Supporting Information

Refractive Indices and Infrared Band Strengths of Amorphous Ices of Key Fluorinated Refrigerants 1,1,1,2-Tetrafluoroethane, 2,3,3,3-Tetrafluoropropene and 3,3,3-Trifluoropropene

Koushik Mondal[a], Mason Mcanally[a], Souvick Biswas[a], Nils W. Melbourne[a], Andrew M. Turner[a], Alexandre Bergantini[a,b], Rui Sun[a*], Ralf I. Kaiser[a*]

[a] Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, United States

[b]Present Address: Valongo Observatory, Federal University of Rio de Janeiro (OV-UFRJ), Rio de Janeiro-RJ, 20080-090, Brazil

* Corresponding author. E-mail: ruisun@hawaii.edu; ralfk@hawaii.edu

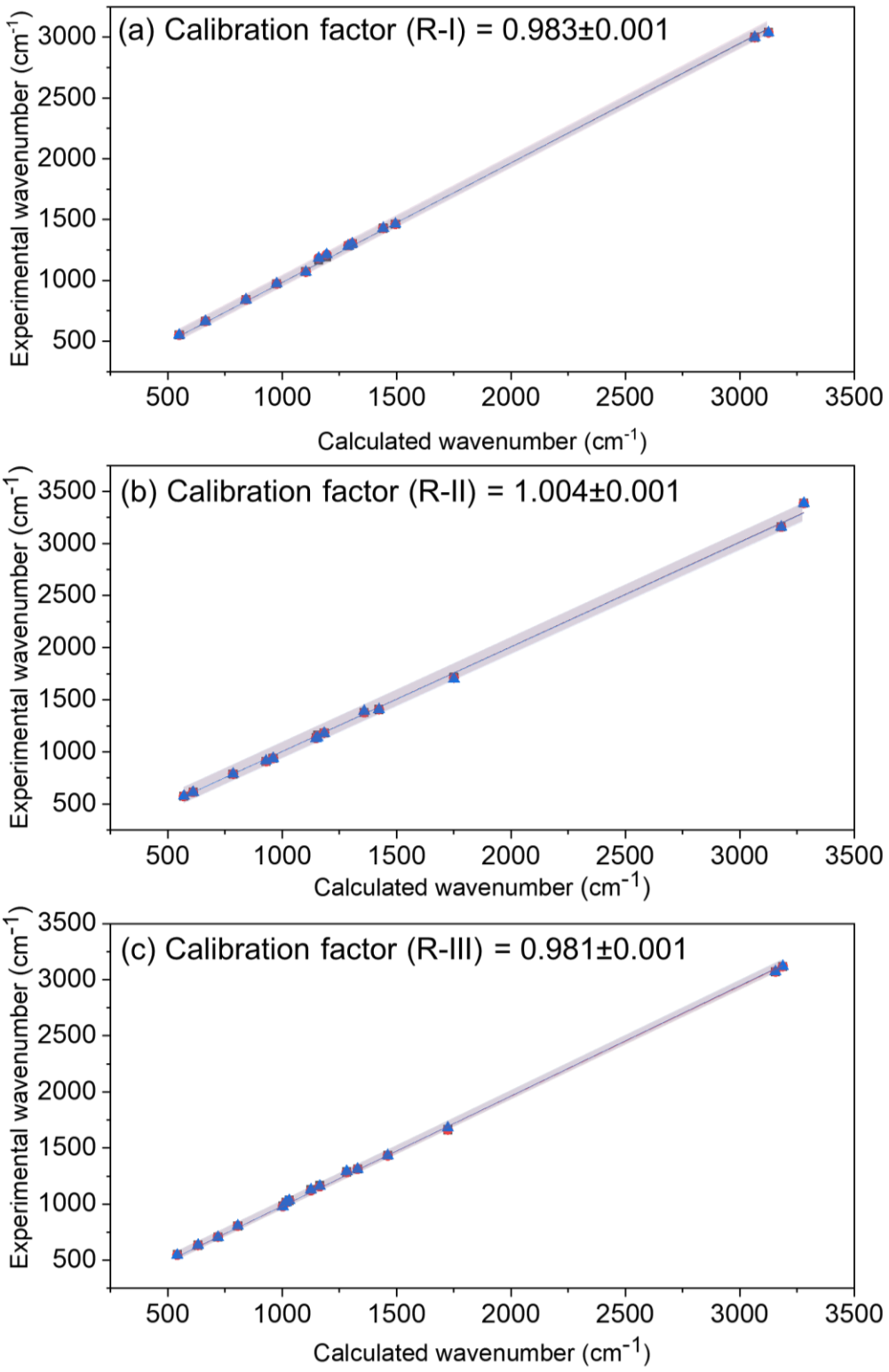

Figure S1: Calibration of calculated frequency with experimental ones; (a) R-I, (b) R-II and (c) R-III.

