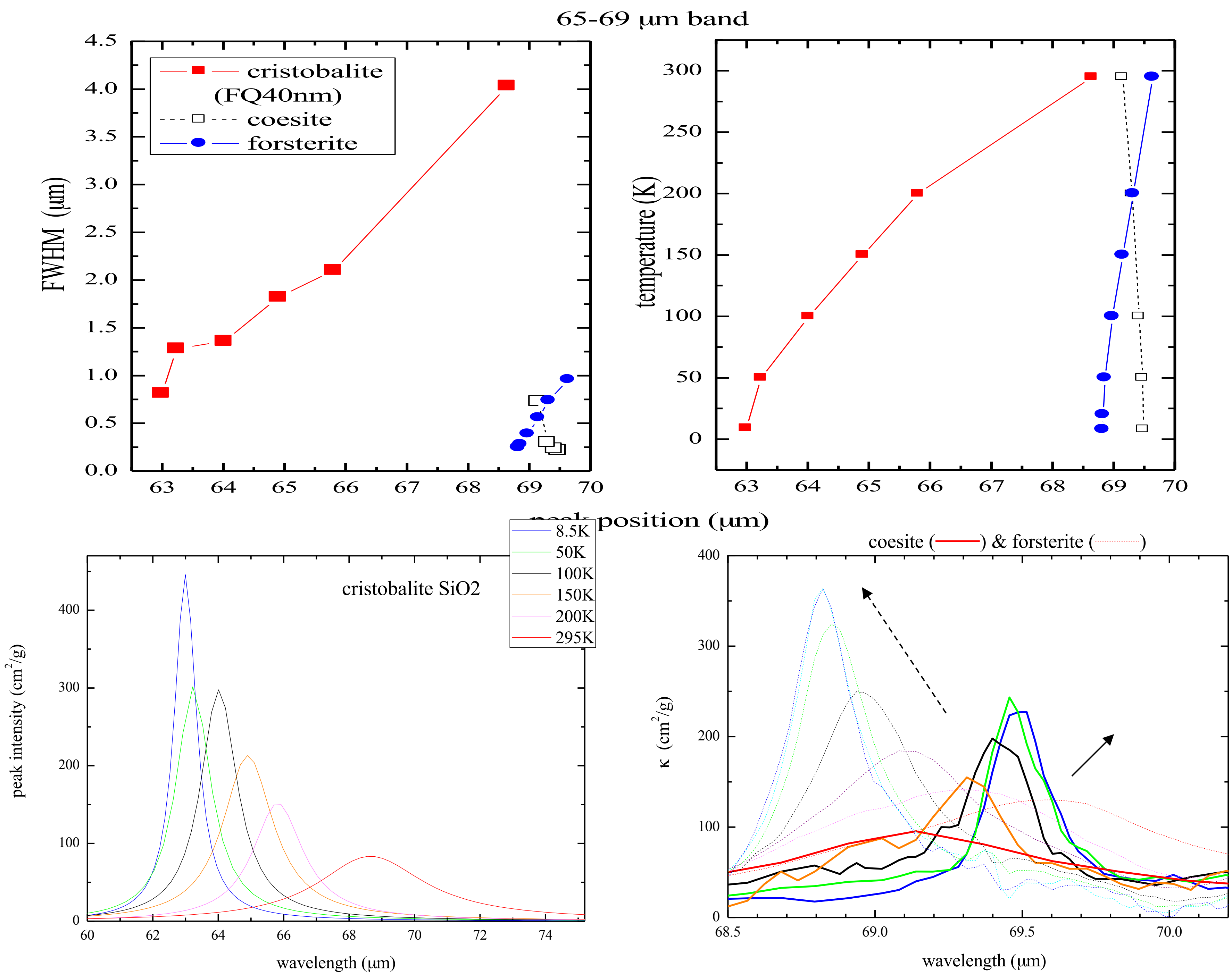


cristobalite_FQ400A-1500C72h
8.5K
50K
100K
150K
200K
295K
κ (cm²/g)
wavelength (μm)
cristobalite_FQ400A-1500C72h
8.5K
50K
100K
150K
200K
295K
κ (cm²/g)
wavelength (μm)
coesite
8 K
50 K
100K
200K
RT
κ (cm²/g)
wavelength (μm)
coesite SiO2
8 K
50 K
100K
200K
RT
wavelength (μm)



