Vacuum Ultraviolet Photolysis of Condensed Methyl Chloride in Interstellar Model Conditions and Trapping of Intermediates at Intergrain Interfaces

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This PDF file includes:

Supporting information 1:

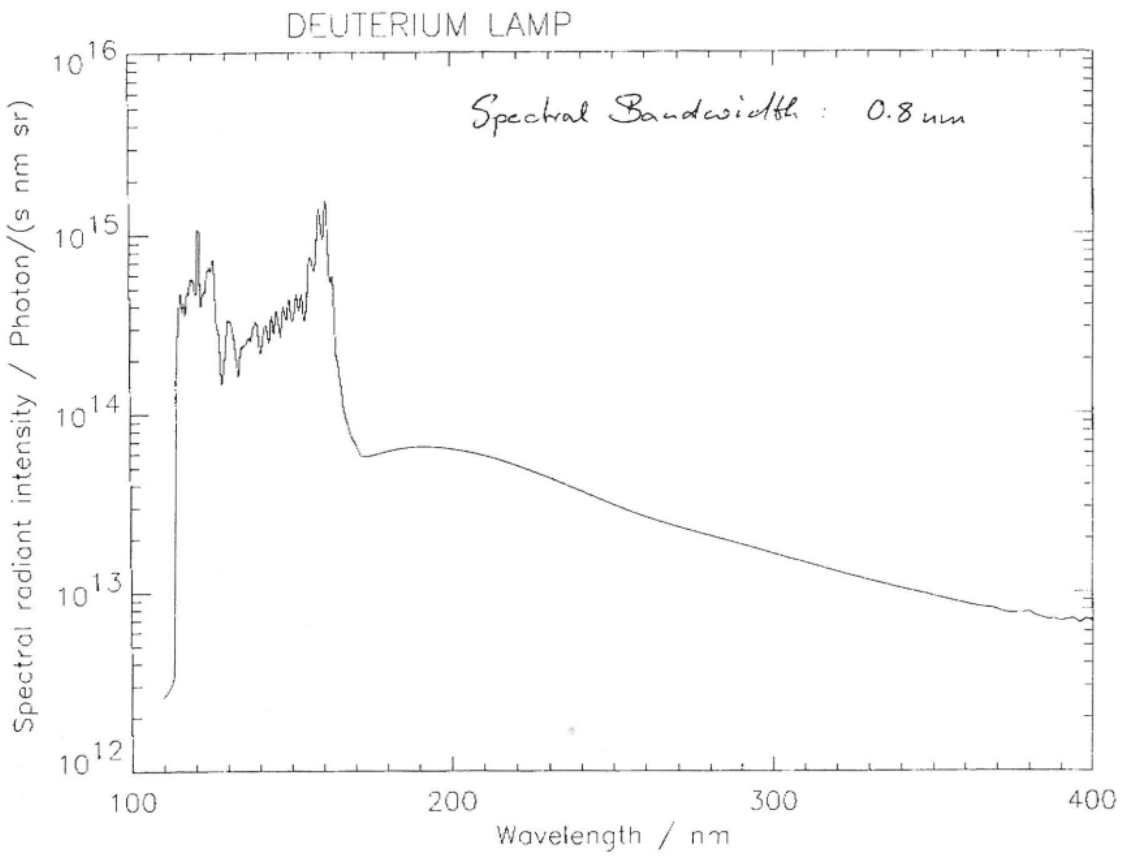

Figure S1. Emission spectrum of Model 634 Deuterium lamp, provided by the McPherson.

Supporting information 2:

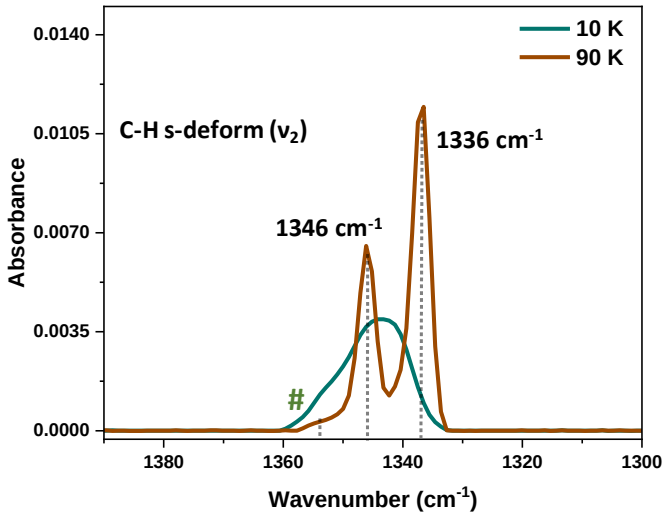

Figure S2. RAIR spectra of 63 ML of methyl chloride in C-H symmetric bending region. The pure methyl chloride was vapor-deposited on Ru(0001) substrate at 10 K and further annealed to 90 K with a ramping rate of 10 K/min, and it was waited for 2 hours.

