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Infrared band strengths for amorphous and crystalline methyl propionate, a candidate interstellar molecule

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ABSTRACT

Mid-infrared spectra of amorphous and crystalline methyl propionate, $\text{CH}_3\text{CH}_2\text{COOCH}_3$, are presented for the first time from a single laboratory, along with measurements of the refractive index of each solid form. Density estimates are made and IR band strengths and absorption coefficients are calculated. Vapor pressures of crystalline methyl propionate at 140–150 K are reported along with an enthalpy of sublimation. Spectroscopic results are compared to a recent study of this compound, and the phase of methyl propionate in that work is identified. Several applications are described.

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1. Introduction

Studies of the infrared (IR) spectra and radiation chemistry of icy solids of astrochemical interest are often hindered by the scarcity of absolute-intensity data for mid-IR features. In our own case, we have encountered such problems in our study of nitriles related to the chemistry of Titan [1], Saturn's largest moon, and also in our work on molecules relevant to the chemistry of the interstellar medium (ISM), such as CO_2 , CH_4 , the C_2 hydrocarbons, and acetone [2,3,4,5,6]. Such fundamental spectroscopic information is important for laboratory studies of a variety of molecules known or suspected to be present in icy solids of the solar system and interstellar space, and also for the calculation of molecular abundances in extraterrestrial objects from remote IR-spectroscopic observations [7].

This paper is a continuation of our solid-phase spectroscopic work, but with a different type of compound, an organic ester. Few laboratory studies of esters are in the astrochemical literature, with work on methyl formate and methyl acetate being two examples [8,9]. Given that both methyl formate and methyl acetate are known interstellar molecules, it is appropriate to consider the next most complex ester, methyl propionate ($\text{CH}_3\text{CH}_2\text{COOCH}_3$) to be an interstellar candidate. Here we examine methyl propionate, for which little solid-phase IR laboratory data exists, and none that reports spectral intensities.

Aside from astrochemical connections, this paper also addresses an ambiguity in the literature. Papers by Moravie and Corset presented

part of the mid-IR spectrum of solid methyl propionate, but their spectrum disagrees with one recorded over a larger wavenumber range by Sivaraman et al., obtained with a sample at 85 K, suggesting the possible existence of more than one solid form of this compound [10,11,12]. We have not located relevant calorimetric data for solid methyl propionate, and so we have recorded IR spectra over a wide range of temperatures in case an undocumented phase change exists and can be observed.

A third motivation for this paper is the importance of characterizing different forms of solids, such as methyl propionate, to aid in their future identification and to reduce the likelihood of misidentifications. Several examples can be cited from this journal alone. An early IR study of methanethiol (CH_3SH) by May and Pace characterized two crystalline forms of the compound [13]. However, in a subsequent publication by the same authors [14] the identifications of the phases were reversed, an error that propagated through the literature for nearly 50 years until a recent correction [15]. A study of nitrous oxide (N_2O) which appeared here, presented unusual IR band shapes consisting of pairs of rounded and sharp components [16]. A subsequent analysis showed that the published spectra were from an ice having two solid forms [17]. A third example concerns ethanethiol ($\text{CH}_3\text{CH}_2\text{SH}$). A crystalline sample of this compound was described by the authors as undergoing "a remarkable transformation" on warming to 125–130 K [18]. A later analysis suggested that the more likely explanation for the authors' observations was that the crystalline solid simply liquefied on warming to 125 K, the melting point of ethanethiol [19].

In this brief paper we investigate methyl propionate, reporting mid-IR spectra for two forms, the temperature region for a solid-solid transition, indices of refraction for both solid forms, density estimates, vapor

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pressure measurements, an enthalpy of sublimation, and band intensities and absorption coefficients for several prominent IR features from which other band strengths can be calculated. Although our focus is on spectral intensities, assignments of a few peaks are included.