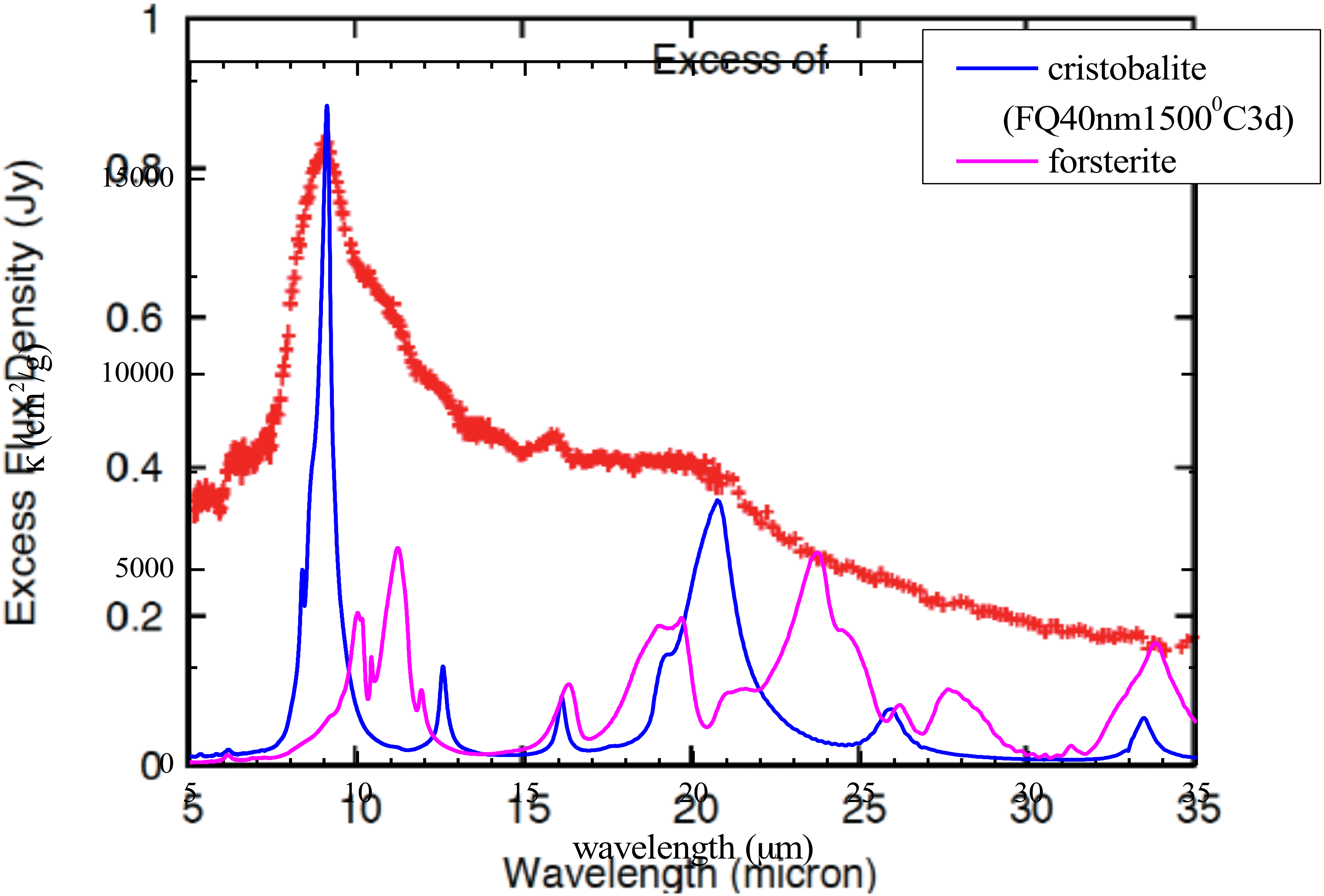
cristobalite
coesite
peak shift
inverse
temperature (K)
peak position (μm)
8.5K
50K
100K
150K
200K
295K
cristobalite SiO2
peak intensity (cm²/g)
wavelength (μm)
cristobalite
coesite
temperature (K)
peak position (μm)


cristobalite
coesite
forsterite
temperature (K)
300
250
200
150
100
50
0
28
30
32
34
36
38
40
16
18
20
22
24
26
peak position (μm)
κ (cm²/g)
3000
2000
1000
0
15.5
16.0
16.5
17.0
32
33
34
35
36
37
wavelength (μm)
63
64
65
66
67
68
69
70