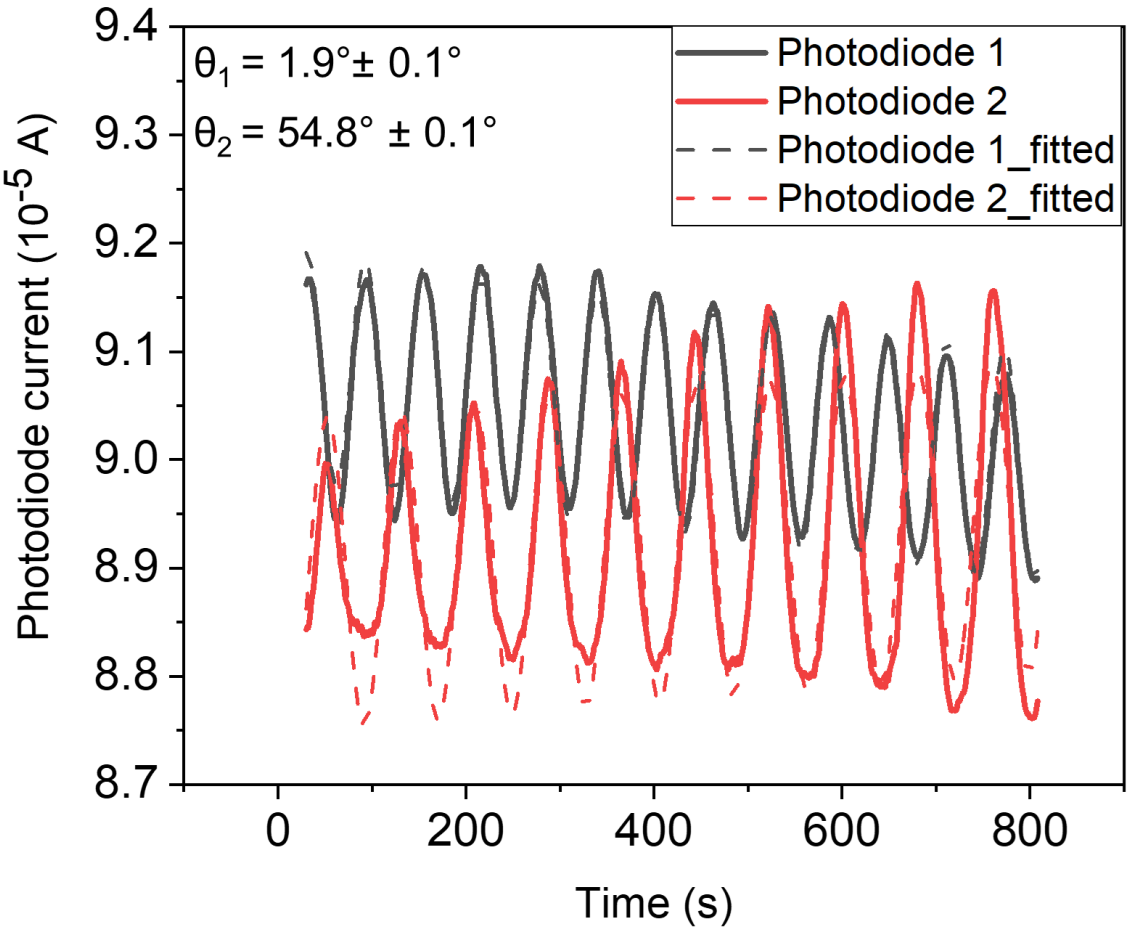

Figure S2: Experimentally measured interference patterns for methane in a two-laser interferometry setup; Laser 1 at angle θ_1 = 1.9°± 0.1° and Laser 2 at an angle θ_2 = 54.8°± 0.1°.