2. Experimental

Our methods and laboratory equipment have been described in several of our recent publications [1–6]. In brief, we deposited methyl propionate (Sigma Aldrich, 99%) vapor onto a pre-cooled KBr substrate in a vacuum chamber ($\sim 10^{-8}$ Torr). Deposition times were 10–60 min with rates of increase for ice thickness of about $1\text{--}8\ \mu\text{m hr}^{-1}$, with ice thicknesses of about $0.5\text{--}4\ \mu\text{m}$. Mid-infrared transmission spectra were recorded at the deposition temperature and after warming and cooling the amorphous ice sample. Most of our spectra were recorded at 16 K for amorphous ices and 130 K for crystalline ones. With few exceptions, a resolution of $2\ \text{cm}^{-1}$ was used over the spectrometer's range of $4000\text{--}650\ \text{cm}^{-1}$, with 100 accumulations per spectrum. The IR bands of the solid compound were sufficiently broad that little, if any, additional information was found at higher resolutions.

The thickness (h) of each of our ice samples was measured by counting the number of interference fringes (N_{fr}) formed by a 670-nm laser's beam reflecting from the sample and the underlying substrate as the methyl propionate was deposited, the laser being aligned almost perpendicular to the plane of the ice. Eq. (1) is the relevant relation [20,21].

$$h = \frac{N_{fr}\lambda}{2n} \quad (1)$$

The use of Eq. (1) requires that the sample's index of refraction (n) be known at 670 nm. We measured n with two-laser interferometry, with one laser's beam at an angle of about $\theta_1 = 6^\circ$, again with respect to a line perpendicular to the plane of the ice sample, and the second laser's beam at an angle of $\theta_2 = 45^\circ$. During the deposition of a sample, each laser produced an interference pattern with period (t). From the periods, t_1 and t_2 , of the two interference patterns, the ice's index of refraction at 670 nm was calculated with Eq. (2) below [22].

$$n = \sqrt{\frac{\sin^2\theta_2 - (t_1/t_2)^2 \sin^2\theta_1}{1 - (t_1/t_2)^2}} \quad (2)$$

See the papers of Satorre et al. [23] and Molpeceres et al. [24] for additional information and examples from other laboratories. Although n can be determined with just one laser, such measurements require an absolute photometric measurement of intensity and a knowledge of the substrate's refractive index at the temperature of interest, but such n values usually are unknown. They are not needed in the method we used.

The number of IR bands and their extensive overlap made it difficult to interpret many IR features of solid methyl propionate in terms of simple atomic displacements. Therefore, we used the Spartan software package (Wavefunction, Inc., Irvine California, USA) to assist in visualizing specific vibrational modes, the calculations being done with density functional theory (DFT) at the B3LYP/6–31 + G* level. Our motivation for these calculations was the software's ability to animate individual vibrational modes, as opposed to its ability to generate numerical results to compare with experiments. As already stated, our main goal in this paper was to measure spectral intensities and other properties, as opposed to carrying out a complete vibrational analysis.

3. Results

3.1. Refractive Indices and Densities

Deposition of methyl propionate vapor at 16 K produced an amorphous solid (see Section 3.2), and during such depositions interference fringes were recorded with two 670-nm lasers as just described, and a refractive index was calculated from the results. The average of three measurements gave $n(16\ \text{K}) = 1.282 \pm 0.007$ for amorphous methyl propionate. Similar measurements for 130 K depositions produced crystalline methyl propionate and $n(130\ \text{K}) = 1.436 \pm 0.006$. Room-temperature ($20^\circ\ \text{C}$) data [25] for this compound are $n = 1.3775$ and a density $\rho = 0.9150\ \text{g cm}^{-3}$ from which a specific refraction of $r = 0.2517\ \text{cm}^3\ \text{g}^{-1}$ was found with the Lorentz-Lorenz equation, shown below.

$$\rho = \left(\frac{1}{r}\right) \left(\frac{n^2 - 1}{n^2 + 2}\right) \quad (3)$$

Combining this value of r with Eq. (3) and our two refractive indices gives densities of $\rho(16\ \text{K}) = 0.702$ and $\rho(130\ \text{K}) = 1.04\ \text{g cm}^{-3}$ for amorphous and crystalline methyl propionate, respectively, after rounding off to three significant figures. Our recent measurements of r for N_2O and acetone showed a variation of about 4% between liquid and solid phases, which we take as the uncertainty introduced by Eq. (3) in the present case [6,17]. See Modica and Paulmbo [8] and Fulvio et al. [16] for Eq. (3) applied to other compounds.

