

Implications of self-consistent H₂O ice optical constants on radiative transfer models of disks

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ABSTRACT

Context. Interstellar water (H₂O) ice exhibits significantly varied profiles over its spectral features with temperature and thermal history. No previous radiative transfer model of a protoplanetary disk has fully accounted for these effects over the wavelength range from 3 - 200 μ m simultaneously. A radiative transfer model with region-based distribution of ices and applicable ice optical constant composites (OCCs) are required to properly model the distribution and spectral signatures of water ice in disks.

Aims. First, we build a series of thermal history- and temperature-dependent H₂O ice OCCs with the available literature data from 0.1 - 10,000 μ m. We then self-consistently apply these within a radiative transfer model of a protoplanetary disk according to its thermal structure. Second, we assess the impact that appropriate H₂O optical constants have on the 3 μ m absorption and 45 and 63 μ m emission profiles in disks populated by ice with one of the two thermal history models.

Methods. We combined multiple experiment measurements of the imaginary refractive indices, k , to cover from 0.1 - 10,000 μ m and performed Kramers-Kronig (KK) integrations to derive updated real refractive indices, n . We constructed H₂O ice OCCs for two thermal histories: first, direct deposit and measure at a fixed temperature ices (**DT**) and deposit and cool down (**DC**) ices, for five and eight distinct temperatures, respectively. We ran four RADMC-3D radiative transfer models of edge-on class II disk, HH 48 NE. The four models each use different OCCs; the standard single temperature crystalline (model M0) and amorphous (model M0A) H₂O ice OCCs available from OpToo1 and our own multi-temperature **DT** set of OCCs (model MDT) and **DC** only set of OCCs (model MDC).

Results. We present the first radiative transfer models with temperature-dependent ice opacities over the full wavelength range relevant for H₂O ice. The 3 μ m absorption feature shifts from 3.0 μ m to 3.1 μ m and shows a 3.2 μ m shoulder when using the **DC** OCCs, while the 45 and 63 μ m emission features only appear when using the **DC** OCCs.

Conclusions. Using our new OCCs and temperature-specific opacity zoning within RT models together provides the first self-consistent RT profiles for the two most commonly used spectroscopic tracers of thermal processing of H₂O ice. We find that ices must have been thermally processed at temperatures higher than the local disk temperature in order to produce crystalline spectral profiles at 3, 45, or 63 μ m in disks, suggesting local heating events or outward transport to colder regions, confirming the conclusions of previous radiative transfer models of edge-on classical T Tauri disks.

Key words. interstellar ices – optical constants – radiative transfer modelling – protoplanetary disks

1. Introduction

Water (H₂O), an essential ingredient for life, is thought to be incorporated into forming planets and moons as icy dust grains. H₂O ice is observed across all stellar formation stages, from molecular clouds (Boogert et al. 2011; McClure et al. 2023; Smith et al. 2025) to disks (Boogert et al. 2008; McClure et al. 2015; Sturm et al. 2024; Potapov et al. 2025), comets (Fornasier et al. 2016), and the surfaces of our Solar System's icy moons (Villanueva et al. 2023; Bockelée-Morvan et al. 2024; Cartwright et al. 2025), through its vibrational absorption bands, including the 1–2 μ m overtones, the 3 μ m stretching mode, the 4.5 μ m combination band, the 6 μ m bending mode, the 11 μ m libration mode, and the far-infrared (FIR) 45 and 63 μ m emission ice lattice modes. In planet-forming disks, ices may enhance the sticking properties of dust grains (Musioli & Wurm 2019), and alter the disk's thermal structure due to their optical properties.

The shapes of the 3, 45, and 63 μ m bands reveal H₂O ice's thermal history, as structural changes in the ice matrix alter the spectral profiles (Smith et al. 1994; Mastrapa et al. 2009). The amorphous-to-crystalline phase transition produces characteristic changes: the 3 μ m band narrows and shifts from 3.0 to 3.1 μ m with the emergence of a 3.2 μ m peak, while the FIR 45 μ m band sharpens and the 63 μ m feature appears only in crystalline ice (Smith et al. 1989). If ice crystallises and subsequently cools, it retains its crystalline structure, but subsequent peak strengths and wavelength shifts track the amount by which it has cooled (Smith et al. 1994; Mastrapa et al. 2009). These spectral differences allow thermal histories to be inferred observationally.

H₂O ice has been detected via these features towards a number of Class II classical (K0 and later spectral type) T Tauri protoplanetary disks (Aikawa et al. 2012; Terada & Tokunaga 2012; McClure et al. 2012, 2015; Sturm et al. 2024; Potapov et al. 2025), with a mixture of amorphous and crystalline profiles being observed. This split in the observed H₂O ice phase is still not fully understood. For disks with crystalline profiles, it has been consistently determined that the crystalline ice must reside in the

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disk's cooler, outer regions, where ice would not natively crystallise (McClure et al. 2015; Min et al. 2016; Kamp et al. 2018). This implies that additional dynamical processes within the disk must either generate these crystalline ices locally or transport them there. Dynamical processes such as viscous spreading, extreme heating phenomena such as an accretion heating event, or planetesimal collisions have been speculated to be the cause.

Accurate interpretation of observed disk ice features requires radiative transfer (RT) modelling. Grain size and shape distributions modify ice opacities (McClure et al. 2012; Dartois et al. 2024), and disk geometry affects the resulting spectra (Sturm et al. 2024). The RT models therefore depend on reliable H₂O optical constants across the full wavelength range (0.1–1,000 μ m) needed to compute both stellar-wavelength absorption and scattering and long-wavelength thermal emission. No single laboratory experiment spans this range, so optical constant composites (OCCs) are constructed from multiple datasets.

Commonly used OCCs include the 266 K crystalline dataset of Warren & Brandt (2008) and an amorphous composite distributed through OpTool (Dominik et al. 2021), which merges 10 K measurements from Hudgins et al. (1993) (2.5 – 90 μ m) with Warren & Brandt (2008) outside that range. Although widely adopted, these fixed-temperature OCCs are often applied uniformly across disk models despite strong radial temperature gradients. This approach neglects temperature dependence and thermal history effects, resulting in ice band profiles that reflect inconsistent ice structures between commonly studied bands; for example, the 3 μ m versus 63 μ m features. Ad hoc substitution of individual laboratory datasets into these OCCs is common (Cheng et al. 2010; Sturm et al. 2024; Thang et al. 2024; Bergner et al. 2024), but lacks standardisation and limits the consistency across studies. Min et al. (2016) and Kamp et al. (2018) both began to address the thermal history issue in their studies, by including temperature-appropriate ice opacities throughout their disk models in a locally self-consistent way for the FIR features. With the advent of JWST and future FIR missions on the horizon, H₂O ice optical constants and RT models that treat ice temperatures in a globally self-consistent way across the full 3–200 μ m wavelength range are essential tools with which to probe different thermal histories of disks.

Here, we present new H₂O OCCs that are globally self-consistent over the 3–200 μ m range for two thermal histories: deposit-and-measure at fixed temperature and deposit-and-cool-down, spanning five and eight temperatures. We extend these OCCs to 0.1 – 1,000 μ m in order to implement them in the RADMC-3D RT code and expand the ice zoning in the established RT model of HH 48 NE (Sturm et al. 2023c, 2024) to include corresponding ice temperature regions. By comparing the resulting 3, 45, and 63 μ m spectral profiles with those of models employing the standard Warren & Brandt (2008) crystalline and Hudgins et al. (1993) OpTool amorphous OCCs, we assess whether crystalline features should be detectable when distributed according to the intrinsic disk temperature gradient. If not, this would imply that additional dynamical processes, such as viscous spreading or transient heating events, are required to bring or produce thermally processed ice in the outer regions of disks, in order to explain observed crystalline ice signatures in classical T Tauri disks.

2. Building thermal history- and temperature-dependent OCCs of pure H₂O ice

In this section, we construct OCCs for n and k of the complex refractive index, $m = n + ik$, from 0.1 – 10,000 μ m for pure H₂O.

Two sets of OCCs are built, split by the thermal history of the experimentally grown ices.

The first set of pure H₂O ice OCCs combine optical constant measurements of the deposit and measure at fixed temperatures thermal history for five temperatures. These are subsequently denoted as the **DT** set from herein. The low temperature measurements (30 K) emulate an amorphous ice layer formed atop a dust grain in the early cloud stages of star formation or to the icy dust towards the outer regions of a disk. The higher temperature measurements (75 K and above) more closely emulate ice formation occurring in the natively warmer inner regions of a disk. The second set of OCCs combines optical constant measurements of the deposit and cool down thermal history for eight temperatures and is subsequently denoted as the **DC** set from herein. All **DC** experimental measurements across the full wavelength range deposit the ice at 150 K and are then cooled; therefore, they are all crystalline in the ice phase. These measurements allow us to emulate interstellar ices that have undergone thermal processing in the inner disk regions and been transported to the cold outer regions.

The laboratory experimental data used to build our OCCs are all measured under slightly different conditions, which are discussed in the following sections, but all produce transmission spectra and then derive the imaginary component of the refractive index, k , values using the transmission spectra. In our OCCs, we collated k values across different wavelength ranges for each temperature and thermal history combination and stitched them together. These datasets are shown in Table 1. In most cases, the k values match across experiments but where discrepancies exist between experimental data, we performed interpolation to ensure a smooth transition from one dataset to another. The space in which the interpolation was chosen to be performed aims to best match the overall profile of the already existing data. The instances in which interpolation was used are outlined in the following sections. This same approach was employed in Warren (1984) when building the widely used H₂O at 266 K composite. Once we had the k values in terms of the wave number, ν , we calculated the real component of the refractive index, n , using the Kramers-Kronig (KK) relation:

$$n(\nu) = n_{632\text{nm}} + \frac{2}{\pi} \mathcal{P} \int_{\nu_1}^{\nu_2} \frac{\nu' k(\nu')}{\nu'^2 - \nu^2} d\nu, \quad (1)$$

where $n_{632\text{nm}}$ is the real refractive index at the reference wavelength of 632 nm. For our **DT** OCCs, we used the directly measured $n_{632\text{nm}}$ from He et al. (2022), which was measured to vary with temperature. However, for the **DC** OCCs, no temperature-dependent measurements in this wavelength range have been taken; therefore, we used $n_{632\text{nm}} = 1.32$ from Hale & Querry (1973). ν' is the wave number used to calculate the integral against the wave number being calculated for, ν . The Cauchy principle, $\mathcal{P}$, was used to overcome the singularity, $\nu' = \nu$. We chose to perform KK calculations using the k values across the total wavelength range of the OCCs rather than for each dataset individually as would have been done in their original studies, as this provides the most accurate n values. To derive usable n values, we performed the KK integral numerically using Simpson integration over a grid of 100,000 evenly spaced wave numbers in $\log(\nu)$ and then we downsampled these n values back to the native frequency grid of each datasets experiments. Warren (1984) state that solving Equation 1 with such fine gridding and singularity that is of type 0/0 means that there is a minimal impact on the final KK integral if one performs an analytical integration at the singularity to account

for the missing integral area. The KK integral runs from zero to infinity, meaning that the wider the range of wavenumbers that you have data for, the more accurate the n values that can be derived. By creating these self-consistent OCCs, we are able to improve on the derivation of the n values for each experimental dataset in isolation. An additional impact of the integral running from zero to infinity is that the ends of the calculated wavelength range suffer from truncation errors. Therefore, an estimate of n values outside of our desired composite frequency range is required to ensure that reliable n values are derived for our end wavelengths, 0.1 and 10,000 μm . How we approach the truncation error is described in Section 2.1.