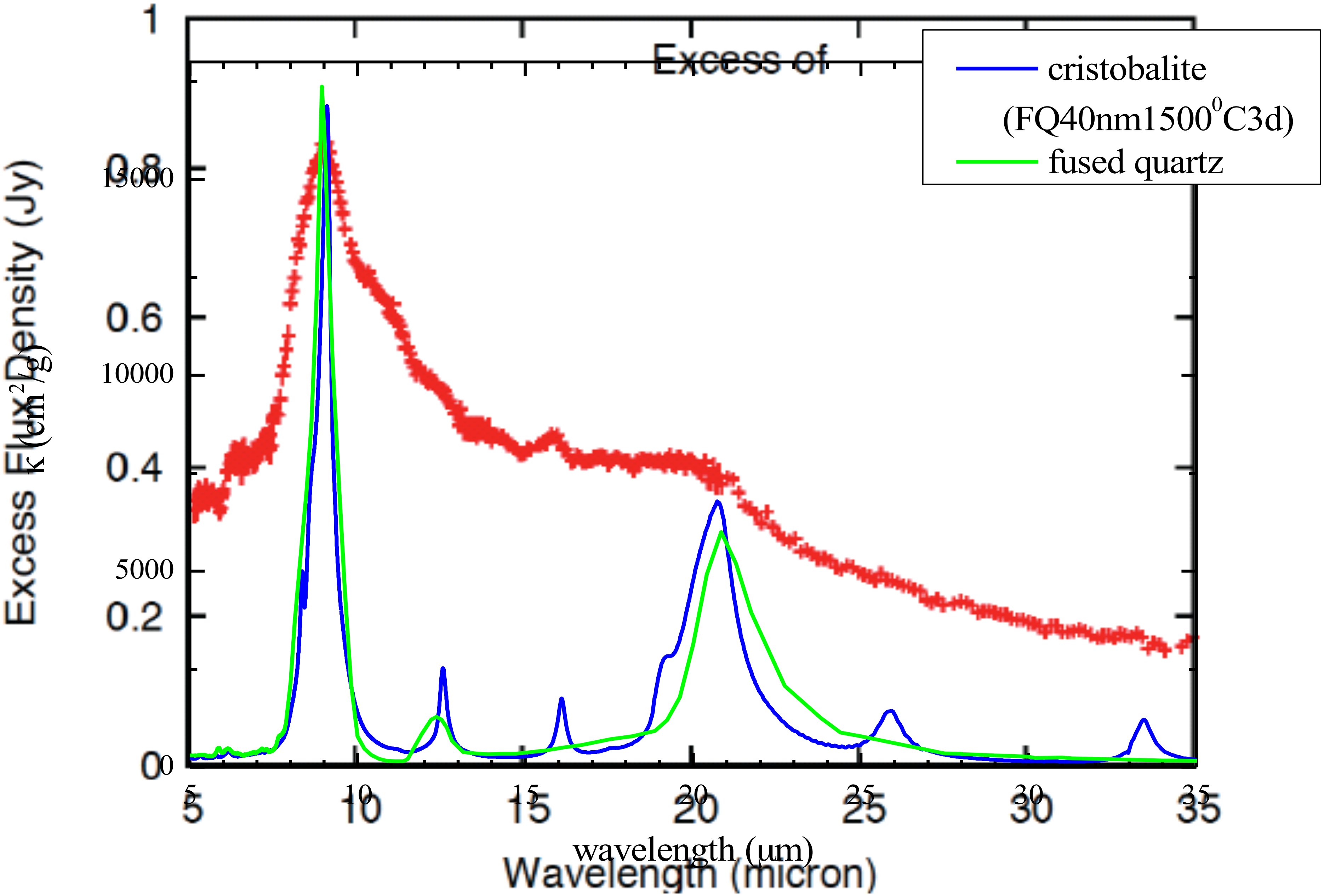
65-69 μm band
cristobalite (FQ40nm)
coesite
forsterite
FWHM (μm)
temperature (K)
peak position (μm)
cristobalite SiO2
8.5K
50K
100K
150K
200K
295K
peak intensity (cm^2/g)
wavelength (μm)
coesite ( ) & forsterite ( )
κ (cm^2/g)
wavelength (μm)