Values of n were needed to determine ice thicknesses using Eq. (1), which in turn were needed to measure absorption coefficients. Both n and ρ were required to determine IR band strengths, and the latter were required for determining vapor pressures, which led to an enthalpy of sublimation.

3.2. Infrared Spectra and Band Strengths

Fig. 1 shows mid-IR survey spectra of methyl propionate deposited at (a) 16 K and (b) 130 K. The broad, rounded peaks of the 16-K spectrum are typical of those for amorphous solids, whereas the sharper narrower features of the upper spectrum suggest a crystalline sample [26]. Little change was seen on slowly warming the 16-K ice to 90 K, but a distinct transition occurred in the 100–110 K region, generating a spectrum like the one shown in Fig. 1(b), and suggesting crystallization of the initially amorphous ice. Enlargements of four regions of these spectra are shown in Figs. 2 and 3. Note that in all three figures,

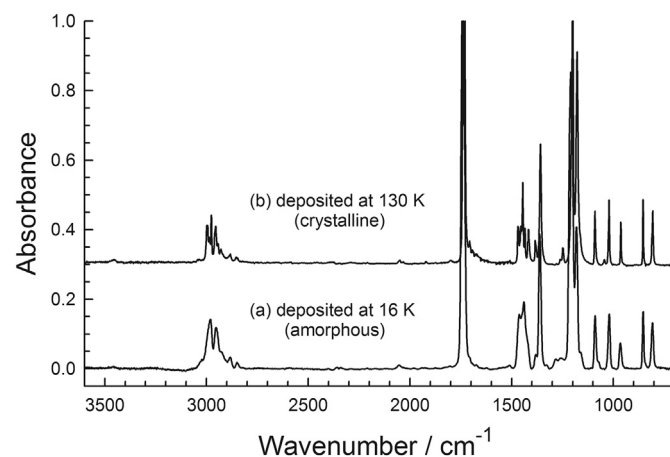


Fig. 1. Mid-infrared survey spectra of methyl propionate (a) deposited at 16 K and (b) deposited at 130 K. The ice thicknesses were about (a) 2.6 and (b) 1.2 μm . The upper spectrum has been offset vertically for clarity.

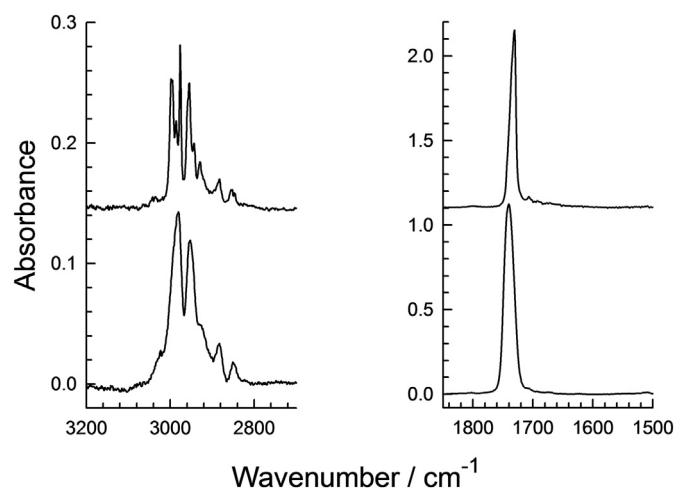


Fig. 2. Enlargements of the 3200–2700 and 1900–1500 cm^{-1} regions of the mid-infrared spectra of amorphous (lower) and crystalline (upper) methyl propionate. The ices' temperatures and thicknesses were the same as in Fig. 1. The upper spectrum in each panel has been offset vertically for clarity.

the crystalline sample's thickness was about half that of the amorphous ice.

The amorphous-to-crystalline transition we observed on warming methyl propionate was irreversible (i.e., recooling to 16 K did not regenerate the amorphous solid). On cooling a crystalline ice that was made at 130 K, most of the IR features became slightly sharper, but otherwise little change was seen, and certainly nothing that would indicate a solid-solid phase change. Rapid sublimation of all methyl propionate ices occurred on warming above 150 K.