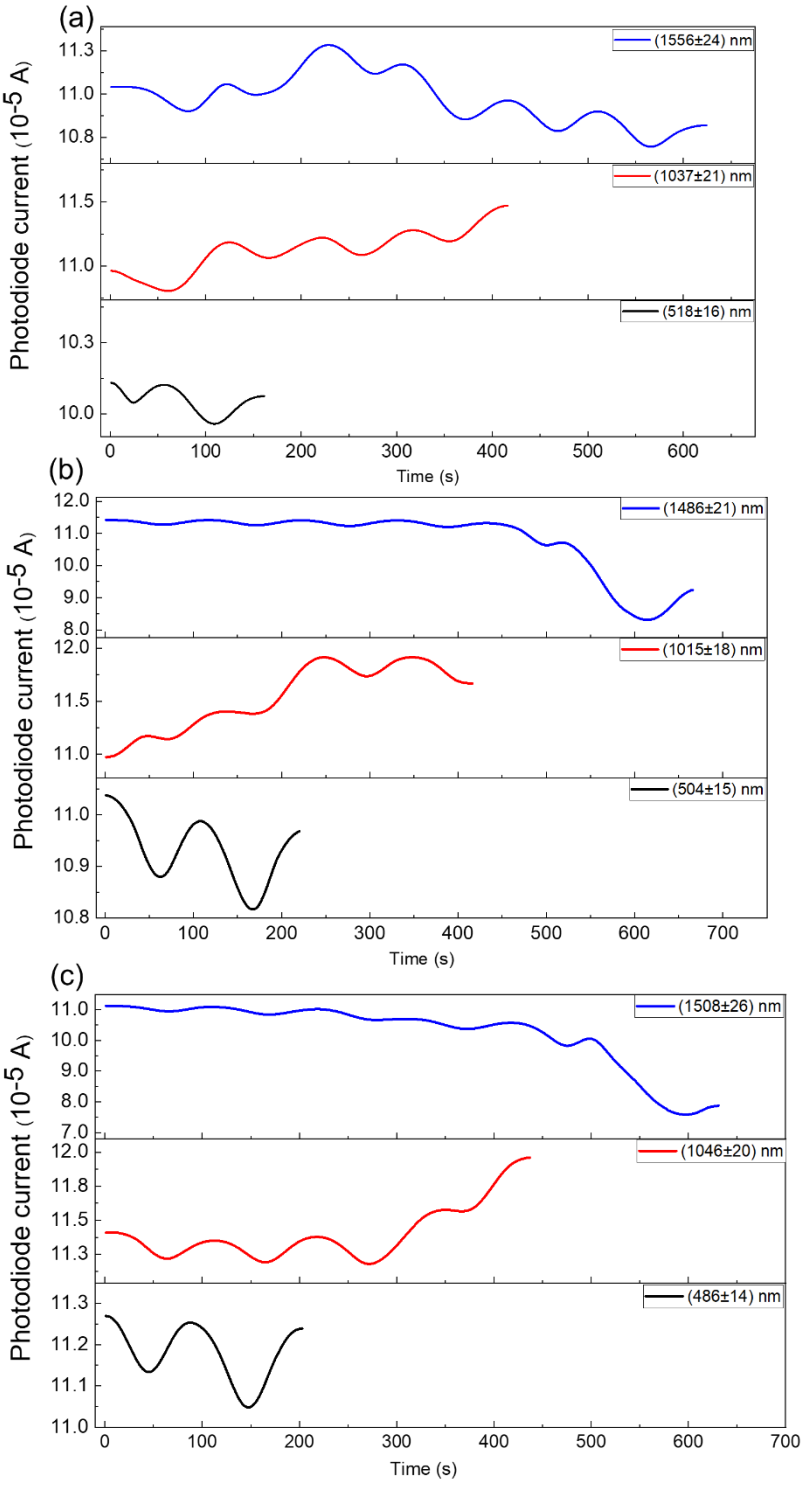

Figure S3: Interference patterns of different refrigerants observed during deposition of distinct thicknesses of ices (a) R-I, (b) R-II, and (c) R-III.

Table S1: Combination bands arise at higher thicknesses of refrigerant ices (a) R-I, (b) R-II, and (c) R-III.

Name of the molecule	Combination frequencies appeared in thicker ice (cm^{-1})	Thickness of ice (d) (nm)
1,1,1,2-tetrafluoroethane (R-I)	-	518±16
	2627, 2708, 2747, 2814, 2837, 3977, 4104, 4220, 4279, 4333	1037±21
		1556±24
2,3,3,3-tetrafluoropropene (R-II)	-	504±15
	1964,1113	1015±18
		1486±21
3,3,3-trifluoropropene (R-III)	-	486±14
	2459, 4035, 4257, 4277, 4415, 4672, 4796	1046±20
	2175, 2459, 2559, 4035, 4257, 4277, 4415, 4672, 4796	1508±26

Table S2: Optimized coordinates (Angstrom) of the refrigerants at the B3LYP-D3/def2-TZVP level. (a) R-I, (b) R-II, and (c) R-III.