Table 1: Laboratory datasets used to construct the fixed temperature thermal history (**DT**) and cool down thermal history (**DC**) H₂O OCCs.

Wavelength range (μm)	DT composite experimental dataset	DC composite experimental dataset
0.1 - 1.2	Warren & Brandt (2008)	
1.2 - 2.64	Mastrapa et al. (2009)	
2.64 - 2.82	Log-log interpolation	
2.82 - 15	Rocha et al. (2024); Gerakines et al. (1996)	Mastrapa et al. (2009)
	160 K; Öberg et al. (2007) <160 K	
15 - 18	Log-log interpolation	
18 - 20		
	Smith et al. (1994) <75 K; Curtis et al. (2005) >75 K	Smith et al. (1994)
20 - 74.5		
74.5 - 94	Linear interpolation	Log-log interpolation
94 - 10,000	Reinert et al. (2015)	

Notes. All datasets except the one of Warren & Brandt (2008) contain temperature-dependent measurements. The interpolation method listed was chosen to best match the profile of the experimental data. See Appendix A for interpolation plots. Where references are listed in both **DT** and **DC** series, there are multiple thermal histories in that study, except for Warren & Brandt (2008), which uses **DT** data, and Reinert et al. (2015), which uses **DC** data.

Table 2 shows the temperatures available in each thermal history's composite set and the according ice phase for each measurement. The number of temperatures we can build OCCs for is limited by the available spectroscopic data from laboratory experiments across the required wavelength range for RT modelling. When creating each set of H₂O ice OCCs, we aim to match the temperatures across the full wavelength range and between thermal histories as closely as possible. These matched temperatures for the **DT** and **DC** OCCs can have a 5 K difference but this is deemed a reasonable match within the temperature range sampled. These matching temperature subsets are denoted by double-barred boxes in Table 2.

In the following sections, for each set of thermal-history and temperature-dependent OCCs, we describe the details of the ex-

Table 2: Temperature, ice phase, and thermal history for each H₂O OCC that we made.

Temperature (K)	Phase	Thermal History
20	I _c	DC
30	I _a	DT
30	I _c	DC
40	I _c	DC
50	I _c	DC
75	I _a	DT
80	I _c	DC
105	I _a	DT
110	I _c	DC
135	I _c	DT
140	I _c	DC
150	I _c	DC
160	I _c	DT

Notes. Temperatures have grouped into closest matches between the two measurement techniques, **DT** and **DC**. I_a = amorphous phase and I_c = crystalline phase.

perimental setup, covered wavelength ranges and any required interpolation between datasets used to produce each OCCs final k values. We also note wavelength regions where potential mismatches in the thermal history, temperature, or ice phase with the target thermal history and temperature for a composite exist and our chosen approach to ensure continuity. We describe the experimental datasets first, followed by the interpolation between them, so that the reader has the full experimental data context. Figures showing the interpolation that we performed can be found in Appendices A.1 and A.2.

2.1. Common **DT** and **DC** experimental data

Table 1 shows that the two sets of thermal history-dependent OCCs use k values from the same datasets in the 0.1 - 1.2 μm and 94 - 10,000 μm wavelength ranges. This is due to very limited experimental data at these wavelengths. We describe the experimental data used and the n values that we calculated in the following sections.

2.1.1. 0.1 - 1.2 μm : Warren & Brandt (2008)

The Warren & Brandt (2008) composite was derived for pure H₂O ice in its hexagonal structure (I_h) at 266 K, with a focus on Solar System and terrestrial ice measurements. From 0.04 - 0.16 μm , they used Seki et al. (1981)'s experimental data of crystalline H₂O ice at 80 K, which remains unchanged from their original composite (Warren 1984). From 0.16 - 1.2 μm , they combined a complex series of experimental data and interpolation, so we refer the reader to the original Warren & Brandt (2008) paper for the details to keep this paper within a reasonable scope. They addressed the clear mismatch of temperature in the 0.04 - 0.16 μm regime (80 K to the target 266 K) in Warren (1984), in which they noted that experiments have shown that the k values appear to show very little variation with temperature or ice phase. Due to this lack of temperature or ice phase dependence and a lack of more recent data in this wavelength regime, we used the Warren & Brandt (2008) composite k values for every **DT** and **DC** composite. Their composite extends far beyond

1.2 μm but we only used it to 1.2 μm as this is the wavelength from which much better-suited data from Mastrapa et al. (2009) is available. Finally, to overcome the truncation issue for the KK integral, we used the Warren & Brandt (2008) data down to 0.04 μm when calculating our n values and then cut our composite's n values at 0.1 μm .

Between 0.1 - 1.2 μm , the k values are identical for all **DT** and **DC** OCCs but Figure 1 demonstrates the impact of the temperature dependence of the $n_{632\text{nm}}$ values as measured by He et al. (2022) on each **DT** composite, with Figure 2 showing that the **DC** OCCs are fixed in place at $n_{632\text{nm}} = 1.32$ from Hale & Querry (1973). He et al. (2022)'s experiments measured n values every 10 K from 30 K up to 160 K. Each temperature measurement was taken as the H_2O was deposited onto the aluminium mirror when it was at the fixed deposition temperature.

2.1.2. 94 - 10,000 μm : Reinert et al. (2015)

Reinert et al. (2015) built a temperature-dependent far-infrared analytical model of hexagonal crystalline ice H_2O (I_h) for wavelengths of 94 μm and above. Their experiments placed distilled liquid H_2O between two windows of polyethylene, $(\text{C}_2\text{H}_4)_n$ inside of a continuous flow helium cryostat and cooling the liquid H_2O to 250 K, resulting in a H_2O I_h ice. They then cooled and measured their ice sample at six different temperatures: 250 K, 200 K, 150 K, 100 K, 50 K, and 10 K. Spectroscopic measurements at each temperature were taken across three distinct wavelength ranges (80 - 192 μm , 149-385 μm , and 225 - 625 μm). Each experimental temperature had a slightly different wavelength range measured within the three ranges; therefore, the model was built using only the data where $\lambda > 94 \mu\text{m}$ to keep consistency at the shorter wavelengths.

This dataset does match the thermal history of the **DC** set, making it the ideal dataset to use. It does not match the thermal history of the **DT** set; however, we chose to use their analytical model over other available data to ensure temperature dependence in our OCCs. This highlights another significant missing temperature-dependent measurement for the fixed temperature thermal history for H_2O ice. We used the Reinert et al. (2015) analytical models from 94 μm in every composite and cut off the shorter wavelength experimental data to ensure consistent temperature dependence across each set of OCCs. Additionally, we were able to generate k values beyond the required 1,000 μm with the analytical models; therefore, we did so out to 10,000 μm to overcome the truncation issue of the KK integral.

Figures 3 and 4 show that the $>94 \mu\text{m}$ k values show much steeper slopes than in Warren & Brandt (2008), as shown in Reinert et al. (2015); Kim et al. (2019). Due to two different datasets being used in the 20-74.4 μm range for the **DT** OCCs, we see in Figure 3 that the temperature-dependent trend does not hold in the n values beyond 94 μm . Until new self-consistent experimental data of the FIR region across our temperature range are measured, we are unable to address this.

2.2. Deposition temperature (**DT**) measurement pure H_2O OCCs

2.2.1. 1.2 - 2.64 μm : Mastrapa et al. (2009)

We used the Mastrapa et al. (2009) deposit and measured at a fixed temperature experimental data from 1.2 - 2.64 μm to include the H_2O overtone transitions in our **DT** OCCs. For these data, Mastrapa et al. (2009) deposited water vapour at a series of temperatures (15, 25, 40, 50, 60, 80, 100, and 120 K) onto

a potassium bromide (KBr), zinc selenide (ZnSe), or cesium iodide (CsI) substrate and immediately took the spectroscopic measurements. This means that for our 30 K and 75 K **DT** OCCs, there is a 5 K mismatch at these wavelengths. Figure 5 shows the temperature dependence of the H_2O overtone transitions in our OCCs.

2.2.2. 2.82 - 20 μm : Gerakines et al. (1996); Öberg et al. (2007); Rocha et al. (2024)

The data we used to describe the 3 μm H_2O ice band in our **DT** OCCs are the k values from the Leiden Ice Database for Astrochemistry (LIDA) (Rocha et al. 2022). LIDA contains k values for five fixed temperatures of 30 K, 75 K, 105 K, 135 K, and 160 K. The 30 K, 75 K, 105 K, and 135 K measurements were taken by Öberg et al. (2007) and the 160 K data from Gerakines et al. (1996), both of which cover 2.5 - 20 μm . In both of the experimental setups, water vapour was deposited onto a cesium iodide (CsI) substrate and measurements were taken at the fixed deposition temperature. The k values were calculated from the experimentally measured absorption spectra by Rocha et al. (2024). There is a small range of negative values from ~ 8.5 - 10.3 μm , which is unphysical. The origin of the negative values is not explained in Rocha et al. (2024); therefore, we replaced them with a constant value of 10^{-3} as the largest neighbouring, positive k value across all temperatures. Using the constant k value in place of the negative k values has a negligible impact on the calculated n values, whilst providing a reasonable estimate for physically possible k values. The refractive indices are shown in Figure 5.

2.2.3. 2.64 - 2.82: Our interpolation

A common cut-off wavelength for every temperature in the **DT** was required for consistency. 2.64 μm was determined to be an applicable wavelength to cut the Mastrapa et al. (2009) k values to include the H_2O overtones and exclude the beginning of the 3 μm absorption band profile. We did not use the Rocha et al. (2024) k values directly from the 2.64 μm cut-off because negative k values are observed in this region for the 75 K, 105 K, and 135 K measurements. Instead, we decided to interpolate the k values from Mastrapa et al. (2009) at 2.64 μm for all temperatures for consistency through all temperatures. We interpolated to 2.82 μm for all temperatures except 30 K, where we interpolated to 2.75 μm for the best profile match. We used log - log interpolation for all temperatures except for 160 K, where we used linear interpolation for the best profile match.

2.2.4. 18 - 22 μm : Temperature-specific interpolation

$\text{Log}(\nu)$ - $\text{log}(k)$ interpolation was performed to smoothly transition from the Rocha et al. (2024) data to the FIR experimental dataset for each temperature. Each interpolation is shown in Appendix A.1.2. For 30 K and 135 K, the interpolation was performed between 20 - 22 μm , and for 105 K it was performed between 20 - 21 μm . The 75 K is extended to 18 - 22 μm due to a mismatch in the Rocha et al. (2024) and Smith et al. (1994) and 160 K interpolates between 19-20 μm because the Rocha et al. (2024) is very noisy beyond 19 μm .