Depositions at 16 K of ices of increasing thickness gave IR spectra where each feature grew in intensity, as seen for several peaks in Fig. 4. Peak heights were multiplied by $\ln(10) = 2.303$ to convert from base-10 to base-e logarithms, and then were plotted as a function of ice thickness. The slopes of such Beer's Law plots equaled apparent absorption coefficients (α'). Similarly, IR band areas multiplied by 2.303 were plotted as a function of ice thickness h . Using Eq. (4), the slopes of such graphs were then divided by ρ_N , the molecular number

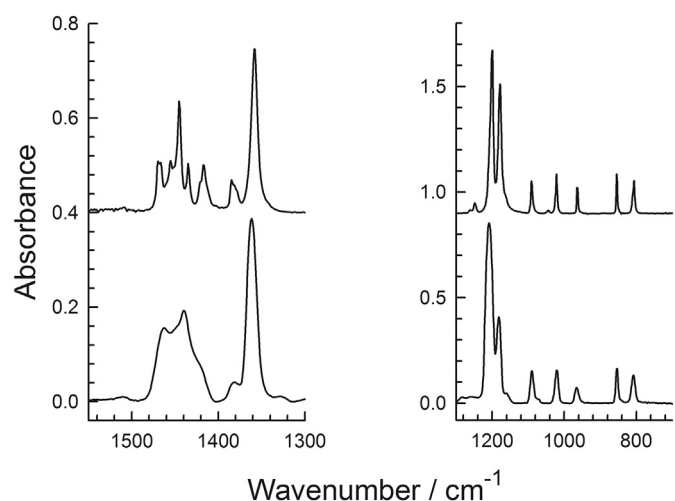


Fig. 3. Enlargements of the 1550–1300 and 1250–750 cm^{-1} regions of the mid-infrared spectra of amorphous (lower) and crystalline (upper) methyl propionate. The ices' temperatures and thicknesses were the same as in Fig. 1. The upper spectrum in each panel has been offset vertically for clarity.

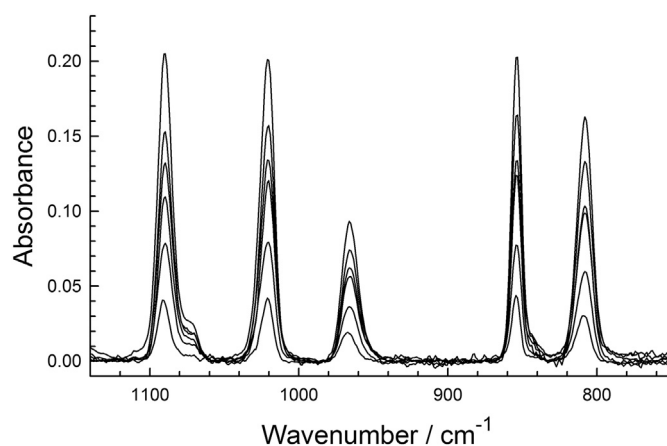


Fig. 4. Five mid-infrared features of amorphous methyl propionate deposited at 16 K for thicknesses of about 0.65, 1.31, 1.70, 2.14, 2.61, and 3.40 μm .

density, to give apparent band strengths (A') for each IR feature of interest [27]. See Fig. 5 for three examples.

$$2.303 \int_{\text{band}} (\text{Absorbance}) d\tilde{\nu} = (\rho_N A') h \quad (4)$$

This same procedure was followed for crystalline methyl propionate made by deposition at 130 K. For more on these methods, including the differences in apparent and absolute absorption coefficients and band strengths, see our earlier papers on the C_2 -hydrocarbons [4,5].

Tables 1–3 summarize peak positions, absorption coefficients, and band strengths for our amorphous and crystalline ices. The IR features selected for these tables are those that were the most prominent in the spectra, and thus potentially of most use for astrochemical studies. Note that some of the bands and regions in the tables cover multiple vibrational modes, such as the C–H stretching region at 3000 cm^{-1} . Many weaker bands also were observed, such as the carbonyl stretch's first overtone ($\sim 3470 \text{ cm}^{-1}$). These have not been tabulated.

3.3. Vapor Pressures

The vapor pressure of crystalline methyl propionate was measured at three temperatures with the method of Khanna et al., a low-temperature modification of the well-known Knudsen-cell technique [28]. The decreases in the areas of the sharp, unobscured IR bands at 1021, 963, 854, and 807 cm^{-1} were followed over time at 140, 145, and 150 K, giving vapor pressures of 1.514×10^{-7} , 5.06×10^{-7} , and 2.89×10^{-6} Torr, respectively, with an uncertainty of about 10%.