(a) R-I

Atom	X-Coord	Y-Coord	Z-Coord
C	-1.14139345	0.32919079	0.05647186
C	0.35051540	0.06832620	0.17960693
F	-1.66080793	-0.42619374	-0.97048926
H	-1.62241816	0.05104522	0.99539163
H	-1.29373317	1.38867702	-0.15471729
F	0.61338142	-1.21889599	0.44996910
F	1.01087080	0.39753920	-0.94053502
F	0.84068914	0.81666249	1.18964492

(b) R-II

C	-0.20907617	1.15786358	-0.07537133
C	-0.14090953	-0.32433474	0.11368718
F	1.00546636	-0.86568039	-0.33679149
F	-0.25431712	-0.65235127	1.42120632
C	0.75893204	1.86737531	-0.63025828
F	-1.15791495	-0.94274707	-0.52922113
H	-1.12872945	1.60117290	0.28546263
H	1.66961654	1.40227002	-0.98371767
H	0.66654869	2.93880038	-0.74693247

(c) R-III

C	0.01864935	0.91207482	-0.14370350
C	0.04245631	-0.58198985	0.06642844
F	1.18641763	-1.11807704	-0.38616053
F	-0.07296324	-0.88808752	1.37122549
C	0.97159402	1.63547459	-0.69354138
F	-0.97869721	-1.17643242	-0.57651467
F	-1.12662200	1.44262452	0.30989005
H	1.87509151	1.16194764	-1.04320557
H	0.85547932	2.70449850	-0.79784011

