



Infrared Band Strength of Molecular Oxygen in Astrophysical Ices

William A. Burris¹ , Mark J. Loeffler^{1,2} , Stephen C. Tegler¹ , and William M. Grundy^{1,3}

¹Department of Astronomy and Planetary Science, Northern Arizona University, 527 S. Beaver Street, Flagstaff, AZ 86011, USA

²Center for Materials Research and Applications, Northern Arizona University, 527 S. Beaver Street, Flagstaff, AZ 86011, USA

³Lowell Observatory, 1400 W. Mars Hill Road, Flagstaff, AZ 86001, USA

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Abstract

Some quantity of molecular oxygen (O₂) is likely condensed on the surface of interstellar ice mantles, yet this compound has never been detected in the solid phase in the interstellar medium. With the sensitivity of the James Webb Space Telescope, it seems reasonable that future detections could be possible. Here we present measurements of the band strength of the O₂ infrared fundamental ($\sim 6.46 \mu\text{m}$) in a number of representative astrophysical ice environments. We find that in binary ice mixtures of O₂ and H₂O (or CO₂), the band strengths are the same within error ($2.2 \times 10^{-20} + / - 0.3 \times 10^{-20} \text{ cm molecule}^{-1}$ and $1.9 \times 10^{-20} + / - 0.3 \times 10^{-20} \text{ cm molecule}^{-1}$, respectively), while the band strength in CO mixtures is $\sim 4\times$ lower. Considering the case where O₂ is mixed with H₂O at percentages measured in cometary coma, we estimate that it could take as little as 2 hr to reach a signal-to-noise ratio where O₂ could be detected with the MIRI instrument.

Unified Astronomy Thesaurus concepts: Astrochemistry (75); Interstellar medium (847); Infrared spectroscopy (2285); Interstellar molecules (849); Ice spectroscopy (2250); James Webb Space Telescope (2291); Molecular clouds (1072); Laboratory astrophysics (2004)

1. Introduction

Molecular oxygen (O₂) is believed to play a critical role in the chemical evolution of material in the interstellar medium (ISM) (A. G. G. M. Tielens & W. Hagen 1982). However, detections of O₂ have been limited to submillimeter spectroscopy in three locations: star-forming molecular cloud ρ Ophiuchi A (P. F. Goldsmith et al. 2002; B. Larsson et al. 2007; R. Liseau et al. 2012), Orion (P. F. Goldsmith et al. 2011; J.-H. Chen et al. 2014), and the galaxy Mrk 231 (J. Wang et al. 2020). The lack of more detections in the radio are not, however, for a lack of trying (P. F. Goldsmith et al. 1985; H. S. Liszt 1985; H. S. Liszt & P. A. Vanden Bout 1985; P. F. Goldsmith & J. S. Young 1989; F. Combes et al. 1991; L. Pagani et al. 1993; F. Combes & T. Wiklind 1995; F. Combes et al. 1997; G. Olofsson et al. 1998; P. F. Goldsmith et al. 2000; L. Pagani et al. 2003; G. J. Melnick et al. 2012; U. A. Yldz et al. 2013; N. Kanekar & D. S. Meier 2015; A. Sandqvist et al. 2015; E. S. Wirström et al. 2016; V. Taquet et al. 2018; B. J. Williams et al. 2023; B.-R. Wang et al. 2024). Efforts using infrared (IR) spectroscopy to identify solid O₂, which is presumably present in the outer mantle of interstellar grains, have also been unsuccessful (P. Ehrenfreund & E. F. van Dishoeck 1998; B. Vandenbussche et al. 1999; E. F. van Dishoeck et al. 2025).

The difficulty in confirming the existence of interstellar O₂ via submillimeter or IR spectroscopy is not too surprising. As a homonuclear species, O₂ does not possess a permanent dipole moment, which makes it a weak absorber. Laboratory studies measuring the absorption band strength (A), which is used to calculate column densities of molecules from spectroscopic observations, support this assertion. For instance, the reported values for the IR fundamental O₂ transition at $\sim 6.46 \mu\text{m}$ (1549 cm^{-1}) are generally 3–4 orders of magnitude smaller

than other IR active species, such as H₂O, CO, and CO₂ (P. Ehrenfreund et al. 1992; B. Müller et al. 2018). Interestingly, those studies also report that the O₂ band strength depends on concentration, while P. Ehrenfreund et al. (1992) also report that the companion species can alter the A-value. Reports for N₂ have also shown that the A-value depends on concentration and companion species (M. P. Bernstein & S. A. Sandford 1999).

While the reported laboratory studies support why homonuclear species, such as O₂, have not been more widely detected in the ISM, the wide range of A-values reported (7.6×10^{-21} to $3.0 \times 10^{-18} \text{ cm molecule}^{-1}$; P. Ehrenfreund et al. 1992; B. Müller et al. 2018) suggests that a closer look is warranted. Quantifying what environment would be the most conducive for detecting these molecules could significantly narrow down the breadth of any future observing campaign. It could also give specific estimates for whether current observational capabilities, such as the James Webb Space Telescope (JWST), could effectively identify these homonuclear species.

Here, we present results from a series of experiments measuring the band strength of the O₂ fundamental absorption band in different astrophysical ice mixtures. Specifically, we grew binary ice mixtures of O₂ and H₂O, CO, or CO₂ over a range of concentrations to determine whether there was an environment that would be the most conducive to identifying O₂ in the ISM. We also investigated the effect that thermal annealing and temperature cycling have on the observed absorption features. Finally, we use these results to form observational time estimates for possible future JWST campaigns.

2. Methods

We performed all of our experiments in an ultrahigh vacuum chamber (UHV) capable of reaching temperatures as low as $\sim 12 \text{ K}$ with a base pressure of $\sim 10^{-9} \text{ torr}$ (P. D. Tribbett & M. J. Loeffler 2022). While we have



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previously utilized this system to perform UV-vis and IR reflectance spectroscopy using a gold-coated quartz crystal microbalance (QCM) as our substrate, we have recently added a second substrate (KBr salt window) to the system, which is vertically offset from the QCM, to allow us to perform transmission spectroscopy. We can align either of these substrates with our instrumentation by vertically translating our sample holder. As described below, utilizing both substrates, we can measure the density, refractive index, and thickness of the ices, as well as the band strengths for absorption features of interest.

2.1. Growth and Composition

We deposited pure ices of O₂ (99.997%, Matheson Gas), H₂O (high-performance liquid chromatography grade, Sigma Aldrich), CO₂ (99.99%, Matheson Gas), and CO (99.9% Matheson Gas). We also codeposited binary mixtures of O₂ and either H₂O, CO₂, or CO from separate manifolds into the chamber. For these experiments, we grew our ices via background deposition (105° between intake valve and substrate surface) at 15 K. We also removed the thermal radiation shield from our system so we could deposit films on both substrates simultaneously.