Supporting information 3:

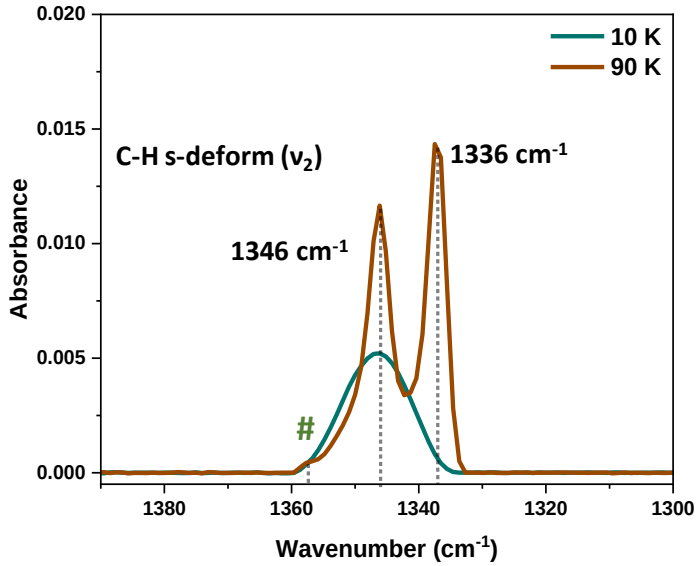

Figure S3. RAIR spectra of 160 ML of methyl chloride:water (2:1) in C-H symmetric bending region. The 160 ML of methyl chloride:water (2:1) was vapor-deposited on Ru(0001) substrate at 10 K and further annealed to 90 K with a ramping rate of 2 K/min.

Supporting information 4:

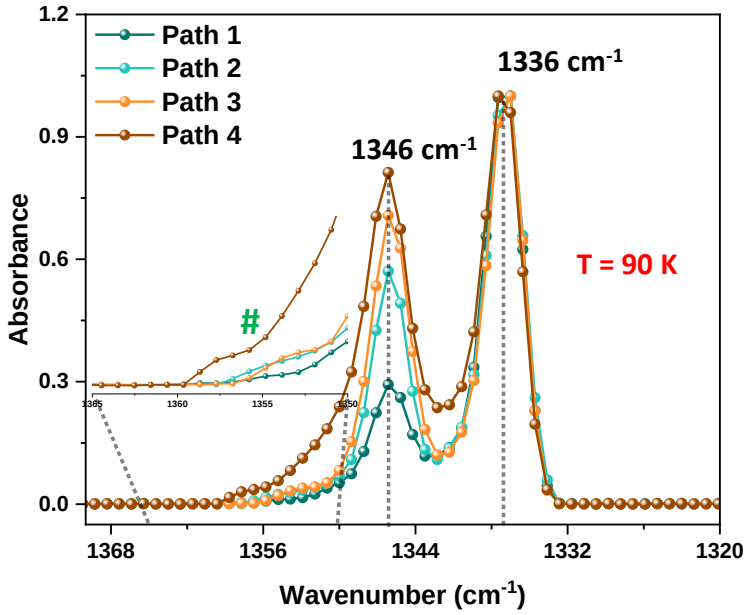

Figure S4. Normalized RAIR spectra of condensed methyl chloride ice in the C-H symmetric bending region at 90 K created by four different paths. In path 1 and path 2, 63 ML of methyl chloride vapor was deposited on Ru(0001) at 10 K substrate and slowly annealed to 90 K at an annealing rate of 2 K/min and 10 K/min, respectively. In path 3, methyl chloride directly vapor deposited on Ru(0001) substrate at 90 K. In path 4, 160 ML of methyl chloride:water (2:1) co-deposited on Ru(0001) substrate at 10 K and slowly annealed to 90 K at an annealing rate of 2 K/min. The enlarged spectra in the inset show a hump around 1354 cm^{-1} (denoted by #), representing the gas phase methyl chloride.