HD 15407 Fujiwara et al., 2009 GFWS



HD 15407

Fujiwara et al., 2009 GFWS



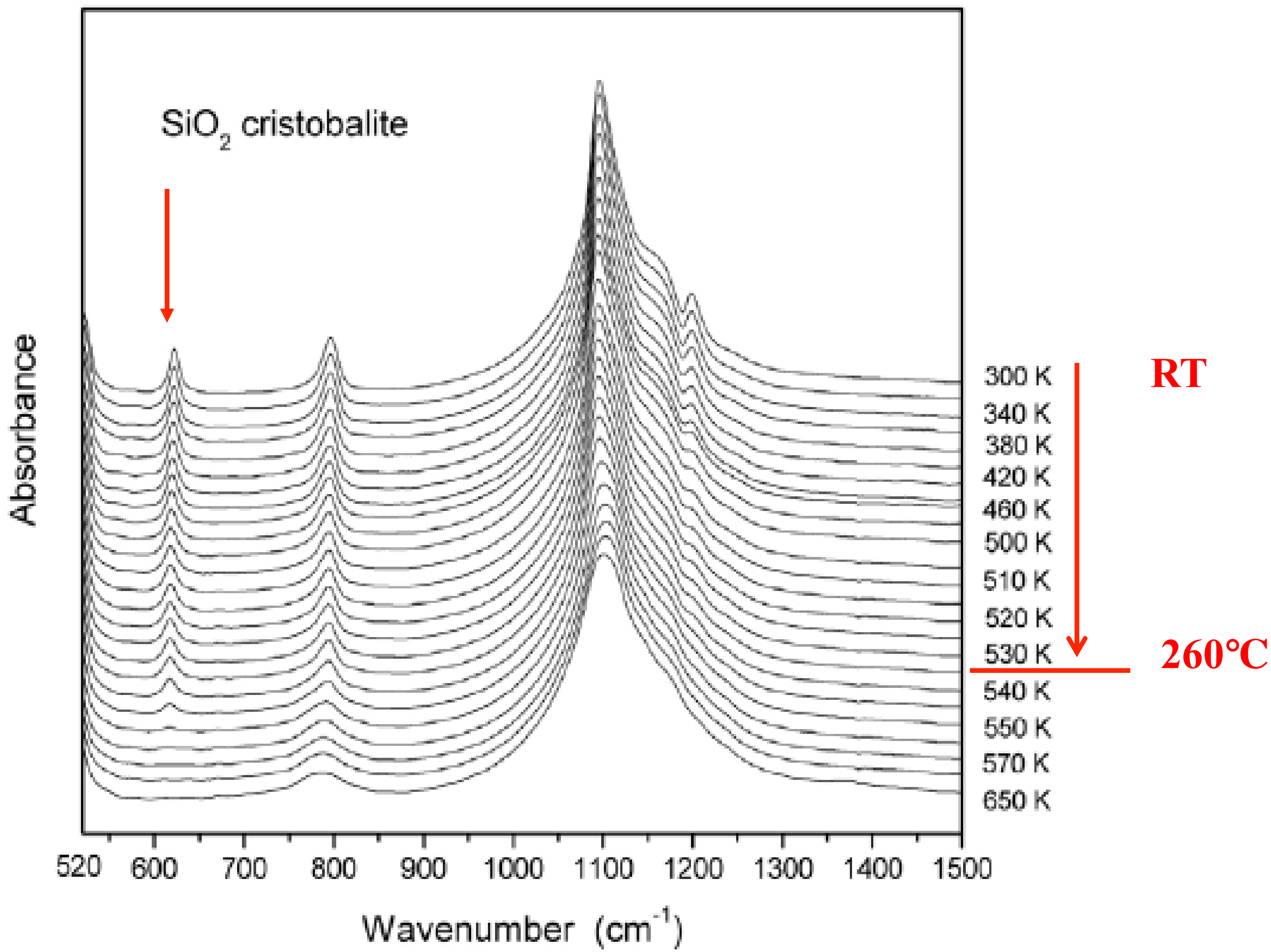


Figure 5. Infrared absorption in cristobalite SiO_2 from 500 to 1500 cm^{-1}, showing persistence of doublet structure near 1100 cm^{-1} up to 650 K. Note that there are too many lines for the O_h space group of references [40, 41].

Conclusion

(1) Silica SiO_2 infrared spectra : characteristic peaks

amorphous (fused quartz) , cristobalite, coesite, quartz

9 μm - all silica have strong peak (almost same intensity)
16 μm - cristobalite & coesite
33 μm - cristobalite & coesite
69 μm - cristobalite (broad) & coesite (sharp)

(2) If cristobalite or coesite dust particles exist around debris disks, charcteristic peak at about 69 μm may be detected, that is, broad peak or sharp peak may be found.

(3) Cristobalite ----- annealing temperature become low due to impurity ?

Stishovite ------ unstable ? (phase transition due to time dependence ??)