Regardless of which substrate is aligned with our instrumentation, we determine the composition of our mixture using the QCM (C.-S. Lu & O. Lewis 1972), taking into account the slight (~8%) difference in the deposition rate in the two QCM positions. We first grow a thin layer of the companion species to establish its growth rate. This results in a layer ~1%–2% of the total sample thickness. Then, we add O₂ to the chamber for the codeposited layer. Near the end of deposition, we stop the flow of O₂ and recheck the growth rate of the companion species. We find that the final growth rate of the companion species is typically within +/–5% of the initial growth rate. The resulting companion species layers are thin compared to the overall thickness of the mixed ice layer, minimizing any impacts at the interface boundaries shared by two layers. As the system pressure drops down to the level prior to leaking O₂ into the chamber within 10–15 s, whereby the growth rate remains constant, we assume that the final growth rate is exclusively the companion species. Thus, we take the average of the initial and final growth rates to establish the mean growth rate of the companion species during codeposition. Knowing the time elapsed, as well as the total mass deposited, we can determine the mass of each species in the mixed portion of the sample. We can then convert this mass (excluding the mass of the pure companion species on both sides of the codeposited layer) into a number ratio (concentration). Finally, we note that although the lowest concentrations reported for each companion species are higher than what cometary observations suggest might be found on a typical interstellar ice mantle (A. Bieler et al. 2015; M. Rubin et al. 2015), they represent the most dilute mixture that we could confidently quantify.

2.2. UV-Vis

We take UV-vis reflection spectra during growth in all experiments. We use the data taken with the gold substrate to solve the Fresnel equations via MCMC modeling (P. R. Behr et al. 2020; P. D. Tribbett & M. J. Loeffler 2022;

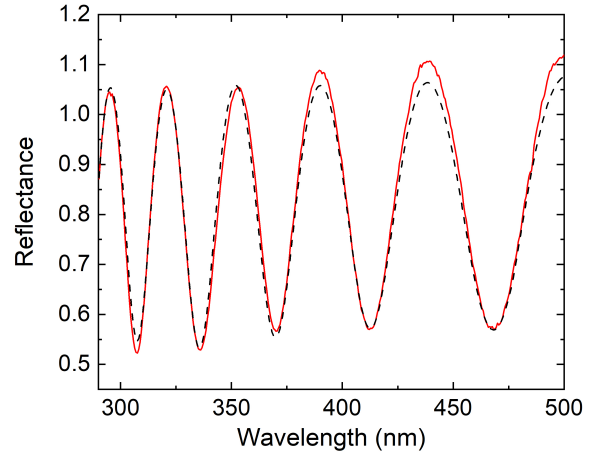


Figure 1. An example of the MCMC best fit (black dashed) of the Fresnel equations to a UV-vis spectrum (red solid) of a 1:1 O₂: H₂O mixture ~1441 nm thick.

R. A. Carmack et al. 2023). The resulting fit includes the refractive index of the ice at all wavelengths, as well as the sample thickness. As the QCM monitors the aerial mass of the sample, we can also calculate the density of the ice (P. R. Behr et al. 2020; P. D. Tribbett & M. J. Loeffler 2022; R. A. Carmack et al. 2023). In Figure 1, we show a typical example of our spectra and the corresponding theoretical fit. As the substrates are in the same orientation when each is aligned with our instrument, we assume that the density and refractive index of the ice deposited on the KBr substrate is the same as what we directly measured on the gold substrate.

We point out that we observed a systematic decrease in the estimated density (ρ) and refractive index (n) with increasing sample thickness. We speculate this is due to scattering in the sample, which we model as a Rayleigh scatterer (B. Hapke 2012; M. Born & E. Wolf 2013). As this decrease is only 4% or less for the majority of thin samples (<1100 nm), we take the mean of ρ and n from fits between, typically, 200–1100 nm, with some variation between different experiments and different species.

When utilizing the KBr substrate, we monitor the UV-vis reflectance spectra as a function of time to directly measure the thickness of our ice sample using

$$t = \frac{N\lambda}{2\sqrt{n^2 - \sin^2(i)}}, \quad (1)$$

where N is the number of fringes, λ is the wavelength of light, n is the refractive index determined from the gold substrate experiments, and i is the angle of incidence (25°) for our light source (O. S. Heavens 1965). Although we have the ability to measure the fringes versus time across a range of wavelengths, we determined the thickness using $\lambda = 500$ nm. With the composition derived from the adjacent QCM, we can use the thickness measurement to determine the column density of each component as a function of time during growth.

2.3. IR Spectroscopy and Band Strengths

While we are measuring the sample thickness on the KBr substrate, we are also collecting transmission spectra between

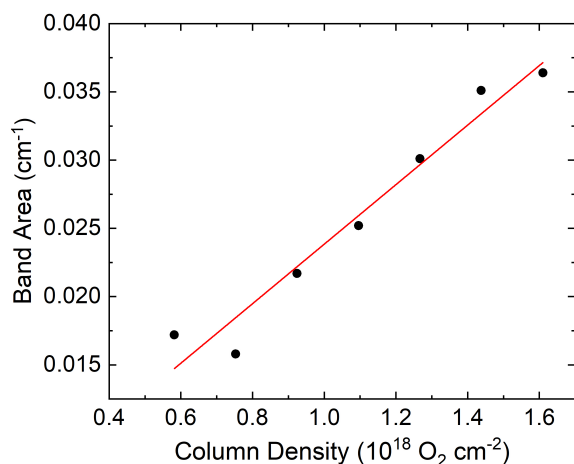


Figure 2. An example of the data used to calculate the band strength for O₂ in a 1:1 O₂: H₂O mixture. The slope of the linear fit (solid line) is A'.

12,000 and 500 cm⁻¹ using the IR light source from a Thermo–Nicolet iS50 Fourier Transform Infrared Spectrometer and an MCT-A detector at a spectral resolution of 2 cm⁻¹. We average 150 individual scans from our sample and 400 scans from our reference prior to converting them to units of optical depth ($\tau = -\ln(T/T_0)$), where T is the transmitted intensity through the sample, and T_0 is the transmitted intensity through the bare KBr substrate.

We use the transmission spectra to determine the apparent band strength (A'), distinct from the absolute band strength (A), of an absorption feature of interest. The difference between the two is that A is derived from the optical constants of the sample, which takes into account the possible influence of surface reflections and optical interference, while A' is derived directly from the band area of the absorption feature. For more details, see R. L. Hudson et al. (2014a, 2014b) and P. A. Gerakines & R. L. Hudson (2015a), and references therein. We minimized the possible contribution from surface reflection effects by growing thicker samples (S. Maeda & P. N. Schatz 1961) while we monitored the potential for interference effects by taking infrared spectra over a wide range of thicknesses to see whether the absorption bands of interest deviated from the straight line predicted by the Beer–Lambert Law (e.g., B. D. Teolis et al. 2007). Plotting the continuum-removed band area of the absorption feature versus its column density and calculating the slope yields A' (Figure 2). We do not constrain the best-fit line to pass through the origin.

To place constraints on our band strengths, we error propagate ρ , n , the mass percentages, and the deposition rate. If the error propagation value is larger than the error of the best-fit line, we adopt the error propagation as the error on the band strength. If the opposite is true, we adopt the error in the best-fit line as the band strength error.