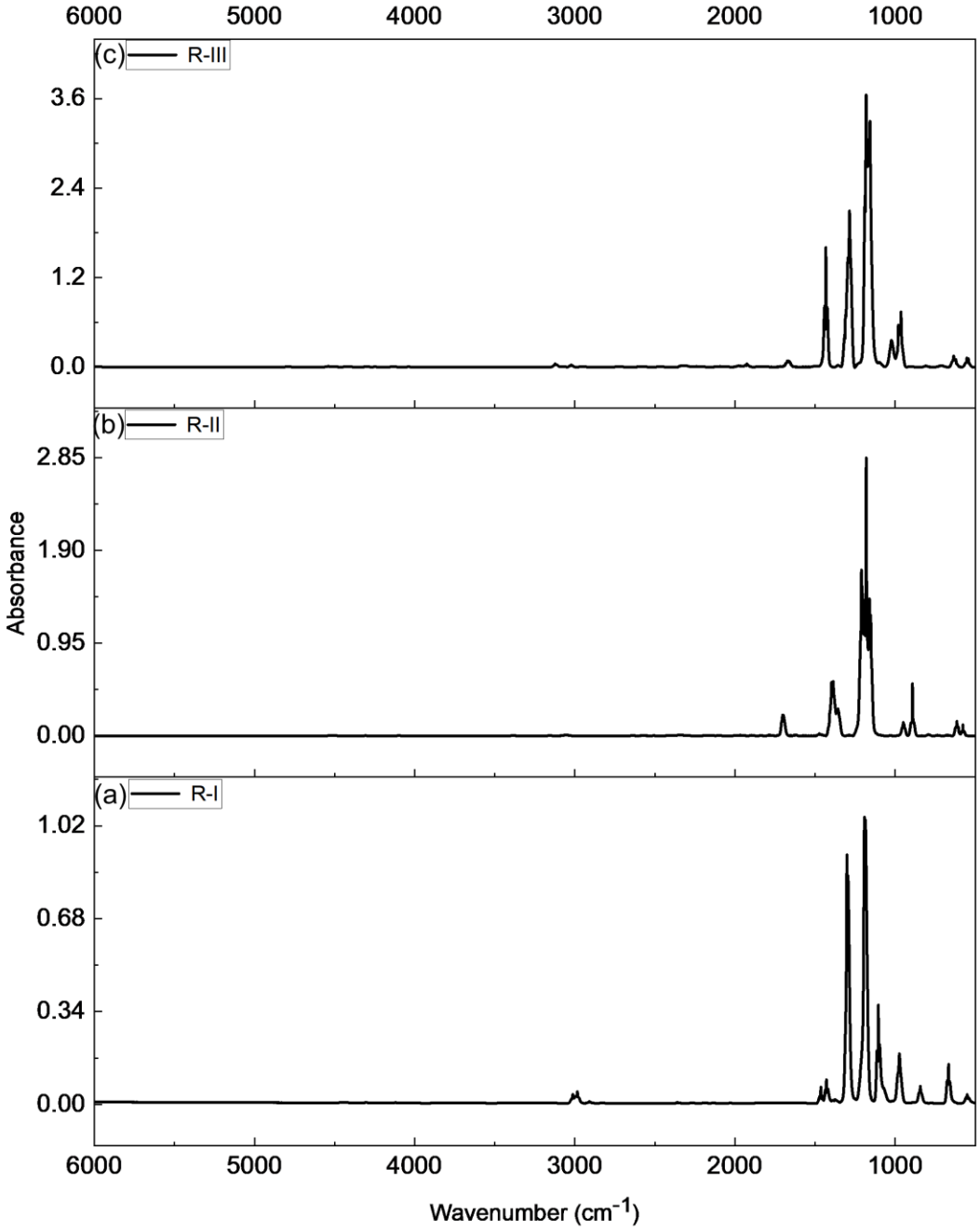

Figure S4: Experimentally measured vapor phase infrared spectra of the refrigerants. (a) R-I, (b) R-II, and (c) R-III.

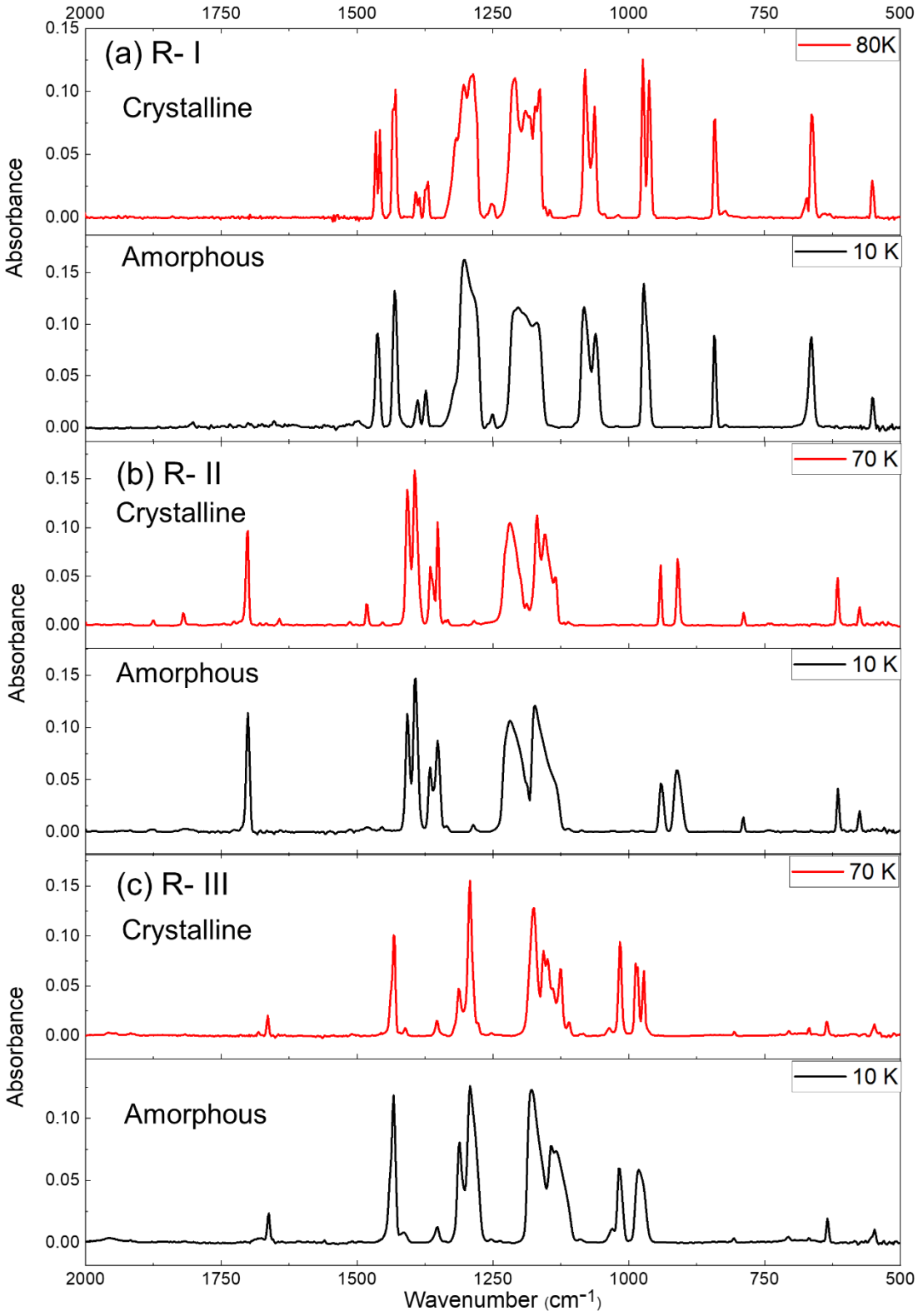
(a) R- I
Crystalline
80K
Amorphous
10 K
(b) R- II
Crystalline
70 K
Amorphous
10 K
(c) R- III
Crystalline
70 K
Amorphous
10 K
Absorbance
Wavenumber (cm-1)
2000
1750
1500
1250
1000
750
500
0.15
0.10
0.05
0.00