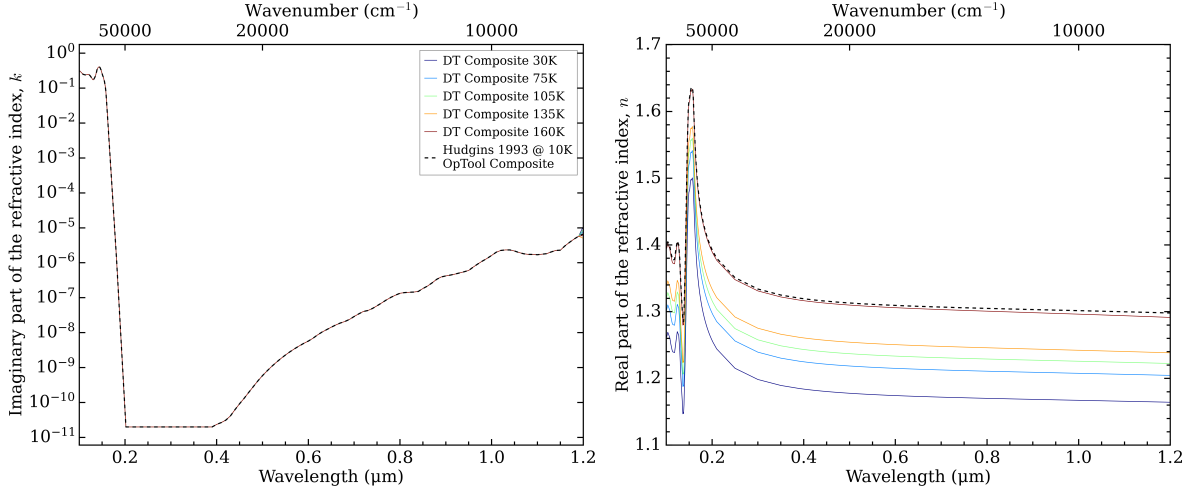


Fig. 1: UV - NIR zoom in of the **DT** OCCs at each temperature shown together with the Hudgins et al. (1993) OpTool composite, which in this region uses the Warren & Brandt (2008) at 266 K data.

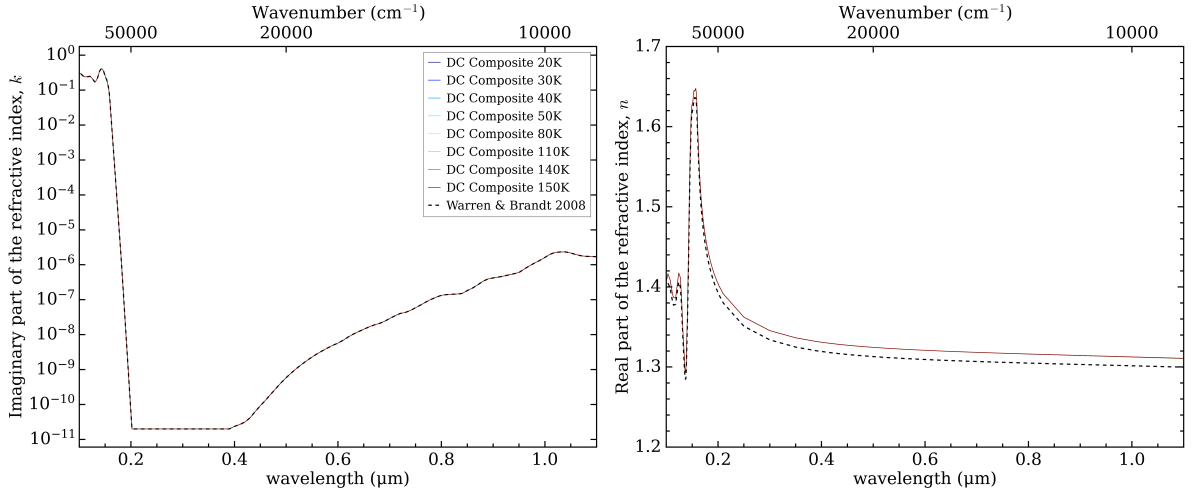


Fig. 2: UV - NIR zoom in of the **DC** OCCs at each temperature shown together with the Warren & Brandt (2008) at 266 K data.

2.2.5. 20 - 74.5 μm: Smith et al. (1994) and Curtis et al. (2005)

We used two different experimental datasets in the FIR wavelength range for our **DT** OCCs. The first is Smith et al. (1994)'s deposit and measure at a fixed temperatures of 30 K and 70 K, used in our 30 K and 75 K **DT** OCCs respectively. In their experiments, they deposited H₂O vapour onto a low-density (C₂H₄)_n substrate to build their ice and collect data from 20 - 110 μm. The second dataset is Curtis et al. (2005)'s deposit and measure at fixed temperatures of 106 K, 136 K, and 156 K, used in our 105 K, 135 K, and 160 K **DT** OCCs, respectively. They deposited H₂O vapour onto a silicon substrate to build their ices and collect data from 15 - 192 μm.

Figure 6 shows the data for all temperatures for which a clear temperature dependence is observed. However, there may be slight differences to true temperature-dependent behaviour in this region due to the two different experimental setups. Both the Smith et al. (1994) and Curtis et al. (2005) datasets become noisy from around 100 μm. This motivated our decision to cut the experimental data at 94 μm and use the k values of the temperature-dependent analytical model of Reinert et al. (2015), as discussed in Section 2.1.2.

2.2.6. 74.5 - 94 μm: Our interpolation

For the 30 K, 75 K, and 105 K, additional interpolation at the longer wavelengths is required. At 94 μm, the Smith et al. (1994) **DT** data are at much higher values than the Reinert et al. (2015) model k values. This may be a thermal history or ice phase effect that distinguishes the two datasets. This discontinuity produces an unphysical sudden drop in the continuum of any spectra derived by RT modelling, and therefore must be addressed. It is noted that Smith et al. (1994) **DT** data at 130 K measures higher k values than an equivalent dataset, Curtis et al. (2005) **DT** data at 136 K measurements, suggesting that this is not a thermal history effect but an experimental issue. We deemed that the Smith et al. (1994) k values are overestimated in this region and performed interpolation between Smith et al. (1994) and Reinert et al. (2015) k values.

To best match the profile of the experimental data, linear interpolation between 74.5 μm for the Smith et al. (1994) 30 K and 75 K data and the start of the Reinert et al. (2015) k values at 94 μm was chosen. Additionally, the Curtis et al. (2005) measurements show larger k values than the Reinert et al. (2015) models between at 94 μm region. This difference may be a true reflection of the effect of thermal history on this wavelength re-

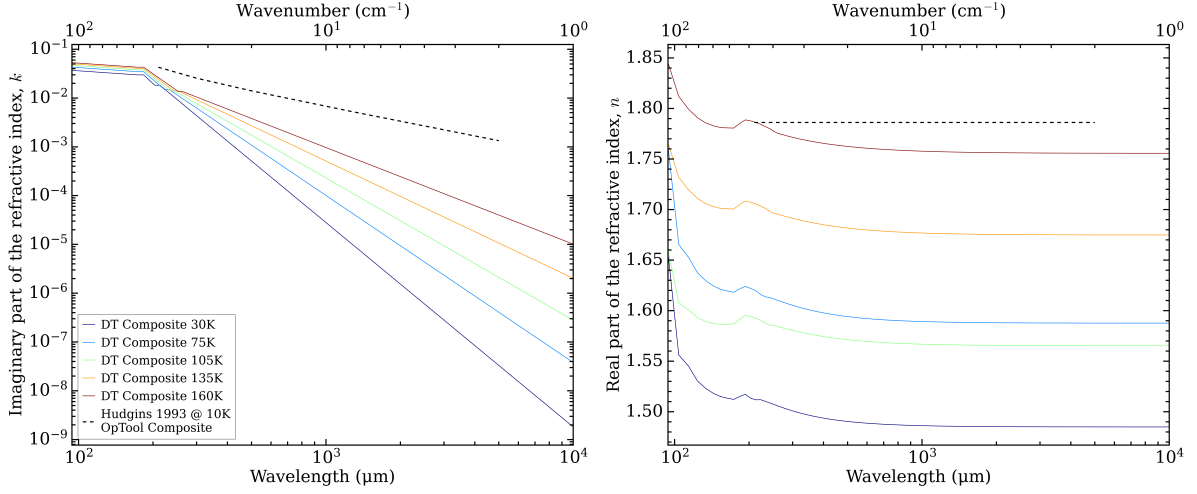


Fig. 3: Beyond FIR zoom in of 94 - 10,000 μm of the **DT** OCCs at each temperature shown together with the Hudgins et al. (1993) OpTool composite, which in this region uses the Warren & Brandt (2008) at 266 K data. All our OCCs use the analytical model of Reinert et al. (2015), deriving values at each composite temperature.

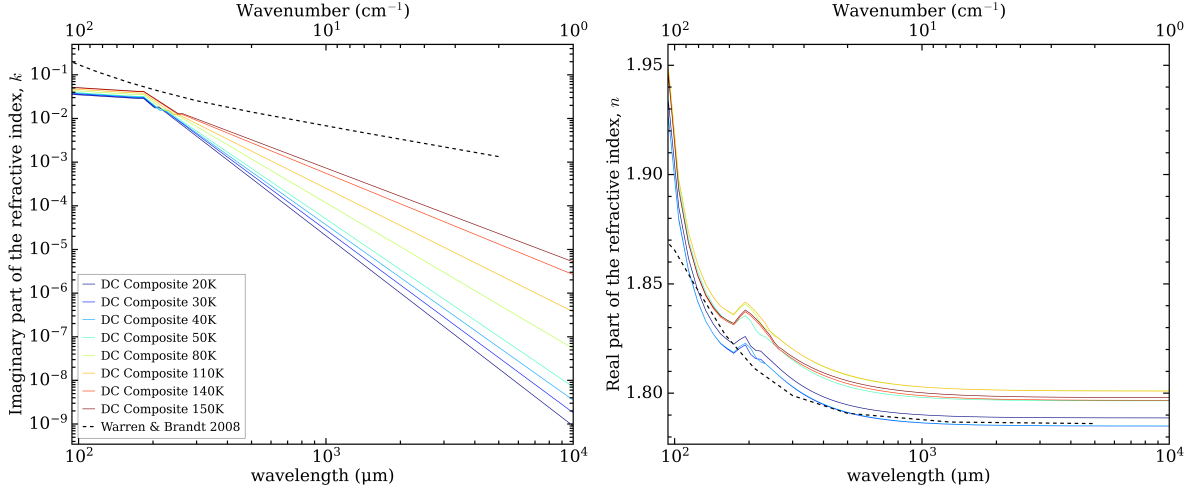


Fig. 4: Beyond FIR zoom in of 94 - 10,000 μm of the **DC** OCCs at each temperature shown together with the Warren & Brandt (2008) at 266 K data. All our OCCs use the analytical model of Reinert et al. (2015), deriving values at each composite temperature.

gion, due to the inconsistency between Curtis et al. (2005) (**DT**) and Reinert et al. (2015) (**DC**). To preserve the temperature dependence in the 94 - 10,000 μm region and to not have a sharp decrease in k values at 94 μm , we performed linear interpolation between 74.5 μm in the 105 K Curtis et al. (2005) data to 94 μm ; see figures in Appendix A.1.3. There is an excellent alignment between Curtis et al. (2005) 136 K and 156 K with the Reinert et al. (2015) models at the same temperatures and no interpolation is required.