3. Results

3.1. IR Spectra and Thermal Stability

In Figures 3–5, we show selected IR spectra of 1:1 O₂: H₂O, O₂: CO₂, and O₂: CO mixtures, focusing on the region that contains the fundamental stretching vibration of O₂ (B. R. Cairns & G. C. Pimentel 1965). The peak position across all concentrations in H₂O and CO mixtures is

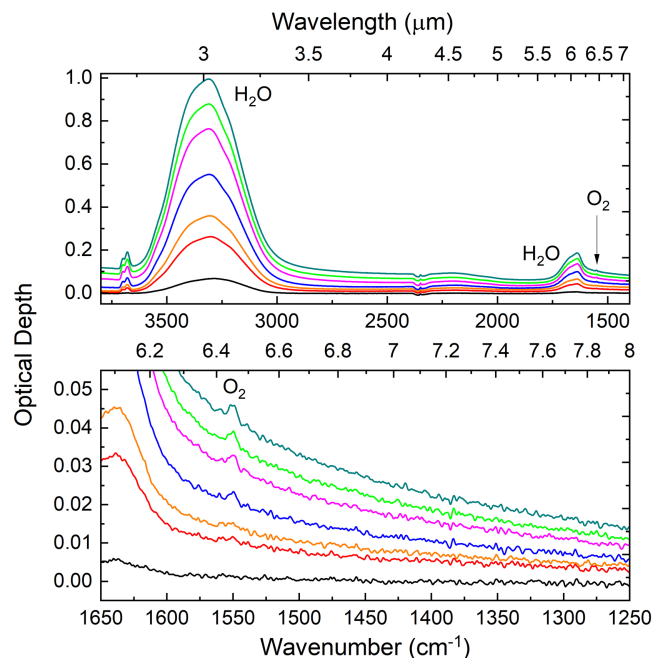


Figure 3. IR spectra of a 1:1 O₂: H₂O mixture during growth. Spectra have been vertically offset for clarity and (from bottom to top in each panel) correspond to a total thickness of ~61, 330, 465, 734, 1005, 1141, and 1275 nm.

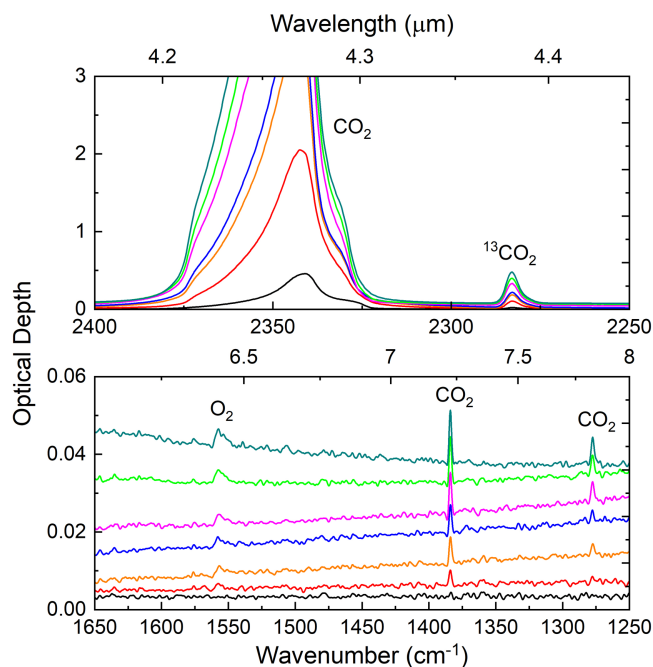


Figure 4. IR spectra of a 1:1 O₂: CO₂ mixture during growth. Spectra have been vertically offset for clarity and (from bottom to top in each panel) correspond to a total thickness of ~64, 450, 857, 963, 1472, 1729, and 2114 nm.

consistent, ~1549 and 1551 cm⁻¹, respectively. The peak position in CO₂ mixtures varied slightly with concentration: in 1:1 mixtures, the position is located at ~1552 cm⁻¹, while at lower concentrations it shifted to ~1558 cm⁻¹. The full width at half-maximum (FWHM) is also similar across all concentrations in H₂O (~8 cm⁻¹) and CO (~5 cm⁻¹). The FWHM in 1:1 CO₂ mixtures is ~8 cm⁻¹ and is ~5 cm⁻¹ in lower concentrations.

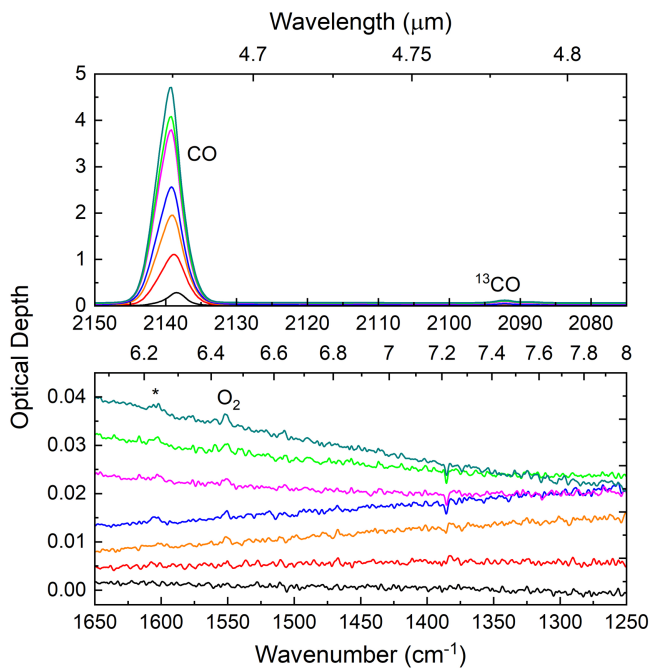


Figure 5. IR spectra of a 1:1 O₂: CO mixture during growth. Spectra have been vertically offset for clarity and (from bottom to top in each panel) correspond to a total thickness of ~ 70 , 444, 818, 1065, 1564, 1689, and 1939 nm. A trace amount of water contamination is marked by an *.

While this spectral region is generally devoid of other absorption features, we find a feature at 1602 cm^{-1} in the CO mixture and features at 1384 and 1277 cm^{-1} in the CO₂ mixture. We attribute the feature in the CO mixture to trace H₂O contamination (P. Ehrenfreund et al. 1996), while the two features in CO₂ are forbidden transitions (M. Falk 1987; P. A. Gerakines & R. L. Hudson 2015b).

We also studied the thermal stability of the O₂ absorption band in the H₂O and CO₂ mixtures by heating the sample to around 30 K, while monitoring the mass loss and the absorption band area. We chose 30 K because the sublimation of pure O₂ at that temperature is negligible on the timescale it takes to collect one spectrum (B. P. Blakley et al. 2024). We are interested in seeing whether annealing would cause the band area to decrease when there is little to no mass loss in the sample, as has been observed previously in pure O₂ (B. R. Cairns & G. C. Pimentel 1965). Using the QCM, we verified that we lost $<1\%$ of our sample upon heating to 30 K and recooling. However, we find that the first annealing causes the band area to permanently decrease by $\sim 5\%$ – 20% , with the largest effect being at 15 K. Subsequent annealing seems to cause no additional decrease. After annealing the sample, we also see that the band area is $\sim 15\%$ lower at 30 K than at 15 K, yet this is reversible.

3.2. Density and Refractive Index

In Figures 6 and 7, we plot ρ and $n(500\text{ nm})$ calculated for pure H₂O, CO₂, and CO, as well as those values for binary mixtures with O₂. For pure H₂O, we find a density of 0.69 g cm^{-3} and $n(500\text{ nm})$ of 1.21. For pure CO₂, we find a density of 1.15 g cm^{-3} and $n(500\text{ nm})$ to be 1.24. For pure CO, we find a density of 0.99 g cm^{-3} and $n(500\text{ nm})$ to be 1.24. For pure O₂, data not shown here, we find a density of 1.50 g cm^{-3} and $n(500\text{ nm})$ of 1.28. In each case, as the

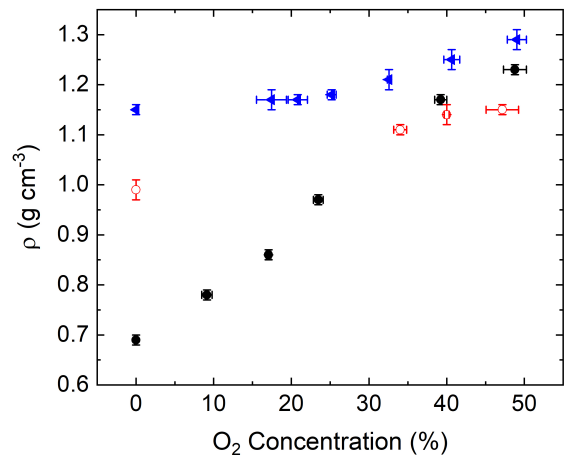


Figure 6. Measured density for O₂: H₂O (black circles), O₂: CO₂ (blue triangles), and O₂: CO (red open circles) mixtures versus O₂ concentration. A number fraction of 0 is a pure ice of the companion species.