Supporting information 5:

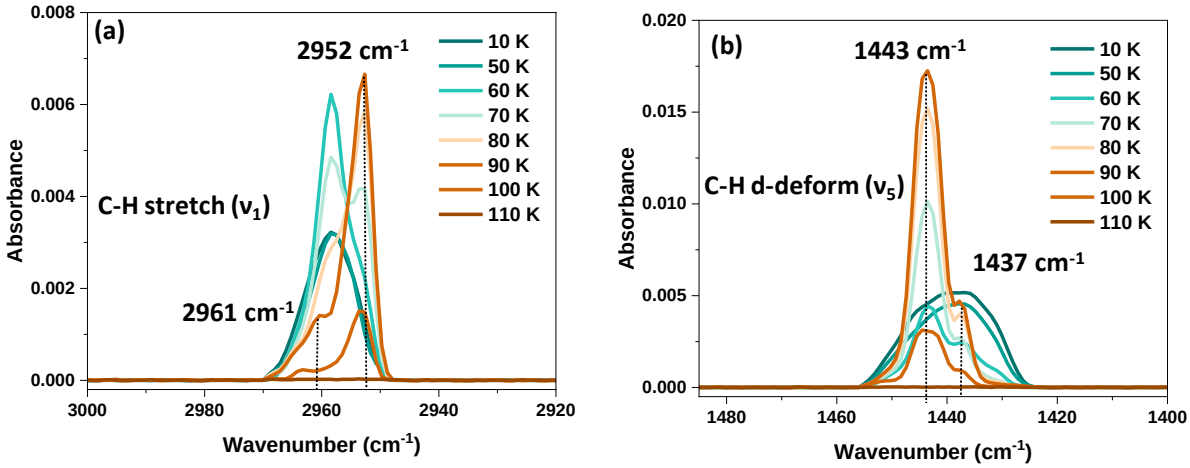

Figure S5. Temperature-dependent RAIR spectra of 63 ML of methyl chloride in (a) C-H stretching region, (b) C-H antisymmetric bending region. The pure methyl chloride was vapor-deposited on Ru(0001) substrate at 10 K and further annealed to 90 K with a ramping rate of 2 K/min.

Supporting information 6:

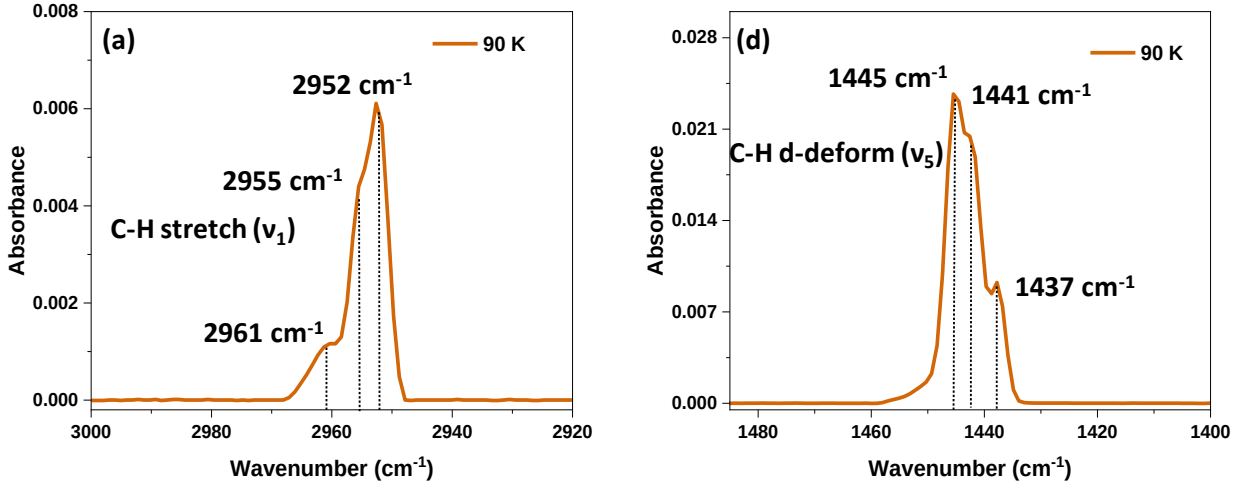

Figure S6. RAIR spectrum of 63 ML of methyl chloride in (a) C-H stretching region, (b) C-H antisymmetric bending region. The pure methyl chloride was vapor-deposited on Ru(0001) substrate at 90 K.