2.3. Deposited and cooled (**DC**) measurement pure H_2O OCCs

2.3.1. 1.2 - 15 μm : Mastrapa et al. (2009)

We used experimental data of Mastrapa et al. (2008, 2009) for the NIR region of our **DC** OCCs. In their experiments, H_2O vapour was deposited at 150 K onto either a potassium bromide (KBr), zinc selenide (ZnSe) or cesium iodide (CsI) substrate, then cooled, with spectroscopic measurements from 1.1 - 15 μm taken at 10 K increments from 150 K down to 20 K. Fig-

ure 2 shows the lack of temperature dependence in this region for the **DC** OCCs. This highlights the need for experiments to test whether the $n_{632\text{nm}}$ value is temperature-dependent for cooled down H_2O ices, as it is for fixed temperature H_2O ice (He et al. 2022).

2.3.2. 20 - 74.5 μm : Smith et al. (1994)

In the FIR wavelength range, we used the Smith et al. (1994) cool down series of measurements, which covers 20 - 110 μm . In these experiments, H_2O vapour is deposited directly onto a low-density $(\text{C}_2\text{H}_4)_n$ substrate, preheated at 140 K, and then cooled with a series of measurements taken at 140, 130, 120, 110, 100, 90, 80, 70, 50, 30, and 10 K. This means that for our 20 K, 40 K, and 150 K **DC** OCCs, we do not have a direct temperature match between the NIR and FIR datasets. Thus, we chose to use the Smith et al. (1994) data that is 10 K lower than the NIR dataset temperature. There is a large discrepancy in k values at 94 μm , with Smith et al. (1994) **DC** data showing much larger k values than the Reinert et al. (2015) **DC** models. This suggests that this

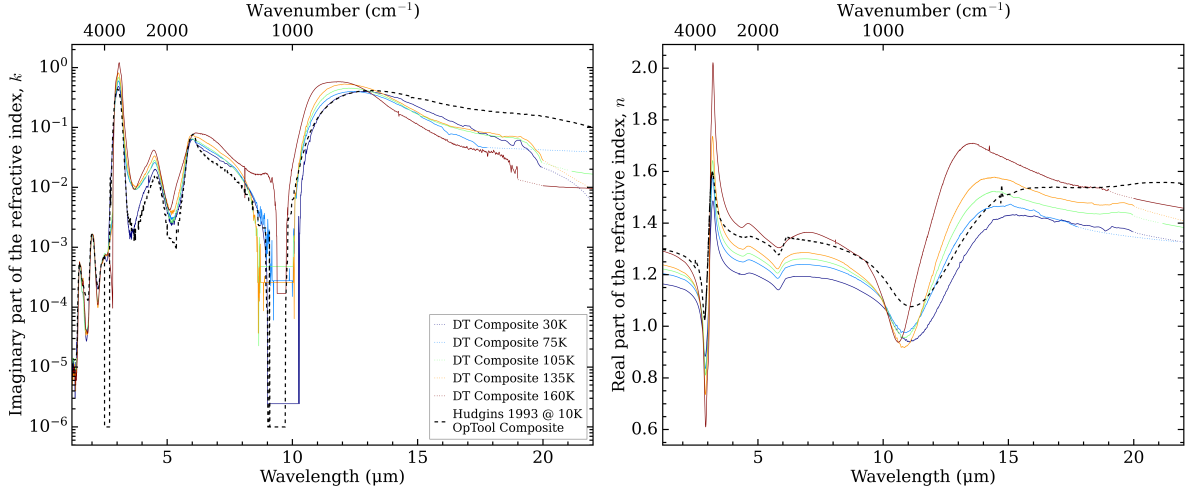


Fig. 5: NIR - MIR zoom-in of 1.2 - 20 μm of the *DT* OCCs at each temperature shown together with the Hudgins et al. (1993) at 10 K data. The dotted regions indicate where the k value interpolation has been performed.

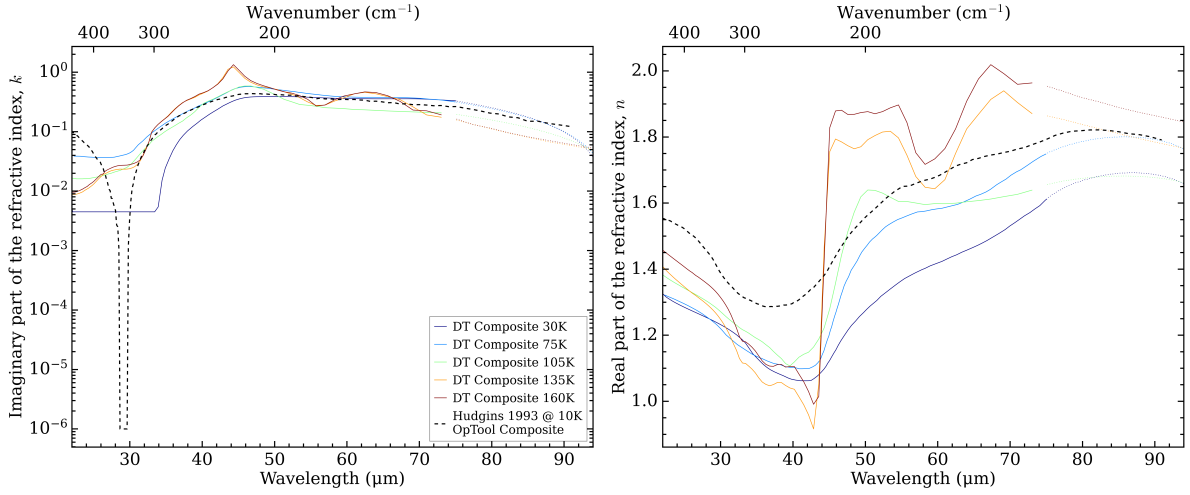


Fig. 6: MIR - FIR zoom-in of 15 - 94 μm of the *DT* OCCs at each temperature shown together with the Hudgins et al. (1993) at 10 K data. The dotted regions indicate where the k value interpolation has been performed.

is not a thermal history issue, as was mentioned in Section 2.2.6, but rather a experiment setup issue. Due to this, we performed an interpolation. Figure 8 shows the experimental data up to 7.45 μm along with the interpolation from 74.5 - 94 μm for all *DC* temperatures.

2.3.3. 15 - 20 μm : Our interpolation

There are missing experimental data between 15 - 20 μm for the *DC* thermal history. To overcome this, we employed the same technique as in Warren (1984) to connect datasets and interpolate k values between the two datasets in $\log(\nu)$ - $\log(k)$ space. The interpolation between the two datasets is shown in the figures of Appendix A.2.1.

2.3.4. 74.5 - 94 μm : Our interpolation

We performed an $\log(\nu)$ - $\log(k)$ interpolation between the Smith et al. (1994) data and Reinert et al. (2015) models that retains the peak and spectral profile of the 63 μm emission feature observed in the Smith et al. (1994) data whilst also providing

a smooth continuum through to 94 μm where the Reinert et al. (2015) k values begin. We started the interpolation from the experimental data point nearest to 74.5 μm through to 94 μm . The interpolation between the two datasets is shown in the figures of Appendix A.2.2.

3. Construction of multi-temperature ice RT models

Our thermal-history and temperature-dependent OCC sets allow us to create the first series of RT disk models with self-consistent H₂O ice optical constants across the full required wavelength range. The HH 48 NE disk's edge-on geometry (inclination $>70^\circ$) allows us to probe the H₂O ice using its 3 μm ice absorption and 45 and 63 μm emission features simultaneously as a background continuum for the absorption feature is provided by the central protostar and its scattered light. This combination of the updated disk model and new globally self-consistent OCCs provides a novel opportunity to:

- Study the effects of ice thermal history on each of these feature's profiles in unison and begin to test the region of the disk contributing to each of these features.

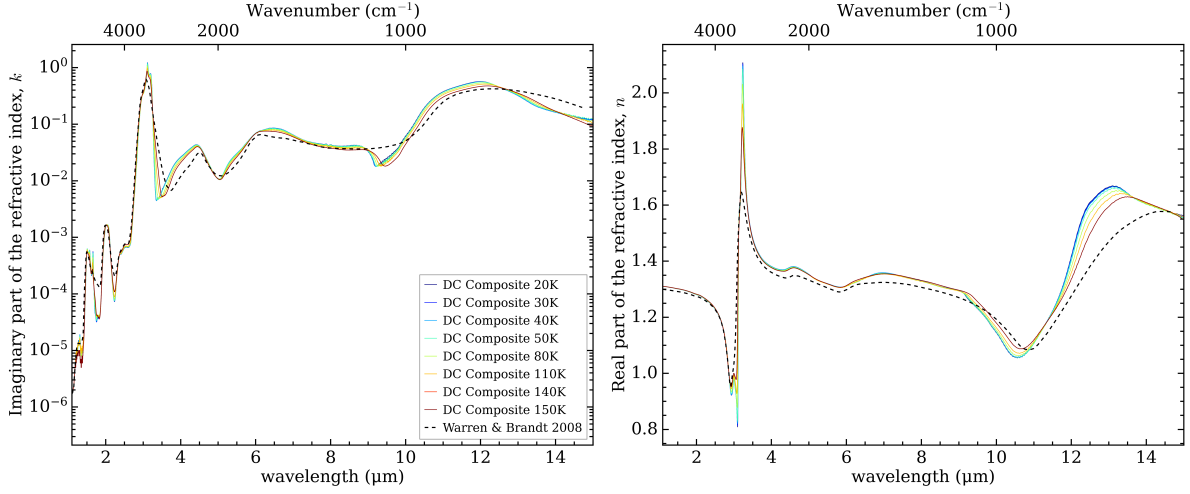


Fig. 7: NIR - MIR zoom-in of 1.1 - 15 μm of the **DC** OCCs at each temperature shown together with the Warren & Brandt (2008) at 266 K data. Our OCCs use the deposited and cooled measurements of Mastrapa et al. (2009).

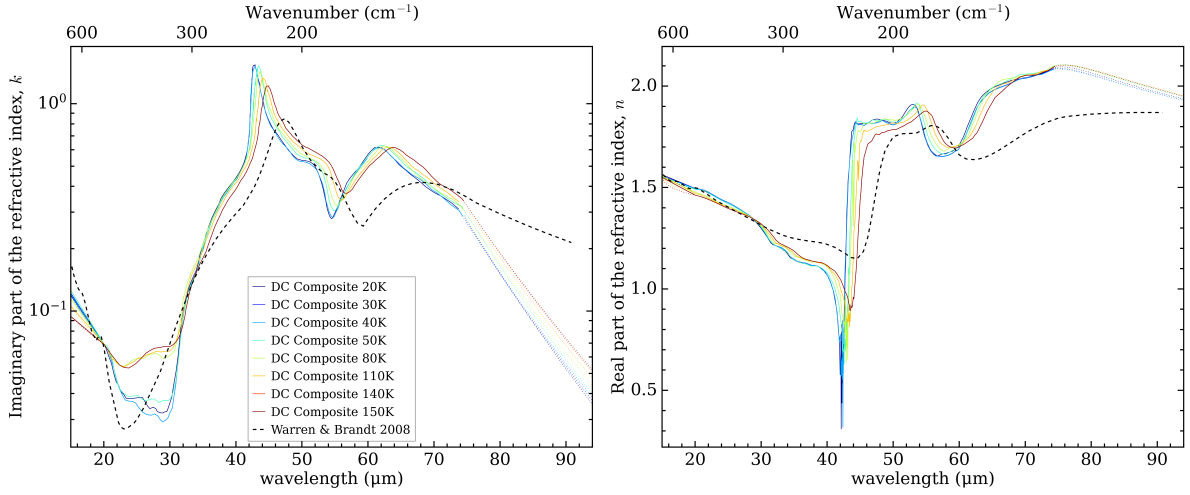


Fig. 8: MIR - FIR zoom-in of 15 - 94 μm of the **DC** OCCs at each temperature shown together with the Warren & Brandt (2008) at 266 K data. All our OCCs use the deposited and cooled measurements of Smith et al. (1994). The dotted regions indicate where the k value interpolation has been performed.