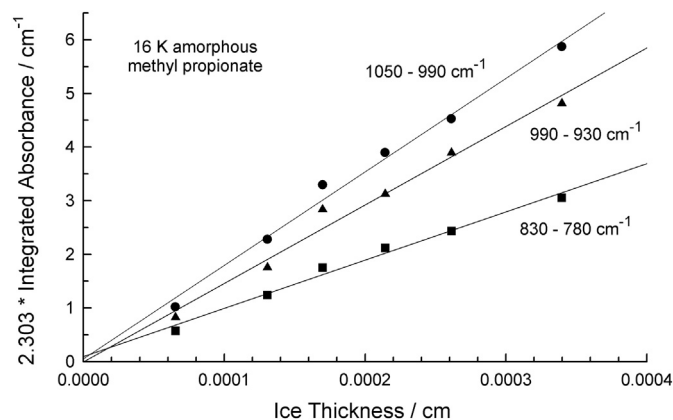


Fig. 5. Beer's law plots for three IR features of amorphous methyl propionate deposited at 16 K. Integration ranges are as indicated in the figure.

Table 1
Positions of Selected IR Features of Methyl Propionate^a.

$\tilde{\nu}$ (amorphous, 16 K)	$\tilde{\nu}$ (crystalline, 130 K)
2980.8	2997.9, 2994.9, 2985.6, 2976.3
2952.7	2958.1, 2955.0, 2943.0
2925.4	2929.0
2882.9	2882.6
2850.6	2855.2, 2846.6
1740.5	1734.5, 1730.8
1462.7	1469.5, 1466.7, 1460.3, 1455.0
1439.4	1445.0, 1434.5, 1421.0, 1417.0
1381.5	1384.6, 1381.9
1361.5	1358.1
1208.3	1199.6
1181.4	1178.2
1089.8	1090.5
1020.5	1021.1
965.5	963.2
853.7	854.2
807.9	809.6, 806.6

^a All positions in units of cm^{-1} . For assignments and approximate descriptions of vibrational motions see Moravie and Corset [11] and references therein. Note that considerable mixing occurs among the vibrations.

These temperatures and vapor pressures were used to construct a Clapeyron plot, the slope of which gave a sublimation enthalpy of 51 kJ mol^{-1} for crystalline methyl propionate, again with an uncertainty on the order of 10%.

4. Discussion

4.1. Infrared Spectra

With 14 atoms, methyl propionate has $3(14) - 6 = 36$ fundamental vibrations. Assignments of peaks in our spectra to these fundamentals are not straightforward, save for the carbonyl stretch near 1740 cm^{-1} and a few others in very general terms. Sivaraman et al. published assignments from density-functional, and other, calculations [12], and earlier work by Moravie and Corset [11] gave assignments based on deuterated isotopologs of methyl propionate. However, in many cases the brief descriptions published by these authors do not agree, although this could well be because many of the vibrations are not simply due to a motion of a single functional group.

In broad terms, for amorphous methyl propionate's spectrum the peaks in the $3100\text{--}2800 \text{ cm}^{-1}$ region are from five asymmetric and three symmetric forms of C—H motions. The strong feature near 1362 cm^{-1} is from a wagging of the ethyl group, the peak near 1208 cm^{-1} is due to a rocking motion of the ethyl group, and the peak near 1181 cm^{-1} is from a rocking of the methoxy group. Continuing

Table 2
Absorption coefficients of selected IR peaks of methyl propionate^a.

Amorphous Ice (16 K)		Crystalline Ice (130 K)	
$\tilde{\nu}$	α'	$\tilde{\nu}$	α'
2981	1303	2976	2490
2953	1094	2955	2249
1741	9961	1731	17,820
1439	1794	1445	3977
1361	3466	1358	6922
1208	7714	1200	13,380
1181	3459	1178	10,671
1090	1390	1091	3128
1021	1354	1021	3086
966	649	963	2379
854	1361	854	2587
808	1135	807	2660

^a Units of $\tilde{\nu}$ and α' are cm^{-1} . Values of α' are from the slopes of Beer's Law graphs of $2.303 \times (\text{peak height})$ against ice thickness. In each case, the slope is the apparent absorption coefficient, α' . See Section 4.2 for a discussion of uncertainties.