Supporting information 7:

Table S1. Vibrational frequencies of methyl chloride in amorphous, crystalline, polycrystalline, and gas phases.[1]

Mode	Amorphous (cm^{-1})	Crystalline (cm^{-1})	Polycrystalline (cm^{-1})	Gas (cm^{-1})
C-Cl stretching (ν_3)	710	704, 700, 695	705, 700, 695	732
C-Cl rocking (ν_6)	1019	1022	1022	1015
C-H symmetric bending (ν_2)	1343	1336, 1346	1336, 1346	1354
C-H antisymmetric bending (ν_5)	1438	1443, 1437	1445, 1441, 1437	1454
C-H symmetric stretching (ν_1)	2958	2952, 2961	2952, 2955, 2961	2966

Supporting information 8:

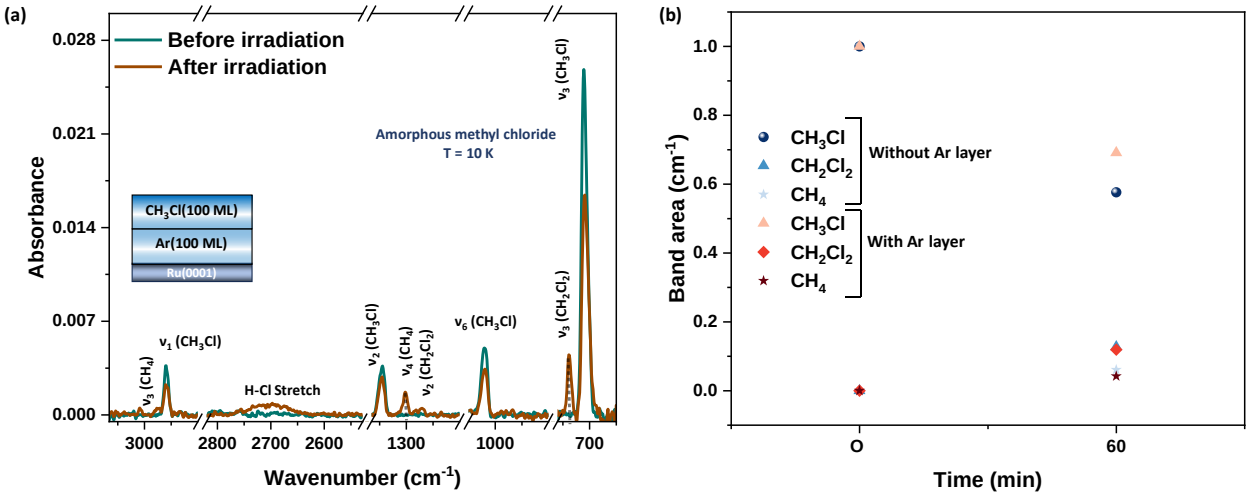

Figure S7. (a) RAIR spectra of 100 ML of methyl chloride before and after irradiation with VUV light at 10 K in the mid-infrared region. At first, 100 ML of Ar vapor was deposited on Ru(0001) substrate, followed by methyl chloride vapor deposited on top of that. The amorphous methyl chloride ice was photo-irradiated for 60 minutes. (b) Normalized band area of methyl chloride, dichloromethane, and methane before and after 60 min irradiation. Two systems were taken: in the first system, 63 ML of methyl chloride was directly vapor deposited on Ru(0001) substrate, and in the second system, 100 ML of methyl chloride was deposited on the top of 100 ML of Ar matrix on Ru(0001) substrate.

Supporting information 9:

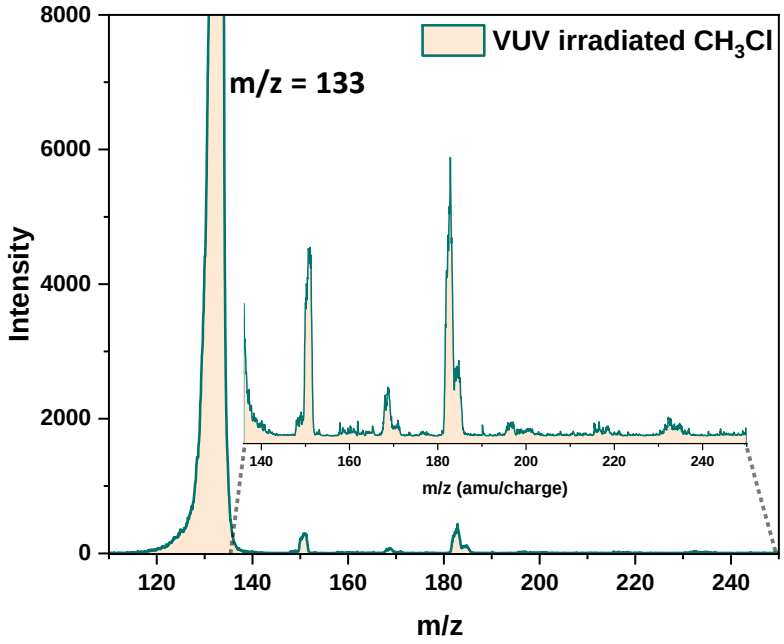

Figure S8. Reactive ion scattering mass spectrum obtained on 60 minutes VUV irradiated amorphous methyl chloride ice at 10 K.