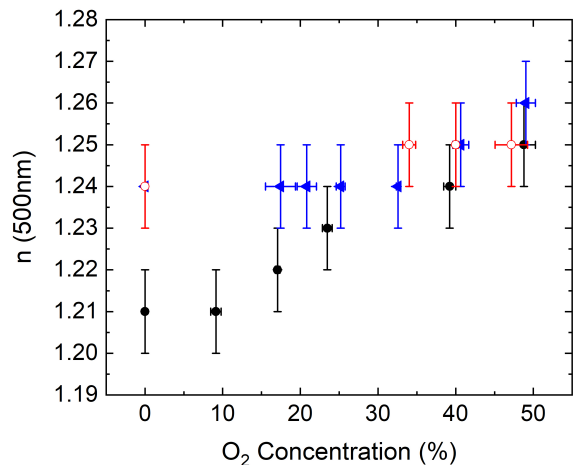


Figure 7. Measured refractive index at 500 nm for O₂: H₂O (black circles), O₂: CO₂ (blue triangles), and O₂: CO (red open circles) mixtures versus O₂ concentration. A number fraction of 0 is a pure ice of the companion species. The data points for pure CO and CO₂ are overlapping.

concentration of O₂ increases in the mixture, the density increases somewhat linearly. While $n(500\text{ nm})$ may also have a similar dependence, the error is too large to say definitively. Finally, we note that the refractive indices of the pure component and codeposited layers are similar, minimizing any potential issues with reflection/refraction at the sandwich layer interface.

3.3. Band Strength

Using the method described in Figure 2, we calculate A' for O₂ as a function of concentration (e.g., O₂/(H₂O + O₂)) and companion species (Figure 8). While the majority of the data spread is likely a consequence of the small nature of the O₂ band, the 1:1 O₂: CO₂ mixture shows repeatable larger band strength values. We suspect that this is because the FWHM of the 1:1 mixture is nearly a factor of 2 larger than in the other CO₂ mixtures. Thus, while the A' -value that we report (Table 1 and dashed/dotted lines in Figure 8) is an average across all mixtures in the H₂O and CO experiments, we

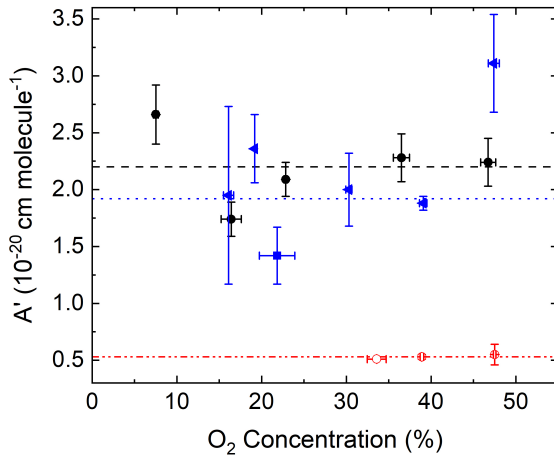


Figure 8. A'-value of O₂ in O₂: H₂O (black circles), O₂: CO₂ (blue triangles), and O₂: CO (red open circles) mixtures versus O₂ concentration. The dashed line is the mean for all of the H₂O experiments, the dotted line is the mean for all of the CO₂ experiments, excluding 1:1 concentrations, and the dashed-dotted line is the mean for all of the CO experiments.

Table 1
A'-values for O₂ in H₂O, CO, and CO₂

Companion Species	Concentration (Species:O ₂)	O ₂ A' (10 ⁻²⁰ cm molecule ⁻¹)	References
H ₂ O	10:1-1:1	2.2 (0.3)	This work
CO	2:1-1:1	0.5 (0.1)	This work
CO ₂	5:1-1:1	1.9 (0.3)	This work
CO ₂	1:1	60	(1)
CO ₂	10:1	300	(1)
CO	1:1	7	(1)
H ₂ O:CO	1:1:1	7	(1)
H ₂ O:CO:CO ₂	2:2:0.5:1	10	(1)
H ₂ O	9:1-1:1	0.76–3.9	(2)
H ₂ O	1:2-1:9	6.4–32	(2)

Note. (1) P. Ehrenfreund et al. (1992); (2) B. Müller et al. (2018).

excluded the 1:1 mixture results when calculating an A'-value in the CO₂ experiments. We find that A' for O₂ in H₂O and CO₂ are the same within error but about 4 times higher than in mixtures with CO.

We also measured the band strength of the main absorption bands in our companion species (Table 2). We show values for both our measurements of pure ices, as well as those obtained by averaging across all concentrations of O₂.

4. Discussion

4.1. Comparison to Previous Studies

4.1.1. ρ , n , and L

Previous studies (e.g., M. S. Westley et al. 1998; R. A. Baragiola 2003; Z. Dohnálek et al. 2003; M. J. Loeffler et al. 2016; V. Kofman et al. 2019) have shown that growth conditions, such as the deposition temperature, deposition tube, deposition angle of incidence, and deposition rate, can have significant effects on the ρ and n of an ice. Thus, below, in addition to n and ρ , we will also compare the Lorentz–Lorenz factor (L) using Equation (2), which relates ρ and n of a material (H. A. Lorentz 1880; L. Lorenz 1881) and should

theoretically be the same regardless of growth conditions.

$$\frac{n^2 - 1}{n^2 + 2} = L\rho. \quad (2)$$

We point out that since n depends on wavelength, we considered whether our comparison would be complicated by many of the previous studies reporting values between 600 and 700 nm. However, we found that, in our samples, the difference in n between 500 and 670 nm is <0.01 , and so we neglect any wavelength dependence in our comparison. Finally, R. Luna et al. (2012) demonstrated that the resulting ρ and n values of ice mixtures is not a simple linear mix of the individual ρ and n values, and so below we limit our comparison to pure ices.

For pure H₂O, we measured a ρ of 0.69 g cm⁻³, which is consistent with the works of Z. Dohnálek et al. (2003), R. A. Baragiola (2003), U. Raut et al. (2007), J. B. Bossa et al. (2014), and R. A. Carmack et al. (2023) who all measured the density of 0.6–0.74 g cm⁻³ for background deposited H₂O ice grown between 20 and 40 K. Z. Dohnálek et al. (2003) and J. B. Bossa et al. (2014) also measured n to be 1.19 and 1.203, respectively, yielding an L -value of 0.196 and 0.190, which is consistent with our value at 0.194. V. Kofman et al. (2019) measured n of background deposited H₂O to be 1.1924 and 1.2104 at 10 and 30 K, consistent with our values.