- Find out whether including crystalline ice only within a temperature-appropriate region (>125 K in Table 3) is enough to produce a crystalline profile without additional dynamical processes.
- Model the effect of dynamical processes on ice spectral profiles through unique distributions of thermally processed and non-thermally processed material throughout a disk.

Upcoming FIR observatories will enable us to compare the impact of ice thermal history on both the NIR and FIR ice features and model different dynamical processes through unique ice distributions within RT models. This work provides an essential tool in identifying excellent candidates for FIR observatories based on previous observations. Such sample selection will be critical given the small number of targets that can be observed during these mission’s lifetimes.

To build this first series of self-consistent ice RT models, we used the RT code RADMC-3D (Dullemond et al. 2012) with its full anisotropic scattering capabilities enabled. Our fiducial model is a disk continuum setup from Sturm et al. (2024), where

they used JWST NIRSpec IFU, MIRI MRS, HST scattered light images, ALMA, and archival spectral energy distribution (SED) data to derive the disk dust density structure and stellar properties. Their dust distribution employs the two dust grain size populations (small: $<12.63 \mu\text{m}$, large: $>12.63 \mu\text{m} - <3000 \mu\text{m}$) with the same dust grain material properties as are used in Sturm et al. (2024).

We added an ice mixture with constant ice abundance fractions with regard to H_2O ice derived by Sturm et al. (2024) for HH 48 NE onto our dust grains. Our ice distribution throughout the disk uses a mix of approaches of Sturm et al. (2023b) and Sturm et al. (2024). The ices have a limited extent through the disk due to photodesorption. This limit is set to include ices on the dust in regions of $z/r \leq 0.6$. The distribution of our ice species follows the approach of Sturm et al. (2023b) whereby the ices are distributed according to their pure ice desorption temperatures, as opposed to by their binding energies as done in Sturm et al. (2024). This is to ensure that our newly derived temperature-dependent optical constants are used in the appropriate regions of the disk. The ice mixture includes a 3:1 mix of CO_2 and CO (15% and 5% with regard to H_2O , respectively),

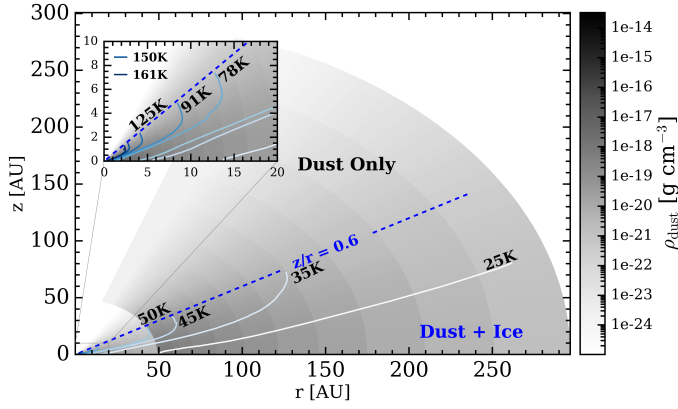


Fig. 9: Temperature regions within our disk models. The bold black outline shows the full extent of the dust within our disk models. The $z/r = 0.6$ dashed line shows the limit set for ices.

NH₃ (1.7%) and CH₄ (<12%) ices, in addition to H₂O. We employed the optical constants provided by OpTool for NH₃ and CH₄ and measurements by Bergner et al. (2024) for the CO₂ and CO mix. This ensures that any continuum effects from the additional ices are modeled, allowing for a true comparison with the 3 μ m spectral profile of Sturm et al. (2024)’s model. Using this ice distribution approach and ice mixture, we are able to split the disk into eleven regions when using the **DC** set and seven regions using the **DT** set. These regions and their according ice species are listed in Table 3 and the full eleven regions are shown in Figure 9 via their dust temperature contours.

To test the impact of the self-consistent models, we performed an initial study of the original H₂O ice OCCs against our self-consistent models. Table 4 outlines the four models we built for this test. Model M0 and M0A use the standard single ice temperature and phase OCCs from OpTool, model M0 uses Warren & Brandt (2008) H₂O I_c at 266 K, and model M0A uses Hudgins et al. (1993) H₂O I_a at 10 K data for the NIR and FIR wavelength regions of interest to this study. M0 is the model fitted in Sturm et al. (2024). We know that disks have radial temperature gradients and this widely used approach is not a realistic representation of ice throughout the disk. The other two models include our self-consistent H₂O ice optical constants. Model MDT uses our **DT** composite series, where crystalline ice is only present in the region of the disk that is 125 K and above. This is determined by the temperature structure calculations from RADMC-3D. Figure 9 shows that this region is deeply embedded in the disk and extends out to 3 AU based on the HH 48 NE system parameters. The rest of the ice in the disk is in the amorphous phase. This is the view of a disk without any additional dynamical processes transport or forming crystalline ice in unexpected outer regions. The final model, MDC, uses our **DC** composite series, meaning that the entire disk is populated by crystalline ice that has either been transported from the hot inner 3 AU region or been crystallised in situ through a thermal processing event, such as a global episodic accretion outburst or local planetesimal collisions. This ice will have subsequently cooled, retaining its crystalline structure. Theoretically, each of these crystallisation routes would produce different distributions of crystalline ices, but modelling each phenomenon individually is outside the scope of this paper. This model could test the reset versus inheritance scenario for sufficiently young disks; however, the age of class II disks is typically beyond the 0.5 Myr timescale on which re-amorphisation of the ices by ex-

ternal high-energy radiation or particles occurs (Grundy et al. 2006; Cook et al. 2007; McClure et al. 2015). Additionally, bulk crystallisation of the entire outer disk through infall and spreading has yet to be demonstrated by chemical models incorporating dynamics (Visser et al. 2011; Drozdovskaya et al. 2016).

In Figure 10, we present the small and large grain population opacities for each of the eleven possible ice mixtures including the cool down H₂O optical constants and the seven including the deposition temperature H₂O optical constants we use within our models. The changes in spectral profile for the 3, 45, and 63 μ m H₂O features between each measurement technique, and thus the ice phase, are evident from the opacities. We see that the small population opacities dominate at the 3, 45, and 63 μ m H₂O features wavelengths. We kept a constant grain size distribution for the dust only and dust and ice opacities, meaning that the dust-only opacities have a larger extinction than the dust and ice opacities in some wavelength regimes.

4. Results

We discuss the impact that self-consistently applying our new temperature-dependent H₂O OCCs to our expanded temperature-zoned RT models makes on the spectral profiles of the strongest water ice features, at 3, 45, and 63 μ m. We compared the spectral profiles to the same edge-on disk model of HH 48 NE using the single temperature OCCs widely used in the literature (e.g. Warren & Brandt 2008; Hudgins et al. 1993). We compare our output 3 μ m profiles to the JWST NIRSpec IFU observations of HH 48 NE, as seen in the left panel of Figure 11 for each of the four models, and make predictions about the spectral profiles of the 45 and 63 μ m features for future FIR space missions (right panel). Our results indicate that these features can effectively probe the thermal history of water ice.

4.1. 3 μ m ice absorption feature

4.1.1. Comparisons with HH 48 NE observations

The M0 model fits the depth of the 3 μ m ice feature but not necessarily the profile. In Sturm et al. (2023a), they suggest that the observed 3.2 μ m feature in the JWST NIRSpec IFU data, shown in Figure 11, could be an indication of crystalline ice in the disk. However, if the ices in HH 48 NE are crystalline, then using the Warren & Brandt (2008) crystalline ice at 266 K, as in the M0 model, is unlikely to match the profile, because the maximum sublimation temperature for water ice is 160 K under typical protoplanetary disk conditions.

Our MDC model, with the temperature-dependent optical constants and their self-consistent zoning throughout the RT model provides a better diagnostic of whether the 3.2 μ m feature arises in crystalline ice. We see that although the MDC model matches the depth of the 3.2 μ m feature given the fitted disk parameters, it also produces an extremely strong 3.085 μ m peaked feature that is completely absent from the observations. Since the bottom of the 3 μ m feature is clearly not saturated and past observations of edge-on disks (Terada & Tokunaga 2012; Terada et al. 2012) have shown that the depth of the 3.1 μ m peak is always stronger than the 3.2 μ m, the 3.2 μ m feature in HH 48 NE is better explained by some other solid state absorption than by crystalline water ice.

We see that the M0A model of the fully amorphous disk and the MDT model of the disk with warmed-up ices distributed according to the intrinsic temperature structure (which are mostly amorphous disk beyond 3 AU) both produce a very similar red

Table 3: Ice mixture and temperatures per region using **DC** and **DT** H₂O OCCs.

Region <i>T</i> range (K)	MDC Ice Species	Opacity Reg. #	MDT Ice Species	Opacity Reg. #
>161	Bare dust grains	10	Bare dust grains	6
161 - 147	H ₂ O[150]	9	H ₂ O[160]	5
147 - 125	H ₂ O[140]	8	H ₂ O[135]	4
125 - 91	H ₂ O[110]	7	H ₂ O[105]	3
91 - 78	H ₂ O[80], NH ₃	6	H ₂ O[75], NH ₃	2
78 - 70	H ₂ O[80], NH ₃ , CO ₂ :CO 3:1	5	H ₂ O[75], NH ₃ , CO ₂ :CO 3:1	1
70 - 50	H ₂ O[50], NH ₃ , CO ₂ :CO 3:1	4	H ₂ O[75], NH ₃ , CO ₂ :CO 3:1	
50 - 45	H ₂ O[50], NH ₃ , CO ₂ :CO 3:1, CH ₄	3	H ₂ O[30], NH ₃ , CO ₂ :CO 3:1, CH ₄	0
45 - 35	H ₂ O[40], NH ₃ , CO ₂ :CO 3:1, CH ₄	2	H ₂ O[30], NH ₃ , CO ₂ :CO 3:1, CH ₄	
35 - 25	H ₂ O[30], NH ₃ , CO ₂ :CO 3:1, CH ₄	1	H ₂ O[30], NH ₃ , CO ₂ :CO 3:1, CH ₄	
25 - 0	H ₂ O[20], NH ₃ , CO ₂ :CO 3:1, CH ₄	0	H ₂ O[30], NH ₃ , CO ₂ :CO 3:1, CH ₄	

Notes. The temperatures have been best matched to each region and in each phase but an exact match is not always possible. The temperature of the H₂O ice in each region is given in square brackets. The opacity region number columns correlate to those in Fig. 10.