Table 3
Integrated intensities of selected IR regions of methyl propionate^a.

Integration range/ cm^{-1}	Amorphous Ice, 16 K $A'/10^{-18} \text{ cm molec}^{-1}$	Crystalline Ice, 130 K $A'/10^{-18} \text{ cm molec}^{-1}$
3100–2750	21.7	17.3
1780–1660	44.8	38.7
1490–1400	16.4	11.8
1400–1313	34.7	10.3
1313–1135	54.7	44.4
1130–1050	4.2	2.8
1050–990	3.6	3.2
990–930	1.9	1.8
870–830	2.7	1.7
830–780	3.0	2.8

^a From the slopes of Beer's Law graphs of $2.303 \times (\text{band area})$ against ice thickness. In each case, the slope divided by $(\rho N_A/\text{MW})$ gives A' , where MW = molecular weight = 88.11 g mol^{-1} , $N_A = 6.022 \times 10^{23} \text{ molecules mol}^{-1}$, and density = 0.702 and 1.04 g cm^{-3} for amorphous and crystalline methyl propionate, respectively. For recent examples see our work on the C_2 hydrocarbons [4,5]. See Section 4.2 for a discussion of uncertainties in A' values.

from left to right in the spectrum, five distinct peaks are seen in the $1100\text{--}800 \text{ cm}^{-1}$ region. Our DFT calculations suggested that they can be assigned to a CH_3 wagging (1090 cm^{-1}), a wagging of the CH_2 group (1020 cm^{-1}), a stretching of the $\text{H}_3\text{C—CH}_2$ bond (966 cm^{-1}), a stretching of the $(\text{O})\text{C—OCH}_3$ bond (854 cm^{-1}), and a rocking motion of the ethyl group (808 cm^{-1}). However, we caution that these are very simplistic descriptions of the vibrations, which often involve both bending and stretching motions of multiple groups. The assignments of specific peaks are particularly challenging for the spectrum of crystalline methyl propionate as it is difficult to determine whether peaks that are close together are for different vibrations or from factor-group splitting. See Katritsky et al. for more on the difficulties of IR assignments of esters [29].

Comparisons of our spectra to those in the literature are hindered by the lack of publications on solid methyl propionate. To our knowledge, only two solid-phase spectra are available, one for a sample made at 85 K and the other for a sample cooled from the room-temperature liquid. The sample that gave the spectrum in Fig. 2 of Sivaraman et al. [12], from an 85 K deposition, was not labeled as either amorphous or crystalline, but a comparison to our Fig. 1 shows that it was indeed an amorphous ice. The only substantial disagreement we have found is that the spectrum of Sivaraman et al. shows much greater absorbance in the 3300 cm^{-1} region than what is seen in our Fig. 1. The only comparison spectrum we have for crystalline methyl propionate is from Moravie and Corset [11], which is missing the $2800\text{--}1500 \text{ cm}^{-1}$ region, but otherwise resembles what we report here.

We note also that our spectrum for amorphous solid methyl propionate closely resembles that of liquid methyl propionate [30], as expected. Table 4 compares peak positions in our spectrum of amorphous methyl propionate to those at 85 K (solid) and 298 K (liquid) from the literature just cited.

Few spectral changes were seen on cooling crystalline samples of methyl propionate, suggesting that either only one crystalline phase exists under our conditions or perhaps that conversions among phases are slow. The fact that no significant changes are seen on warming our ices, other than crystallization, suggests that the methyl propionate molecules are frozen into just one conformation on deposition, most likely the one in which all carbon and oxygen atoms are in the same plane, with the carbonyl group eclipsing the methyl group, which has been reported to be the only conformer present in crystalline methyl propionate at 83 K [10].

4.2. Spectral Intensities

We have not found previous work on spectral intensities of methyl propionate with which to compare our values of α' and A' . Earlier papers tend to lack either an ice thickness, a vertical scale with numbers,

Table 4
Comparison of positions of selected IR features of methyl propionate^a.