For pure CO₂, we measured a ρ of 1.15 g cm⁻³ and an n of 1.24, yielding $L = 0.132$ cm³ g⁻¹. W. Schulze & H. Abe (1980), B. E. Wood & J. A. Roux (1982), M. Satorre et al. (2008), and M. J. Loeffler et al. (2016) report n values of 1.22–1.27 and ρ -values of 0.98–1.20 g cm⁻³ for pure CO₂ grown between 4 and 20 K. Our L -value is slightly lower than the derived values in the literature of 0.141–0.157 cm³ g⁻¹ but is within 10% of the 0.141 derived using a number of different deposition conditions in the same experimental setup (M. J. Loeffler et al. 2016).

For pure CO, we measured a ρ of 0.99 g cm⁻³ and an n of 1.24, yielding $L = 0.154$ cm³ g⁻¹. The density value is higher than the 0.8 g cm⁻³ often cited in the literature (J. A. Roux et al. 1980) but is more consistent with other studies that have reported values in the range of 1.029–1.04 g cm⁻³ (I. N. Krupskii et al. 1973; L. Wang et al. 2020; P. A. Gerakines et al. 2023; I. Vegard 1930). The n -value is slightly lower than the 1.294 reported by P. A. Gerakines et al. (2023), which is also why our derived L -value is slightly lower than their derived value of $L = 0.178$ cm³ g⁻¹.

For pure O₂, we measured a ρ of 1.50 g cm⁻³ and an n of 1.28, yielding $L = 0.117$ cm³ g⁻¹. Our ρ -value is similar to that reported by I. N. Krupskii et al. (1979) but slightly higher than reported by J. A. Roux et al. (1980) (1.534 g cm⁻³ at 16 K and 1.22 g cm⁻³ at 20 K, respectively), while our refractive index value is similar to that reported by J. Kruger & W. J. Ambs (1959), J. A. Roux et al. (1980), and D. Fulvio et al. (2009) (1.25 at 4.2 K, 1.22 at 20 K, and 1.322 at 16 K, respectively). Interestingly, J. A. Roux et al. (1980) reported an L -value of 0.112 cm³ g⁻¹, which is essentially the same as our derived value.

4.1.2. O₂ A'

In Table 1, we compare our measured O₂ band strengths to previous studies. Our results are, at worst, within a factor of ~ 2 for similar concentrations studied by B. Müller et al. (2018),

Table 2
A'-values for H₂O, CO, and CO₂ in Pure and Mixed Ices

Species	Band (cm ⁻¹)	Concentrations (Species:O ₂)	A' (cm molecule ⁻¹) Pure Ice	A' (cm molecule ⁻¹) Mixture
H ₂ O	3280	pure, 10:1-1:1	2.0×10^{-16} (0.1)	1.8×10^{-16} (0.1)
H ₂ O	1660	pure, 10:1-1:1	1.0×10^{-17} (0.1)	1.0×10^{-17} (0.1)
CO ₂	2340	pure, 5:1-1:1	9.4×10^{-17} (0.2)	9.9×10^{-17} (0.4)
CO ₂	3700	pure, 5:1-1:1	1.5×10^{-18} (0.1)	1.3×10^{-18} (0.1)
CO ₂	3600	pure, 5:1-1:1	7.0×10^{-19} (0.2)	7.2×10^{-19} (0.6)
CO ₂	650	pure, 5:1-1:1	8.4×10^{-18} (0.3)	8.6×10^{-18} (0.2)
CO ₂	1384	pure, 5:1-1:1	...	1.4×10^{-20} (0.2)
CO ₂	1277	pure, 5:1-1:1	...	7.2×10^{-21} (3.5) ^a
CO	2140	pure, 2:1-1:1	7.5×10^{-18} (0.3)	7.9×10^{-18} (0.2)
CO	4252	pure, 2:1-1:1	6.9×10^{-20} (0.5)	7.1×10^{-20} (0.1)

Note. During pure CO₂ experiments, the 1384 and 1277 cm⁻¹ bands were not observed (...).

^a The 1277 cm⁻¹ band showed significant variation among the different concentrations and therefore has a large error.

while they are ~3–150 times smaller than the values reported by P. Ehrenfreund et al. (1992). Interestingly, P. Ehrenfreund et al. (1992) also measured a lower O₂ band strength in CO mixtures than in CO₂ mixtures.

The general lack of a concentration dependence observed in our experiments also differs from previous work on homonuclear species (P. Ehrenfreund et al. 1992; M. P. Bernstein & S. A. Sandford 1999; B. Müller et al. 2018). However, we speculate that the concentration dependence seen in M. P. Bernstein & S. A. Sandford (1999) is because their homonuclear compound, N₂, was the dominant species. In that case, the intermolecular forces with the other species would not perturb the dipole moment of N₂ molecules as much as if N₂ were thoroughly mixed, which is consistent with the observation that M. P. Bernstein & S. A. Sandford (1999) saw an increase in band strength with less N₂. Furthermore, in a subset of their experiments, they also found that the measured N₂ band strength was the same within error for 1:1 and 1:10 N₂/H₂O mixtures, which is consistent with our results. Thus, we do not have an explanation for why the largest band strengths reported by B. Müller et al. (2018) were in the O₂-dominant mixtures. As we do not have a firm explanation for the differing concentration dependencies reported between our group and those two previous studies (P. Ehrenfreund et al. 1992; B. Müller et al. 2018), below we compared the consistency of our companion species' band strengths with what has been reported in the literature.

4.1.3. Companion A'

To compare our measured H₂O band strengths, we can turn to the work of W. Hagen et al. (1981), D. M. Hudgins et al. (1993), P. A. Gerakines et al. (1995), R. M. Mastrapa et al. (2009), and M. Bouilloud et al. (2015). Our mean H₂O band strengths across all concentrations, and as a pure species, presented in Table 2, are consistent with the listed literature values.

Published band strengths of pure crystalline CO₂ ice can be found in H. Yamada & W. B. Person (1964), D. M. Hudgins et al. (1993), M. Bouilloud et al. (2015), and R. L. Hudson et al. (2025). P. A. Gerakines & R. L. Hudson (2015b) measured the band strength for pure amorphous CO₂, while P. A. Gerakines et al. (1995) reported a band strength for CO₂ in a 1:1 CO₂: O₂ mixture, which is the most direct comparison to our work. Our band strengths for the 660, 2340, 3600, and

3700 cm⁻¹ bands match those of P. A. Gerakines et al. (1995) within ~20%.

Published band strengths of pure CO include the works of G. J. Jiang et al. (1975), P. A. Gerakines et al. (1995, 2005), M. Bouilloud et al. (2015), and C. González Díaz et al. (2022). Recently, P. A. Gerakines et al. (2023) highlighted the difference in spectral resolution and its effect on CO band strength values. At our resolution (2 cm⁻¹), we find that our band strength value for the CO 2140 cm⁻¹ band is within 10% of what is reported by P. A. Gerakines et al. (2023). We did, however, see a break in linearity in the band area versus column density curve at column densities greater than 1.1×10^{18} molecule cm⁻², which is the largest CO data point reported in P. A. Gerakines et al. (2023). If we had chosen that region to measure the band strength, we would have estimated a value that was about ~30% lower. Interestingly, we do not see a similar effect for the CO overtone feature (4252 cm⁻¹). Follow-up checks with reported optical constants of CO (P. A. Gerakines et al. 2023) do not predict such a large break in slope here for the fundamental band, suggesting that our observed decrease is likely not an interference effect (B. D. Teolis et al. 2007). This is consistent with what we observed in the 6 μm band of H₂O, which shows evidence of small interference oscillations in the band area with increasing column density that amounts to only a few percent variation in the band strength (if we include enough data points to see the oscillation).