Supporting information 10:

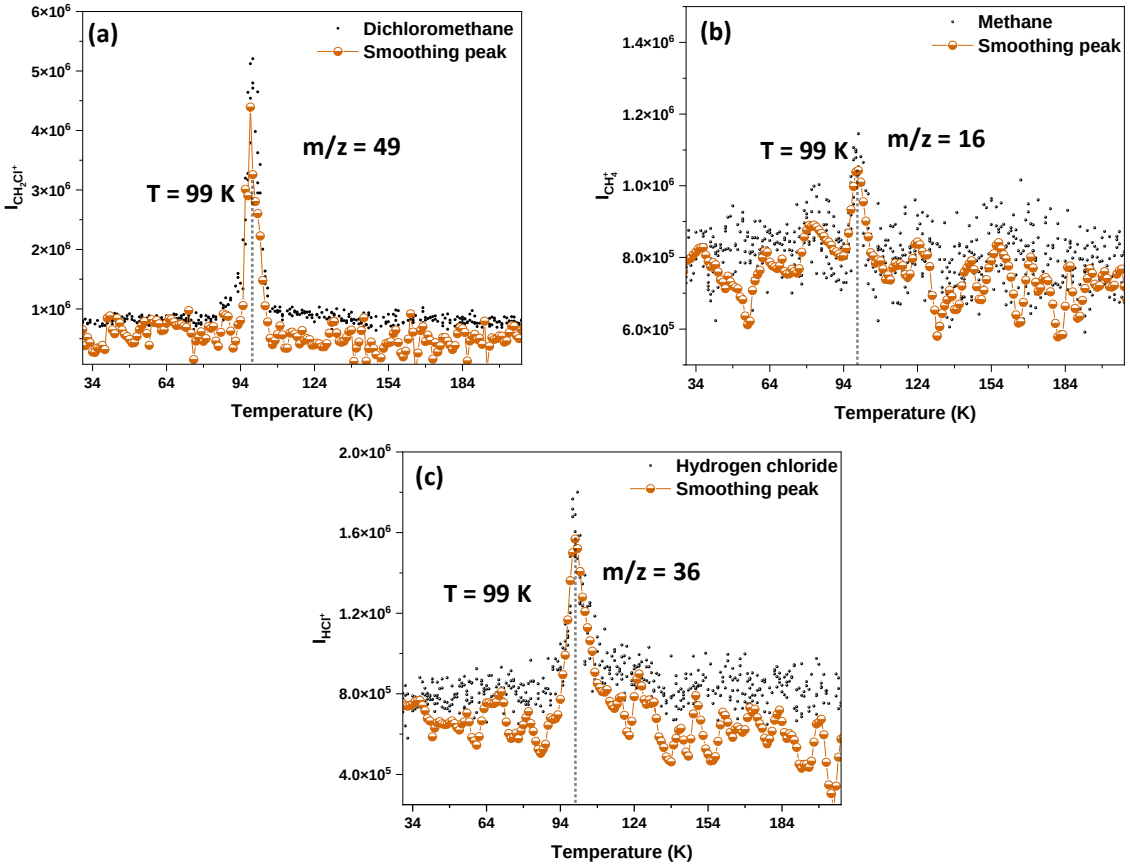

Figure S9. Sublimation profile of integrated ion counts in (a) at m/z = 49 (CH_2Cl_2) in (b) at m/z = 16 (CH_4) in (c) at m/z = 36 (HCl) recorded by quadrupole mass spectrometer. 63 ML of pure methyl chloride was deposited on Ru(0001) substrate, followed by 60 min of VUV light irradiation. The irradiated sample was annealed to 200 K with a 10 K/min ramping rate; subsequently, mass spectra were taken.

REFERENCES

(1) Dows, D. A. Vibrational Spectra of the Crystalline Methyl Halides. *J. Chem. Phys.* **1958**, *29* (3), 484. https://doi.org/10.1063/1.1744528.