Amorphous ice (16 K) ^b	Amorphous ice (85 K) ^c	Liquid phase (298 K) ^d
2980.8	2982	~2980
2952.7	2951.7	~2950
2925.4	2926.9	2930
2882.9	2883.7	2888
2850.6	2848	2847
1740.5	1739.2	1745
1462.7	1461	1465
1439.4	1439.4	1437
1381.5	1378.7	1382
1361.5	1362.1	1357
1208.3	1207	1204
1181.4	1180.5	1177
1089.8	1089	1087
1020.5	1020.6	1023
965.5	965.2	966
853.7	854.2	849
807.9	807.7	809

^a All positions in units of cm^{-1} .

^b This work.

^c From Table 3 of Sivaraman et al. [12]

^d From Table 1 of Moravie and Corset, with the positions of the peaks near 2980 and 2950 cm^{-1} being read from that work's Fig. 3 [11].

or both. Certainly the *relative* intensities across our spectra closely resemble those in publications already cited. The uncertainty in our α' and A' values mostly derives from determinations of ice thickness, which are based on the refractive indices of amorphous and crystalline methyl propionate. Since these are thought to be accurate to within 10%, based on our work with other compounds, that is a generous outside limit on α' and A' in the present case. A more realistic limit is an uncertainty of 5%.

Lacking solid phase data for intensity comparisons, we turned to the work of Katritsky et al. on liquid-phase esters [29]. Those authors reported that the intensity (absorptivity) of the C=O peak of methyl propionate was less than that of the corresponding feature of methyl formate. Our work agrees with this order, our C=O band strength for solid methyl propionate being about 10% less than that found by Modica and Palumbo for solid methyl formate [8].

4.3. Other Comparisons

Few reports of ice sublimation energies have appeared using the method we employed, perhaps because it requires knowing IR band strengths, which in turn usually require both an ice density and thickness, which in turn usually require knowing the sample's refractive index. Lucas et al. employed mass spectral measurements to determine vapor pressures of solid methanol over a range of temperatures, and from them the molecule's sublimation energy [31]. Satorre and co-workers have published several papers on ice sublimation energies based on measurements with a quartz crystal microbalance [32,33,34]. Burke et al. determined the desorption energies of frozen methyl formate, glycolaldehyde, and acetic acid using mass spectral results [35]. However, to our knowledge no detailed comparisons of these techniques with the IR method we used have been published. From the three papers just cited, the result of Burke et al. is most relevant to our own work. Those authors reported a sublimation energy of 35 kJ mol^{-1} for methyl formate. Methyl propionate is a larger ester, and so can be expected to have a somewhat larger sublimation energy, so that our 51 kJ mol^{-1} seems reasonable.

Another area of interest concerns the possibility of using computational-chemistry methods to calculate IR band strengths of amorphous ices. The laboratory methods we have used here have a long heritage [27], but are sufficiently difficult and time-consuming that accurate computational alternatives would be attractive. In Fig. 6 we compare calculated (MP2, second-order Möller-Plesset theory)