The consistency seen between our reported H₂O, CO, and CO₂ A'-values and those previously reported in the literature supports using our updated O₂ values for future estimates of O₂ abundances in these types of astrophysical ices.

5. Astrophysical Implications

In addition to reporting an updated A'-value for O₂, we can also estimate the time required to observe this species with the JWST MIRI instrument. While the Low Resolution Spectroscopy (LRS) mode of MIRI will likely not be able to resolve this narrow feature, the Medium Resolution Spectroscopy (MRS) mode (with a resolving power $R \sim 3190$ –3700 in the Channel 1 Medium (b) sub-band) should be sufficient. Typical icy mantles coating grains in the ISM are dominated by either polar molecules (e.g., H₂O) or nonpolar molecules (e.g., CO or CO₂) (e.g., A. G. G. M. Tielens et al. 1991; J. E. Chiar et al. 1995; T. de Graauw et al. 1996; P. A. Gerakines et al. 1999). Given that the band strength of O₂ in H₂O and CO₂ mixtures is

the same, we explore scenarios where O_2 exists in an H_2O -dominant environment and in a CO -dominant environment, assuming that the estimates for CO_2 would be similar to H_2O .

Through the JOYS program, E. F. van Dishoeck et al. (2025) recently used JWST in MRS mode to look for solid-phase O_2 in the line of sight of B1-c, a low-mass protostar. Under their observational conditions, and using the most recently published A' -value for O_2 in an H_2O -dominated ice environment (B. Müller et al. 2018), they concluded that they could only set an upper limit of $4.9 \times 10^{18} \text{ O}_2 \text{ cm}^{-2}$ ($\sim 20\%$ relative to H_2O -ice). Furthermore, as B. Müller et al. (2018) showed that A' of O_2 weakened at lower concentrations relative to H_2O , E. F. van Dishoeck et al. (2025) concluded that detecting O_2 at a level predicted by cometary observations ($\sim 3.8\%$ relative to H_2O -ice; A. Bieler et al. 2015; M. Rubin et al. 2015) would be extremely difficult.

With our updated A' -value, which is roughly 3 times larger than the B. Müller et al. (2018) value for an $\text{H}_2\text{O}:\text{O}_2$ ratio of 10:1, and noting that our A' -values are essentially constant with concentration, whereas the B. Müller et al. (2018) values strongly decrease with decreasing concentration, we used the JWST Exposure Time Calculator (ETC) to estimate the time required for a 3σ detection of the O_2 band along the line of sight to B1-c. Using $N_{\text{H}_2\text{O}} = 2.5 \times 10^{19} \text{ cm}^{-2}$ (Y. Chen et al. 2024), $\text{O}_2/\text{H}_2\text{O} = 0.038$ (A. Bieler et al. 2015; M. Rubin et al. 2015), $A' = 2.2 \times 10^{-20} \text{ cm molecule}^{-1}$, $\Delta\nu_{\text{fwhm}} = 8 \text{ cm}^{-1}$, and assuming a Gaussian shape of the O_2 band, we calculate $\tau_{\text{max}} \sim 2.4 \times 10^{-3}$ at the band center. Such a τ_{max} requires a signal-to-noise ratio (SNR) of approximately 1250 for a 3σ detection. However, we can lower the required SNR by $\sqrt{2}$ to ~ 883 if we bin the data from 16 (the number of data points contained within the FWHM of the O_2 band embedded in H_2O ice) down to eight data points. Assuming the flux density from Figure 24 in E. F. van Dishoeck et al. (2025), we estimate it would take $\sim 2 \text{ hr}$ to reach the SNR for a detection ($\text{SNR} \sim 892$, 200 groups per integration, 3 integrations per exposure, and 4 dithers). Applying the same procedure for a CO -dominated ice, we estimate that we would need an SNR of ~ 3370 for a 3σ detection. Even with binning this narrowed band, the observability appears beyond the scope of JWST, as the highest SNR we could achieve, using similar parameters to what we used above (280 groups per integration, 100 integrations per exposure, and 4 dithers), was ~ 1460 . Thus, we suspect that JWST may only be able to detect O_2 in H_2O (and possibly CO_2) dominant environments down to abundances consistent with measurements of cometary coma in the solar system.

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ORCID iDs

William A. Burris  <https://orcid.org/0000-0002-6023-7291>
Mark J. Loeffler  <https://orcid.org/0000-0002-1551-3197>

Stephen C. Tegler  <https://orcid.org/0000-0002-6794-495X>
William M. Grundy  <https://orcid.org/0000-0002-8296-6540>

References

- Baragiola, R. A. 2003, Water Ice on Outer Solar System Surfaces: Basic Properties and Radiation Effects, *P&SS*, **51**, 953
- Behr, P. R., Tribbett, P. D., Robinson, T. D., & Loeffler, M. J. 2020, Compaction of Porous H_2O Ice via Energetic Electrons, *ApJ*, **900**, 147
- Bernstein, M. P., & Sandford, S. A. 1999, Variations in the Strength of the Infrared Forbidden 2328.2 cm^{-1} Fundamental of Solid N_2 in Binary Mixtures, *AcSpA*, **55**, 2455
- Bieler, A., Altwegg, K., Balsiger, H., et al. 2015, Abundant Molecular Oxygen in the Coma Of Comet 67P/Churyumov-Gerasimenko, *Natur*, **526**, 678
- Blakley, B. P., Grundy, W. M., Steckloff, J. K., et al. 2024, The Equilibrium Vapor Pressures of Ammonia and Oxygen Ices at Outer Solar System Temperatures, *P&SS*, **244**, 105863
- Born, M., & Wolf, E. 2013, Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light (Elsevier)
- Bossa, J. B., Isokoski, K., Paardekooper, D. M., et al. 2014, Porosity Measurements of Interstellar Ice Mixtures Using Optical Laser Interference and Extended Effective Medium Approximations, *A&A*, **561**, A136
- Bouilloud, M., Fray, N., Bénilan, Y., et al. 2015, Bibliographic Review and New Measurements of the Infrared Band Strengths of Pure Molecules at 25 K: H_2O , CO_2 , CO , CH_4 , NH_3 , CH_3OH , HCOOH and H_2CO , *MNRAS*, **451**, 2145
- Cairns, B. R., & Pimentel, G. C. 1965, Infrared Spectra of Solid α - and β -Oxygen, *JChPh*, **43**, 3432
- Carmack, R. A., Tribbett, P. D., & Loeffler, M. J. 2023, Pore Accessibility in Amorphous Solid Water, *ApJ*, **942**, 1
- Chen, J.-H., Goldsmith, P. F., Viti, S., et al. 2014, Herschel Hifi Observations of O_2 Toward Orion: Special Conditions for Shock Enhanced Emission, *ApJ*, **793**, 111
- Chen, Y., Rocha, W. R. M., van Dishoeck, E. F., et al. 2024, JOYS+: The Link Between the Ice and Gas of Complex Organic Molecules: Comparing JWST and ALMA Data of Two Low-mass Protostars, *A&A*, **690**, A205
- Chiar, J. E., Adamson, A. J., Kerr, T. H., & Whittet, D. C. B. 1995, High-resolution Studies of Solid CO in the Taurus Dark Cloud: Characterizing the Ices in Quiescent Clouds, *ApJ*, **455**, 234
- Combes, F., Casoli, F., Encrenaz, P., Gerin, M., & Laurent, C. 1991, Search for Molecular Oxygen in Galactic and Extragalactic Sources, *A&A*, **248**, 607
- Combes, F., & Wiklind, T. 1995, Direct Search for O_2 in a Single Molecular Cloud, *A&A*, **303**, L61
- Combes, F., Wiklind, T., & Nakai, N. 1997, New Upper Limits on the Interstellar O_2 Abundance, *A&A*, **327**, L17
- de Graauw, T., Whittet, D. C. B., Gerakines, P. A., et al. 1996, SWS Observations of Solid CO_2 in Molecular Clouds, *A&A*, **315**, L345
- Dohnálek, Z., Kimmel, G. A., Ayotte, P., Smith, R. S., & Kay, B. D. 2003, The Deposition Angle-dependent Density of Amorphous Solid Water Films, *JChPh*, **118**, 364
- Ehrenfreund, P., Breukers, R., D'Hendecourt, L., & Greenberg, J. M. 1992, On the Possibility of Detecting Solid O_2 in Interstellar Grain Mantles, *A&A*, **260**, 431
- Ehrenfreund, P., Gerakines, P. A., Schutte, W. A., van Hemert, M. C., & van Dishoeck, E. F. 1996, Infrared Properties of Isolated Water Ice, *A&A*, **312**, 263
- Ehrenfreund, P., & van Dishoeck, E. F. 1998, The Search for Solid O_2 and N_2 with ISO, *AdSpR*, **21**, 15
- Falk, M. 1987, Amorphous Solid Carbon Dioxide, *JChPh*, **86**, 560
- Fulvio, D., Sivaraman, B., Baratta, G. A., Palumbo, M. E., & Mason, N. J. 2009, Novel Measurements of Refractive Index, Density and Mid-Infrared Integrated Band Strengths for Solid O_2 , N_2O and NO_2 : N_2O_4 Mixtures, *AcSpA*, **72**, 1007
- Gerakines, P. A., Bray, J. J., Davis, A., & Richey, C. R. 2005, The Strengths of Near-Infrared Absorption Features Relevant to Interstellar and Planetary Ices, *ApJ*, **620**, 1140
- Gerakines, P. A., & Hudson, R. L. 2015a, Infrared Spectra and Optical Constants of Elusive Amorphous Methane, *ApJ*, **805**, L20
- Gerakines, P. A., & Hudson, R. L. 2015b, First Infrared Band Strengths for Amorphous CO_2 , an Overlooked Component of Interstellar Ices, *ApJ*, **808**, L40
- Gerakines, P. A., Materese, C. K., & Hudson, R. L. 2023, Carbon Monoxide Ices - a Semicentennial Review and Update for Crystalline CO along with