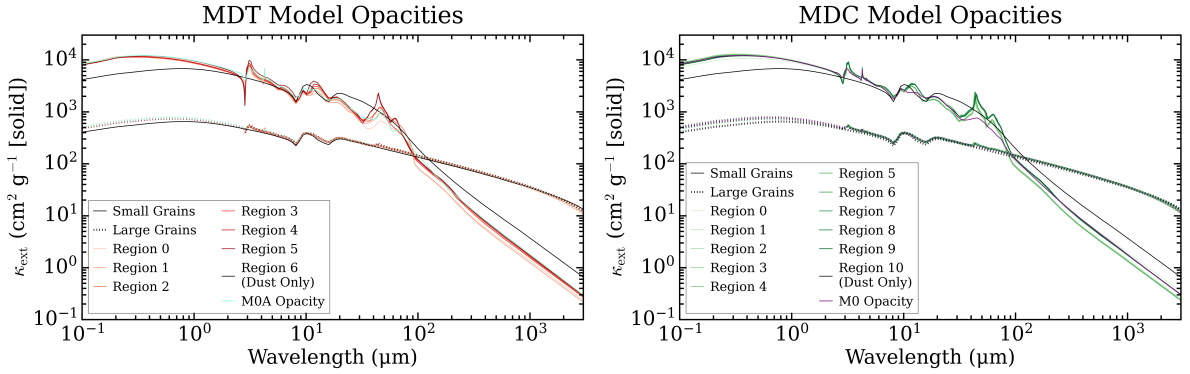


Fig. 10: Opacities of the ice mixtures (see Table 3) from cool down and deposition temperature optical constants. Left: Regional ice mixture opacities using the eight (**DC**) H₂O OCCs. Right: Regional ice mixture opacities using the five (**DT**) H₂O OCCs.

Table 4: Model names and their according H₂O ice OCCs.

Model Name	Optical Constants	H ₂ O Ice Properties
M0	Warren & Brandt (2008)	266 K I _c
M0A	Hudgins et al. (1993)	10 K I _a
MDC	Our DC series	Temp-dep. cooled I _c
MDT	Our DT series	Temp-dep. fixed temperature ices

wing shape to the M0 model. The lack of 3.1 and 3.2 μ m features in the Warren & Brandt (2008) crystalline ice composite demonstrates that it is not suited to modelling the known crystalline 3 μ m disk ice profiles from the literature. The blue wing of the observations does not show as sharp a slope as the M0 or MDC models, matching the amorphous M0A and MDT models more closely. This suggests that the H₂O ice in HH 48 NE is mostly amorphous.

The depth of the 3 μ m feature in model M0A does not match the observations well because Sturm et al. (2024) derived abundances using the Warren & Brandt (2008) optical constants to match the profile. Using the amorphous optical constants from Hudgins et al. (1993) would have required a higher abundance to fit the depth of the ice band in the observations. In the MDT model, the continuum underlying the 3 μ m feature is somewhat lower in flux. This offset is due to the temperature dependence

of n_{632nm} discussed in Section 2. For the same disk parameters, this would alter the SED fit and final ice abundances that would be derived. These results highlight the essential dependence of H₂O ice abundances on accurate optical constant measurements and their self-consistent application in RT models.

4.1.2. Locating the absorbing ices

We would like to use RT models to locate the absorbing ices within disks. Previously this has been accomplished by constructing a contribution function of the ices to the observed feature, which determines the region in which the ice originates within the model, and therefore its temperature. This has been done analytically for certain RT models (e.g. Equation 3 of McClure et al. (2015)). It is difficult to do with Monte Carlo codes such as RADMC-3D because backtracing scattered photons is not practical; however, in principle we should be able to use the temperature information encoded in the observed spectral profiles to provide constraints on the ices' location.

The MDT model, in which crystalline ice exists only in regions hot enough for amorphous ice to crystallise (>125 K), displays no crystalline absorption. This demonstrates that for HH 48 NE, which has typical classical T Tauri stellar and disk parameters, the only way to observe crystalline ice would be for it to be present over a large area of the outer disk. For crystalline ice to exist there, additional dynamical processes must have transported it there from the inner disk or generated it locally through heating events. This finding motivates further study of

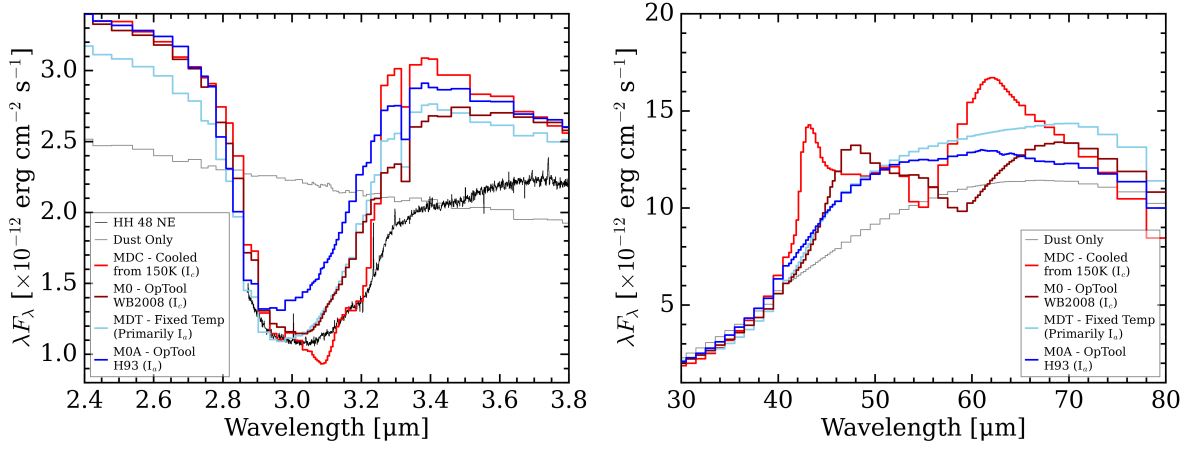


Fig. 11: 3 μm H₂O ice absorption feature and 45 and 63 μm H₂O ice emission feature spectral profiles from RADMC-3D models using the single temperature OCCs from Warren & Brandt (2008) (H₂O I_c - M0) and H₂O I_a based on Hudgins et al. (1993) (M0A) and our temperature-dependent *DT* and *DC* OCCs. These models use the HH 48 NE disk input parameters as determined by Sturm et al. (2024, 2023c); therefore, a profile comparison with the JWST NIRSpec IFU spectra of HH 48 NE (Sturm et al. 2023a) is shown.

similar edge-on classical T Tauri disks with crystalline ice 3 μm profiles, such as HK Tau B (Terada & Tokunaga 2012) and d216-0939 (Terada & Tokunaga 2012; Potapov et al. 2025) to determine the origin of their crystalline ice profiles. This is not necessarily the case for Herbig Ae/Be or F/G type intermediate-mass T Tauri disks, as their hotter central stars may allow ice to crystallise at more distant radii than in classical T Tauri disks and be observed without additional dynamical ice crystallisation mechanisms.

Although the peak wavelength shift from 3.1 μm at 150 K to 3.12 μm at 20 K in Mastrapa et al. (2009) seems like a promising metric with which to locate the crystalline ices beyond the 125 K isotherm from the observations, our MDC model shows that scattering induced by the disk geometry causes the peak wavelength to fall outside of this range, at 3.085 μm . This means we cannot use the peak wavelength of the 3 μm feature as a metric to infer a location of the absorbing ices. The importance of scattering to the 3 μm profile was also demonstrated empirically by Martinien et al. (2025), where they showed that the peak wavelength of the 3 μm feature shifts to shorter wavelengths at higher disk inclinations. HH 48 NE is at an inclination of 83°, an angle at which we expect significant scattering to occur, as demonstrated by Sturm et al. (2024).

4.2. 45 and 63 μm ice emission features

There are no observations of HH 48 NE in the FIR range to compare our models with, but we discuss below the application of these models to potential future FIR ice observations. The right panel of Figure 11 shows our four models. The M0 model exhibits broad emission features peaking at ~ 47 and ~ 70 μm , consistent with Sturm et al. (2024). In contrast, the temperature-dependent MDC model produces features at 43.2 and 62.2 μm , matching the expected peak wavelengths from Smith et al. (1994) for thermally processed crystalline H₂O ice that has cooled to <80 K. We can use these peak wavelengths to constrain the ice’s emission region. Figure 10 shows that the 45 and 63 μm features are dominated by the small-grain population, with $a_{\text{max}}=12.59$ μm , placing the contributing grains in the Rayleigh regime at these wavelengths. In this regime, scattering is negligible, and therefore the peak wavelengths shift only with temperature, not with grain size. Instead, Figure 3 of

McClure et al. (2012) demonstrated that while the 43 μm feature is very sensitive to the power of the grain size distribution, both features become flatter and develop red wings in response to increasing maximum grain size, such that the feature must trace maximum sizes smaller than 30 μm . Figure 6 of Kamp et al. (2018) confirms this finding for the Smith et al. (1994) optical constants as well. Therefore, the agreement between the MDC model peak wavelengths and the Smith et al. (1994) cooled crystalline ice measurements implies that the emitting ice in our model share the same thermally processed and subsequently cooled (<80 K) crystalline structure as in the laboratory experiments. This means ices in the disk atmosphere within ~ 13 AU of the central star do not contribute to the FIR features in our disk models (see Figure 9). Locating the exact radial origin of the strongest emission from our RT models would still require some kind of contribution function as in McClure et al. (2015) or Sturm et al. (2024).

The M0A model shows the clear lack of emission features in the FIR region. This is as expected as these features are specifically a result of crystalline H₂O ice. The MDT model completely emulates the shape of the continuum of the M0A in the FIR wavelength range with a very slight increase in flux.

5. Discussion

Our globally self-consistent H₂O ice OCCs will now enable modellers to retrieve full insights into each H₂O ice feature. Being able to predict spectral profiles of all the H₂O ice features using our OCCs and temperature-specific opacity zoning model setup will have far-reaching implications for RT disk modelling and NIR/FIR observational planning.

Firstly, our study demonstrates that constraints on the crystalline ice distribution can be found even using a single feature. We show that strong crystalline ice signatures in either the NIR and FIR feature profiles, for HH 48 NE’s disk parameters, must arise from ice residing in cool, outer disk regions, far from crystalline ice’s in situ forming region. These results strongly support the findings of McClure et al. (2015), Min et al. (2016), and Kamp et al. (2018) using the 45 and 63 μm features alone, where the FIR crystalline ices were all found to originate in the outer regions of disks as a result of dynamical processing occurring

within the disks. That we see the same effect for the NIR ices in our disk model implies that dynamical processes may also be the cause of ice crystallisation in classical (K0 and later spectral type) T Tauri disks, more generally.

Combining our model setup and OCCs should enable us to vary the ice's thermal history through the disk, allowing us to emulate the effects of different local dynamical processes such as viscous spreading or planetesimal collisions. We explore this in Smith et al. (in prep.), where we vary the ice crystallinity throughout the disk model through abundance ratios throughout the entire disk but also through varying the spatial distribution of crystalline H₂O ice throughout the disk. Such models may identify spectral profile indicators associated with each dynamical process, and therefore greatly enhance the interpretation of edge-on disk observations.