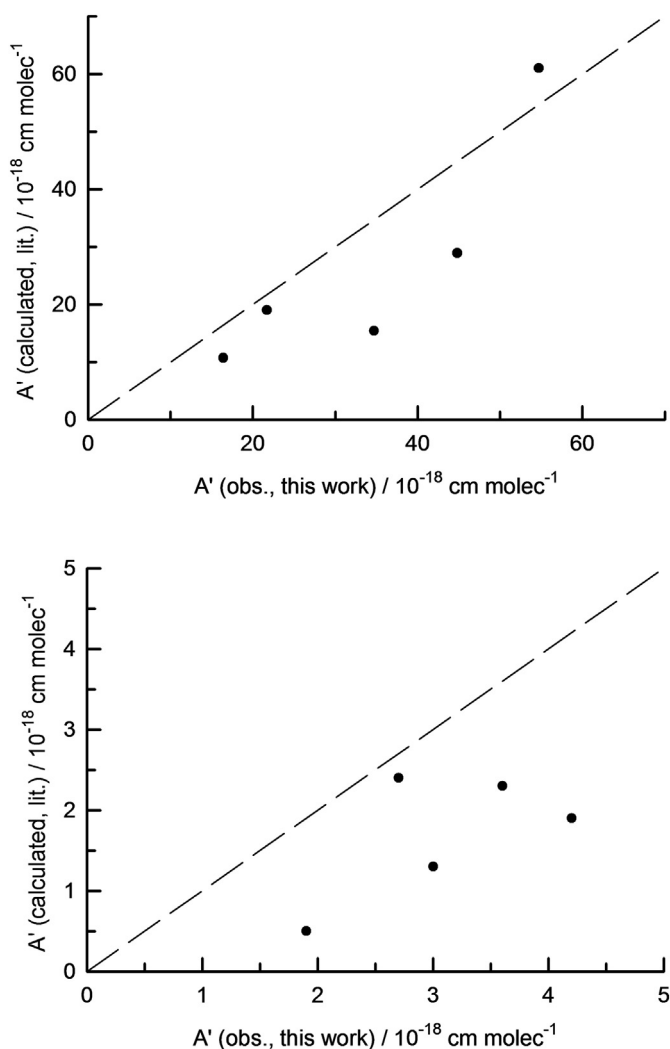


Fig. 6. Comparison of the observed (this work) and calculated [12] apparent band strengths for the ten regions of the mid-IR spectrum of amorphous methyl propionate listed in Table 3. The upper and lower panels are for IR regions above and below 1130 cm^{-1} , respectively.

gas-phase intensities of ten IR regions of gas-phase methyl propionate [12] to our measured integrated intensities for amorphous methyl propionate at 16 K, with the dashed lines at 45° indicating perfect agreement. However, with correlation coefficients of 0.74 and 0.38 for the upper and lower plots, respectively, Fig. 6 suggests that no simple conversion or scaling factor will bring together the observed solid-phase and calculated gas-phase results. Admittedly, it is not quite fair to expect much agreement between these two data sets, but it is not difficult to find examples in the astrochemical literature where gas-phase IR intensities calculated with an ab initio or density-functional method are used to interpret solid-phase experiments, often due to the lack of any solid-phase spectroscopic data. Seen this way, the intensity results reported in the present paper can be used as benchmarks for future work on calculating IR intensities of solids.

4.4. Astrochemical and Other Applications

One motivation for our work was the possible presence and eventual remote identification of methyl propionate and other esters in extraterrestrial solids. However, H_2O , CH_3OH , and silicates, common components of interstellar ices, will obscure methyl propionate bands in the 3000, 1700, and 1000 cm^{-1} regions, making specific identifications difficult, regardless of these esters' abundances. The carbonyl region

(1700 cm^{-1}) is particularly challenging for identifying esters as other compounds, such as H_2CO , also absorb there. In addition, peak positions can vary in the case of a complex extraterrestrial solid due to the presence of H_2O -ice and silicate components. However, it should be possible to use the results in the present paper to determine relative intensities in the near- and far-IR regions where the prospects for identifications might be better, or to place upper limits on astronomical abundances.

The more likely applications of our results are to laboratory studies of methyl propionate. For example, one measurement of astrochemical interest is the stability of this compound (and many others) against ionizing radiation. Our peak and band intensities will be useful in the quantification of such measurements. Solid-phase product abundances, branching ratios for reactions, and elemental balances for methyl-propionate destruction can be determined now that band strengths of the ester have been measured. Conversely, experiments can be envisioned for the low-temperature synthesis of methyl propionate in interstellar ice analogs, such as through variants of the classic Fischer esterification [36]. Again, our spectral results will be useful for identifying methyl propionate and determining reaction yields. We also suggest that the band strengths we have measured can be used for quantitative comparisons to the results of calculated IR intensities of icy solids. Few such solid-phase comparisons have been published, in part due to the lack of laboratory data for comparison.

5. Summary and Conclusions

In this brief paper we have presented results from a low-temperature IR spectroscopic study of the amorphous and crystalline forms of methyl propionate. The temperature region for crystallization was determined as were vapor pressures of the crystalline ice at 140–150 K, along with an enthalpy of sublimation. The first infrared absorption coefficients and band strengths for this compound are reported, as are solid-phase measurements of refractive indices at 670 nm and calculations of ice densities. Comparisons have been made to previous studies.

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