- the First IR Spectrum and Band Strength for Amorphous CO, *MNRAS*, **522**, 3145
- Gerakines, P. A., Schutte, W. A., Greenberg, J. M., & van Dishoeck, E. F. 1995, The Infrared Band Strengths of H₂O, CO and CO₂ in Laboratory Simulations of Astrophysical Ice Mixtures, *A&A*, **296**, 810
- Gerakines, P. A., Whittet, D. C. B., Ehrenfreund, P., et al. 1999, Observations of Solid Carbon Dioxide in Molecular Clouds with the Infrared Space Observatory, *ApJ*, **522**, 357
- Goldsmith, P. F., Li, D., Bergin, E. A., et al. 2002, Tentative Detection of Molecular Oxygen in the ρ Ophiuchi Cloud, *ApJ*, **576**, 814
- Goldsmith, P. F., Snell, R. L., Erickson, N. R., et al. 1985, Search for Molecular Oxygen in Dense Interstellar Clouds, *ApJ*, **289**, 613
- Goldsmith, P. F., & Young, J. S. 1989, Search for Molecular Oxygen in VII ZW 31, *ApJ*, **341**, 718
- Goldsmith, P. F., Melnick, G. J., Bergin, E. A., et al. 2000, O₂ in Interstellar Molecular Clouds, *ApJ*, **539**, L123
- Goldsmith, P. F., Liseau, R., Bell, T. A., et al. 2011, Herschel Measurements of Molecular Oxygen in Orion, *ApJ*, **737**, 96
- González Díaz, C., Carrascosa, H., MuñozCaro, G. M., Satorre, M. Á., & Chen, Y.-J. 2022, Density and Infrared Band Strength of Interstellar Carbon Monoxide (CO) Ice Analogues, *MNRAS*, **517**, 5744
- Hagen, W., Tielens, A. G. G. M., & Greenberg, J. M. 1981, The Infrared Spectra of Amorphous Solid Water and Ice I_c between 10 and 140 K, *CP*, **56**, 367
- Hapke, B. 2012, Theory of Reflectance and Emittance Spectroscopy (Cambridge Univ. Press)
- Heavens, O. S. 1965, Optical Properties of Thin Solid Films (Dover)
- Hudgins, D. M., Sandford, S. A., Allamandola, L. J., & Tielens, A. G. G. M. 1993, Mid- and Far-infrared Spectroscopy of Ices: Optical Constants and Integrated Absorbances, *ApJS*, **86**, 713
- Hudson, R. L., Ferrante, R. F., & Moore, M. H. 2014a, Infrared Spectra and Optical Constants of Astronomical Ices: I. Amorphous and Crystalline Acetylene, *Icar*, **228**, 276
- Hudson, R. L., Gerakines, P. A., & Moore, M. H. 2014b, Infrared Spectra and Optical Constants of Astronomical Ices: II. Ethane and Ethylene, *Icar*, **243**, 148
- Hudson, R. L., Yarnall, Y. Y., & Materese, C. K. 2025, Carbon Dioxide Ices—A Sexagennial Update of Infrared Intensities, Band Shapes, and the Formation and Destruction of Crystalline CO₂, *ApJ*, **995**, 89
- Jiang, G. J., Person, W. B., & Brown, K. G. 1975, Absolute Infrared Intensities and Band Shapes in Pure Solid CO and CO in Some Solid Matrices, *JChPh*, **62**, 1201
- Kanekar, N., & Meier, D. S. 2015, A New Constraint on the Molecular Oxygen Abundance at $z \sim 0.886$, *ApJ*, **811**, L23
- Kofman, V., He, J., Loes ten Kate, I., & Linnartz, H. 2019, The Refractive Index of Amorphous and Crystalline Water Ice in the UV-vis, *ApJ*, **875**, 131
- Kruger, J., & Ambs, W. J. 1959, Optical Measurements on Thin Films of Condensed Gases at Low Temperatures, *JOSA*, **49**, 1195
- Krupskii, I. N., Prokhvatilov, A. I., Erenburg, A. I., & Yantsevich, L. D. 1973, Structure and thermal expansion of α -CO, *PSSAR*, **19**, 519
- Krupskii, I. N., Prokhvatilov, A. I., Freiman, Y. A., & Erenburg, A. I. 1979, Structure, Elementary Excitation Spectrum, and Thermodynamic Properties of Solid Oxygen, *JLTP*, **5**, 130
- Larsson, B., Liseau, R., Pagani, L., et al. 2007, Molecular Oxygen in the ρ Ophiuchi Cloud, *A&A*, **466**, 999
- Liseau, R., Goldsmith, P. F., Larsson, B., et al. 2012, Multi-line Detection of O₂ toward ρ Ophiuchi A, *A&A*, **541**, A73
- Liszt, H. S. 1985, A search for O₂ toward NGC 7674, *ApJ*, **298**, 281
- Liszt, H. S., & Vanden Bout, P. A. 1985, Upper Limits on the O₂/CO Ratio in Two Dense Interstellar Clouds, *ApJ*, **291**, 178
- Loeffler, M. J., Moore, M. H., & Gerakines, P. A. 2016, The Effects of Experimental Conditions on the Refractive Index and Density of Low-temperature Ices: Solid Carbon Dioxide, *ApJ*, **827**, 98
- Lorentz, H. A. 1880, Ueber Die Beziehung Zwischen Der Fortpflanzungsgeschwindigkeit Des Lichtes Und Der Körperdichte, *AnP*, **245**, 641
- Lorenz, L. 1881, Ueber das Leitungsvermögen der Metalle für Wärme und Electricität, *AnP*, **249**, 582
- Lu, C.-S., & Lewis, O. 1972, Investigation of Film-Thickness Determination by Oscillating Quartz Resonators with Large Mass Load, *JAP*, **43**, 4385
- Luna, R., Satorre, M. Á., Domingo, M., Millán, C., & Santonja, C. 2012, Density and Refractive Index of Binary CH₄, N₂ and CO₂ Ice Mixtures, *Icar*, **221**, 186
- Maeda, S., & Schatz, P. N. 1961, Absolute Infrared Intensity Measurements in Thin Films, *JChPh*, **35**, 1617