Unfortunately, very few objects have both NIR and FIR ice observations. Comparative samples will not become available until a FIR observatory becomes operational. These models and OCCs linking the 3 μ m and 45 and 63 μ m features will aid in the interpretation of archival NIR and FIR observations, new JWST NIR observations, and future FIR missions, such as the Planetary Origins and Evolution Multispectral Monochromator (PO-EMM), PRobe far-Infrared Mission for Astrophysics (PRIMA), and the Far-Infrared Great Observatory (FIGO). The ability to accurately select disks that will show crystalline ice features for future observations in the NIR or FIR will require zoned RT models, such as ours, to reveal what information each feature provides observers with.

6. Conclusions

In this study, we build the first set of self-consistent H₂O ice OCCs across the full wavelength range required for RT modelling. We have done so for ices with two different thermal histories: deposited-and-cooled (*DC*) and deposited-and-measured at a fixed temperature (*DT*). By doing so we have improved the derivation of the *n* values for H₂O ice using data across a broad wavelength range, while identifying wavelengths that require new experimental data. These updates enable the derivation of accurate H₂O ice opacities across many different physical and chemical environments. Our OCCs have been uploaded to a Zenodo repository, DOI: 10.5281/zenodo.2031356.

We have also updated the RADMC-3D RT model of the edge-on classical T Tauri disk HH 48 NE (Sturm et al. 2024) to include temperature zoning appropriate for our new OCCs. With these new RT models, we have demonstrated self-consistent ice analysis across the full RT model wavelength, improving on previous local to FIR self-consistent modelling efforts from McClure et al. (2012, 2015); Min et al. (2016) and Kamp et al. (2018). Our models clearly show that observations of the NIR and FIR ice profiles can pinpoint the origin of crystalline ice features in the cold outer regions of classical T Tauri disks, below their nominal crystallisation temperature. These results indicate that classical T Tauri disks with observed crystalline H₂O profiles must host additional dynamical processes such as viscous spreading, accretion event heating, or planetesimal collisions. The combination of our new OCCs and updated RT models enables us to begin testing how these different dynamical processes can be traced via the profiles of the 3, 45, and 63 μ m ice features.

This work provides the basis for self-consistent H₂O ice modelling within RT models, allowing modellers to begin to trace the thermal and structural evolution of H₂O ice from molecular clouds through to planetary systems. Essentially, these OCCs provide the basis for accurate planning of analysis of

observations of complementary datasets across multiple instruments.

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Appendix A: Interpolation regions

A.1. *DT*

A.1.1. 2.64 - 2.82 μm interpolation

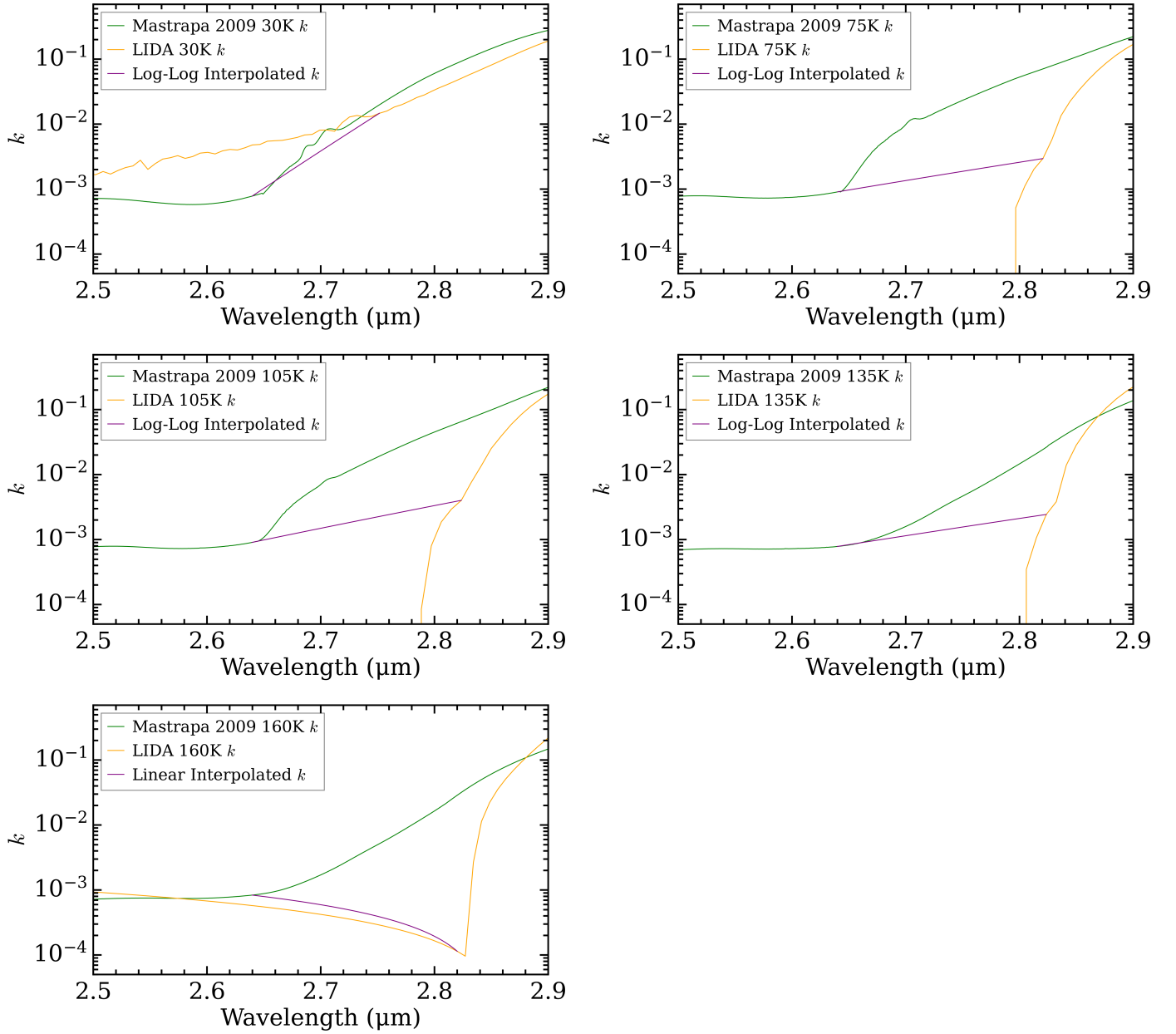


Fig. A.1: k value interpolation between the Mastrapa et al. (2009) and Rocha et al. (2024) NIR data of the *DT* OCC series. Note the 30 K interpolation only reaches 2.75 μm instead of 2.82 μm . Also note that the 160 K composite uses linear interpolation rather than log-log interpolation.

A.1.2. NIR - FIR interpolation

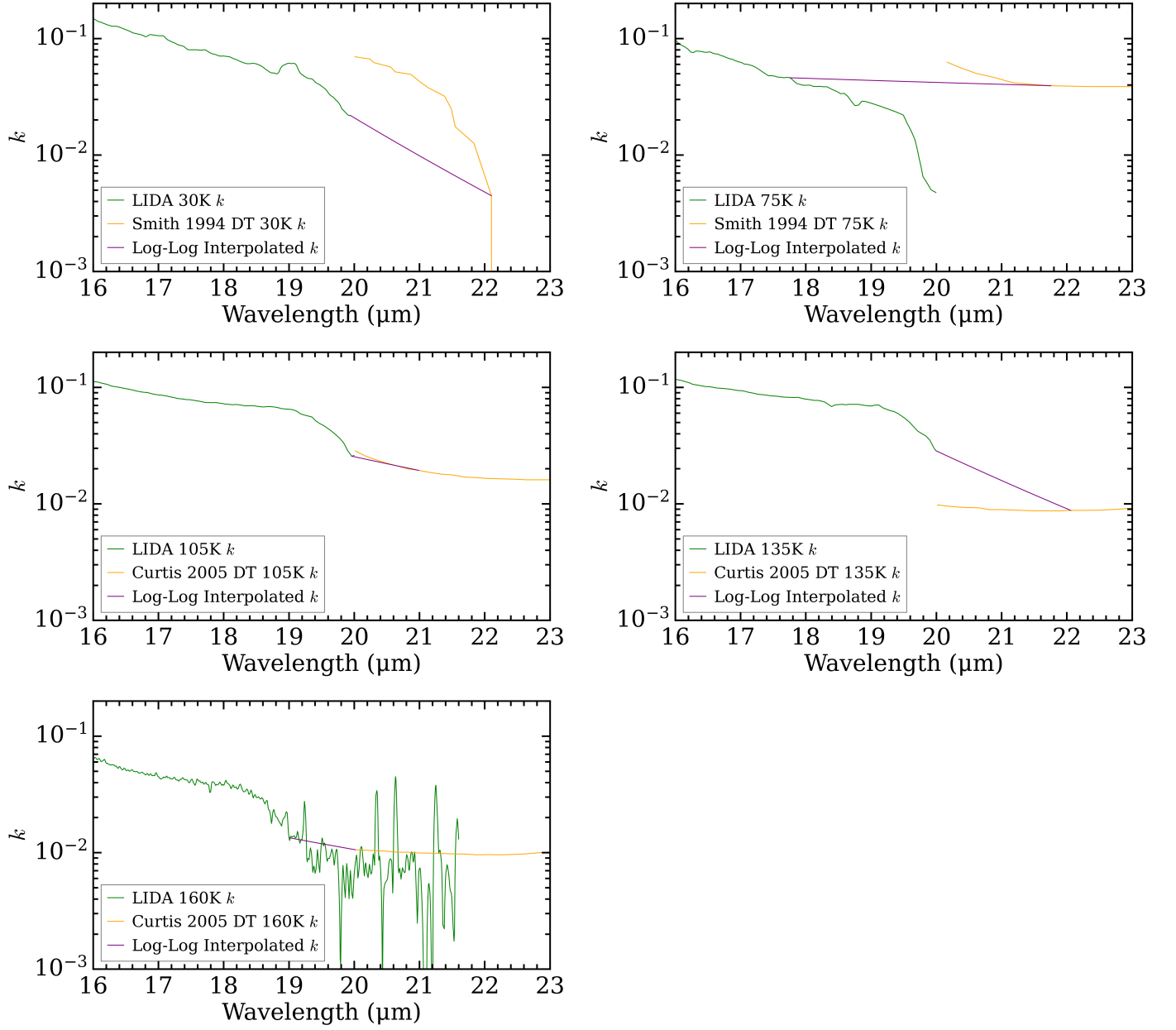


Fig. A.2: k value interpolation between the end of the Rocha et al. (2024) NIR data and the start of the Smith et al. (1994) data of the *DT* composites.