Figure S5: Evidence of amorphous to crystalline phase transition at elevated temperatures of the refrigerants. (a) R-I, (b) R-II, and (c) R-III.

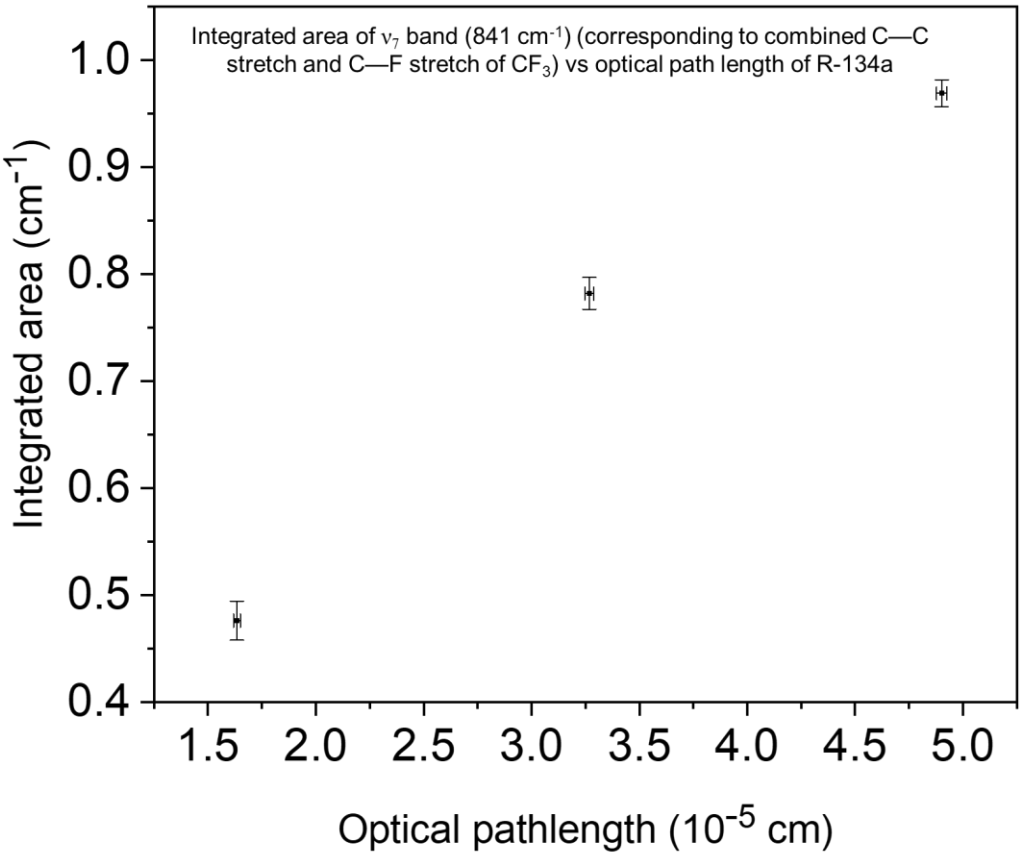

Figure S6: Representative plot of integrated areas versus ice thicknesses utilized to measure band strengths of ν_f^{11} (ν_7) (841 cm^{-1}) band corresponding to C—C stretch and C—F stretch of CF_3 for R-I.