- Mastrapa, R. M., Sandford, S. A., Roush, T. L., Cruikshank, D. P., & Dalle Ore, C. M. 2009, Optical Constants of Amorphous and Crystalline H₂O-ice: 2.5–22 μ m (4000–455 cm⁻¹) Optical Constants of H₂O-ice, *ApJ*, **701**, 1347
- Melnick, G. J., Tolls, V., Goldsmith, P. F., et al. 2012, Herschel Search for O₂ Toward the Orion Bar, *ApJ*, **752**, 26
- Müller, B., Giuliano, B. M., Bizzocchi, L., Vasyunin, A. I., & Caselli, P. 2018, O₂ Signature in Thin and Thick O₂-H₂O Ices, *A&A*, **620**, A46
- Olofsson, G., Pagani, L., Tauber, J., et al. 1998, Low Interstellar Abundance of O₂ Confirmed by the PIROG 8 Balloon Experiment, *A&A*, **339**, L81
- Pagani, L., Langer, W. D., & Castets, A. 1993, First Tentative Detection of the Molecular Oxygen Isotopomer ¹⁶O ¹⁸O in Interstellar Clouds, *A&A*, **274**, L13
- Pagani, L., Olofsson, A. O. H., Bergman, P., et al. 2003, Low Upper Limits on the O₂ Abundance from the Odin Satellite, *A&A*, **402**, L77
- Raut, U., Famá, M., Teolis, B. D., & Baragiola, R. A. 2007, Characterization of Porosity in Vapor-Deposited Amorphous Solid Water from Methane Adsorption, *JChPh*, **127**, 204713
- Roux, J. A., Wood, B. E., Smith, A. M., & Plyer, R. R. 1980, Infrared Optical Properties of Thin CO, NO, CH₄, HCl, N₂O, O₂, AR, and Air Cryofilms, Tech. Rep. **AEDC-TR-79-81**, Arnold Engineering Development Center, Arnold Air Force Station, TN
- Rubin, M., Altwegg, K., Dishoeck, E. F. V., & Schwehm, G. 2015, Molecular Oxygen in Oort Cloud Comet 1p/halley, *ApJ*, **815**, L11
- Sandqvist, A., Larsson, B., Hjalmarsen, A., et al. 2015, Herschel HIFI Observations of the Sgr A +50 Km S-1 Cloud. Deep Searches for O₂ in Emission and Foreground Absorption, *A&A*, **584**, A118
- Satorre, M., Domingo, M., Millán, C., et al. 2008, Density of CH₄, N₂ and CO₂ Ices at Different Temperatures of Deposition, *P&SS*, **56**, 1748
- Schulze, W., & Abe, H. 1980, Density, Refractive Index and Sorption Capacity of Solid CO₂ Layers, *CP*, **52**, 381
- Taquet, V., van Dishoeck, E. F., Swayne, M., et al. 2018, Linking Interstellar and Cometary O₂: A Deep Search for ¹⁶O ¹⁸O in the Solar-Type Protostar IRAS 16293-2422, *A&A*, **618**, A11
- Teolis, B. D., Loeffler, M. J., Raut, U., Famá, M., & Baragiola, R. A. 2007, Infrared Reflectance Spectroscopy on Thin Films: Interference Effects, *Icar*, **190**, 274
- Tielens, A. G. G. M., & Hagen, W. 1982, Model Calculations of the Molecular Composition of Interstellar Grain Mantles, *A&A*, **114**, 245
- Tielens, A. G. G. M., Tokunaga, A. T., Geballe, T. R., & Baas, F. 1991, Interstellar Solid CO: Polar and Nonpolar Interstellar Ices, *ApJ*, **381**, 181
- Tribbett, P. D., & Loeffler, M. J. 2022, Thermal Reactions between H₂S and O₃: Implications for Europa Surface Chemistry, *PSJ*, **3**, 233
- van Dishoeck, E. F., Tychoniec, L., Rocha, W. R. M., et al. 2025, JWST Observations of Young ProtoStars (JOYS): Overview of program and early results, *A&A*, **699**, A361
- Vandenbussche, B., Ehrenfreund, P., Boogert, A. C. A., et al. 1999, Constraints on the Abundance of Solid O₂ in Dense Clouds from ISO-SWS and Ground-Based Observations, *A&A*, **346**, L57
- Vegard, I. 1930, Struktur und Leuchtfähigkeit von Festem Kohlenoxyd, *ZPhy*, **61**, 185
- Wang, B.-R., Li, D., Goldsmith, P. F., et al. 2024, Molecular Oxygen Abundance in Galactic Massive Star Formation Regions Based on SWAS Observations, *RAA*, **24**, 095007
- Wang, J., Li, D., Goldsmith, P. F., et al. 2020, Molecular Oxygen in the Nearest QSO Mrk 231, *ApJ*, **889**, 129
- Wang, L., Sun, C., Xu, H., et al. 2020, Neutron Diffraction Study of Crystal Structure and Temperature Driven Molecular Reorientation in α -CO, *AIPA*, **10**, 045301
- Westley, M. S., Baratta, G. A., & Baragiola, R. A. 1998, Density and Index of Refraction of Water Ice Films Vapor Deposited at Low Temperatures, *JChPh*, **108**, 3321
- Williams, B. J., Cleaves, L. I., Eistrup, C., & Ramsey, J. P. 2023, Deep Search for Molecular Oxygen in TW Hya, *ApJ*, **956**, 135
- Wirström, E. S., Charnley, S. B., Cordiner, M. A., & Ceccarelli, C. 2016, A Search for O₂ in CO-depleted Molecular Cloud Cores with Herschel, *ApJ*, **830**, 102
- Wood, B. E., & Roux, J. A. 1982, Infrared Optical Properties of Thin H₂O, NH₃, and CO₂ and Cryofilms, *JOSA*, **72**, 720
- Yamada, H., & Person, W. B. 1964, Absolute Infrared Intensities of the Fundamental Absorption Bands in Solid CO₂ and N₂O, *JChPh*, **41**, 2478
- Yldz, U. A., Acharyya, K., Goldsmith, P. F., et al. 2013, Deep Observations of O₂ Toward a Low-Mass Protostar with Herschel-HIFI, *A&A*, **558**, A58