A.1.3. 74.5 - 94 μm interpolation

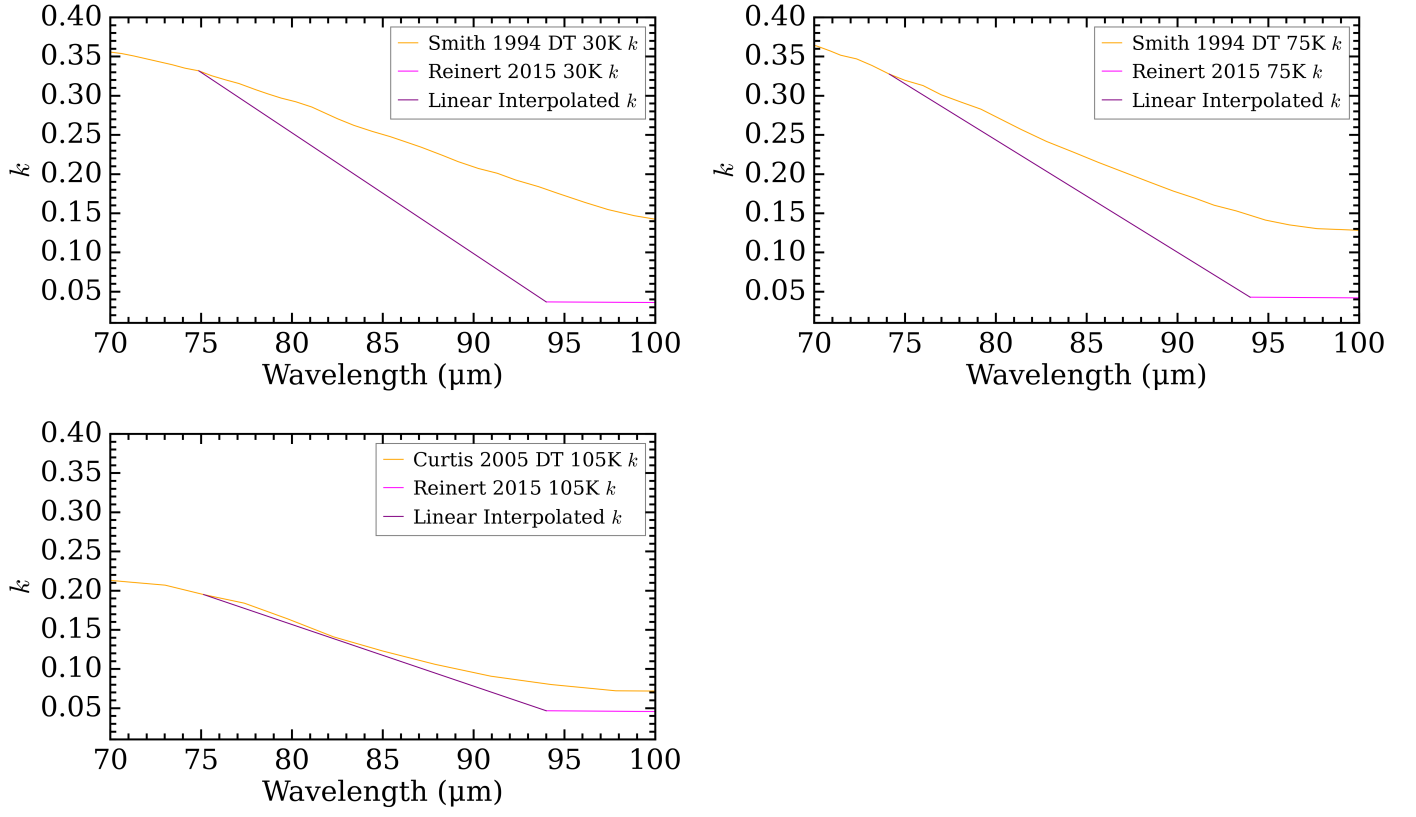


Fig. A.3: k value interpolation between the end of the Smith et al. (1994) FIR data and the start of the Reinert et al. (2015) model of the *DT* 30 K, 75 K and 105 K composites. The 135 K and 160 K required no interpolation.

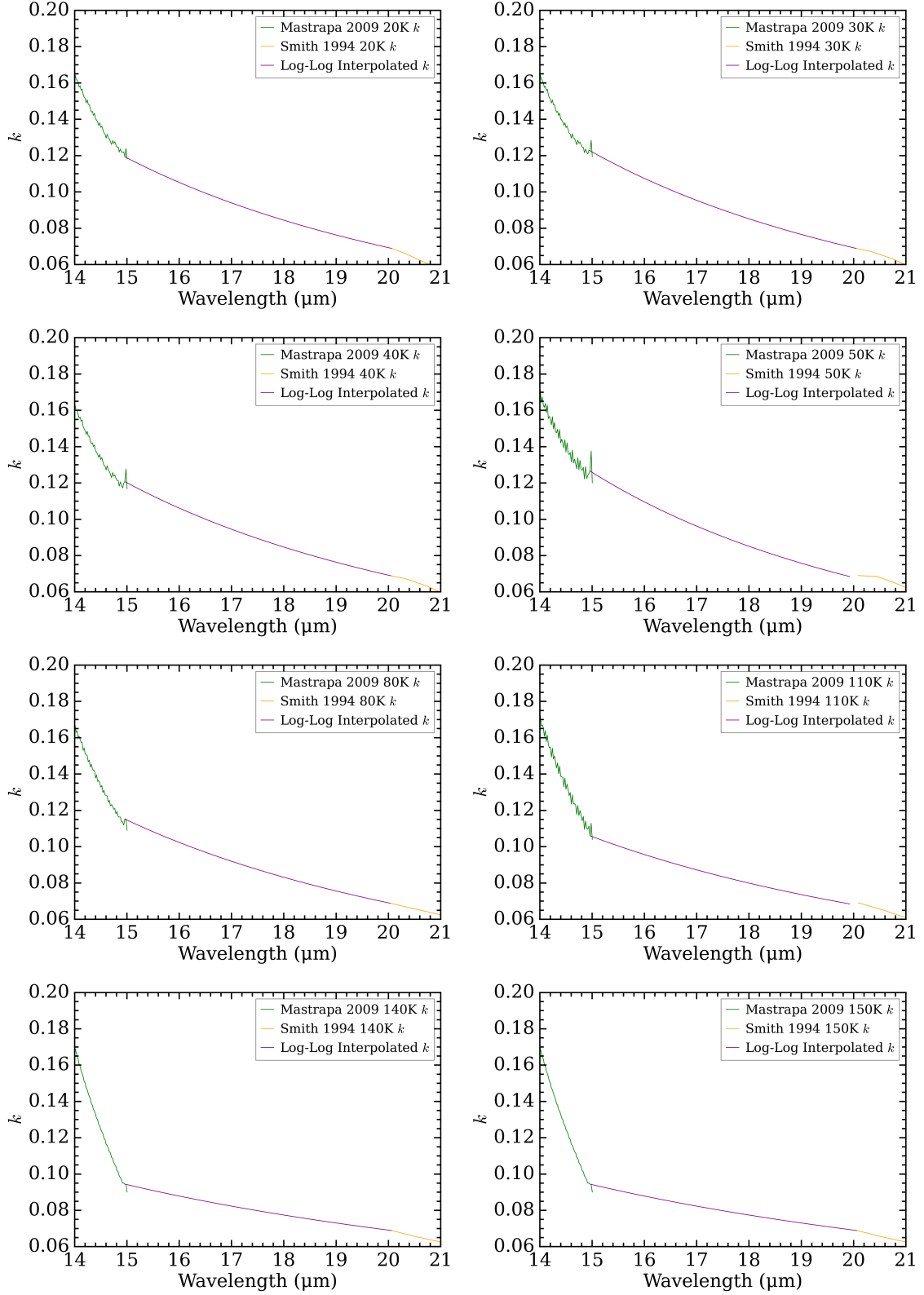
A.2. **DC**A.2.1. 15 - 20 μm interpolation

Fig. A.4: k value interpolation between the end of the Mastrapa et al. (2009) NIR data and the start of the Smith et al. (1994) FIR data of the **DC** composite.

A.2.2. 74.5 - 94 μ m interpolation

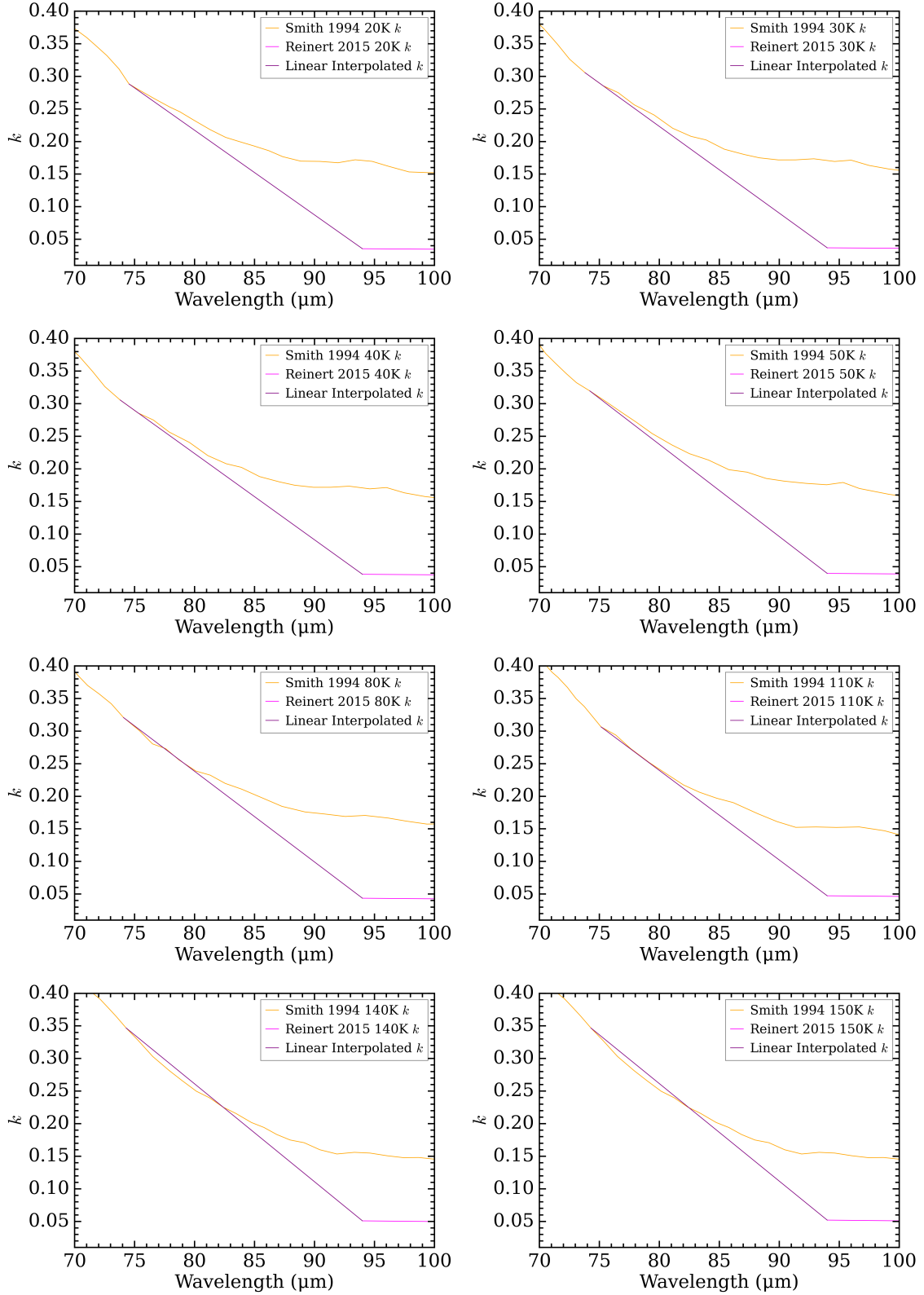


Fig. A.5: k value interpolation between the end of the Smith et al. (1994) FIR data and the start of the Reinert et al. (2015) model for all *DC* composites.