



Universiteit
Leiden
The Netherlands

From clouds to comets: tracing the molecular journey of interstellar ices in the JWST era

Slavicinska, K.

Citation

Slavicinska, K. (2026, June 10). *From clouds to comets: tracing the molecular journey of interstellar ices in the JWST era*. Retrieved from <https://hdl.handle.net/1887/4305137>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/4305137>

Note: To cite this publication please use the final published version (if applicable).

From Clouds to Comets

Tracing the Molecular Journey of Interstellar Ices in the JWST Era

Proefschrift

ter verkrijging van
de graad van doctor aan de Universiteit Leiden,
op gezag van rector magnificus prof. dr. S. de Rijcke,
volgens besluit van het college voor promoties
te verdedigen op woensdag 10 juni 2026
klokke 11:30 uur

door

Kateřina Slavičinská
geboren te Brno, Tsjechische Republiek
in 1997

Promotores

Prof. dr. E. F. van Dishoeck

Prof. dr. H. V. J. Linnartz†

Co-promotor

Dr. K. -J. Chuang

Promotiecommissie

Prof. dr. I. A. G. Snellen

Prof. dr. S. Viti

Prof. dr. P. Ehrenfreund

Dr. M. E. Palumbo

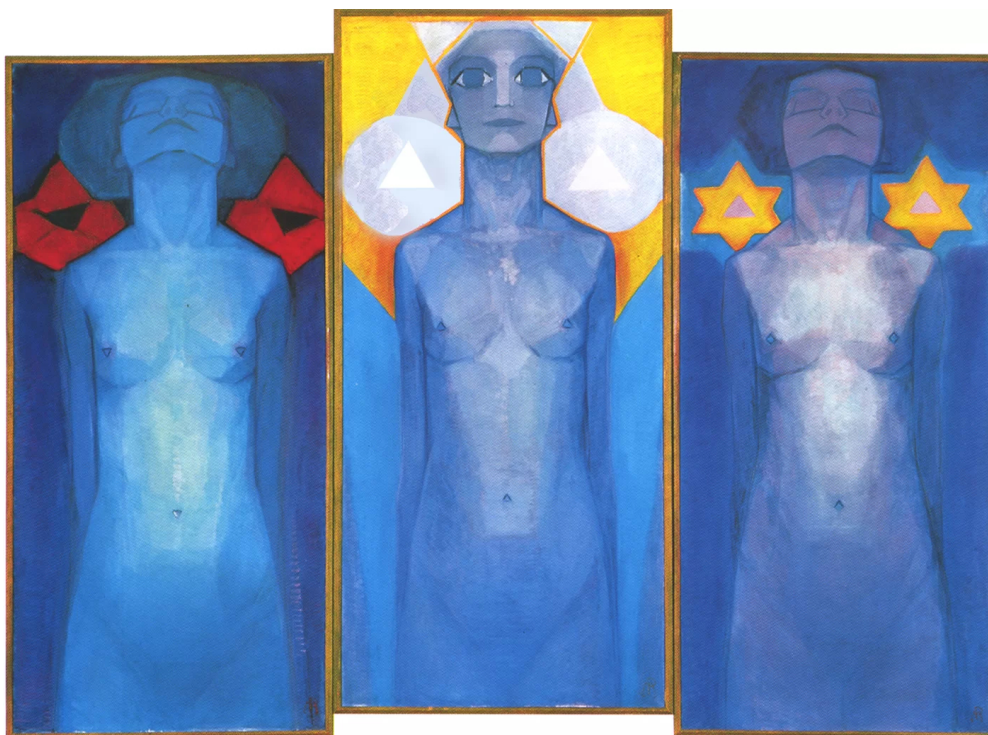
INAF - Osservatorio Astrofisico di Catania

Dr. P. Gerakines

NASA Goddard Space Flight Center

Copyright © 2026 *Katerina Slavicinska*.

Cover art: *Surfaces and Depths (bottom half)*. Illustrated by Katie Slavicinska in Adobe Photoshop. Inspired by the collaborative artworks of Stephen Muldoon and Robert Wyland. See Brian Ferrari's thesis for top half.



Evolution
Piet Mondrian, 1911

Contents

1	Introduction	1
1.1	Seeds of life in surprising places	1
1.2	Ice chemistry during star and planet formation	3
1.2.1	Molecular clouds	3
1.2.2	Protostars and protoplanetary disks	8
1.2.3	Planetary bodies	11
1.3	Infrared spectroscopy of ices	12
1.3.1	Observational methods	14
1.3.2	Laboratory methods	20
1.4	Thesis overview	25
1.4.1	Aims	25
1.4.2	Chapter summary	26
1.4.3	Scientific significance and future directions	27
1.B	Bibliography	29
2	JWST detections of amorphous and crystalline HDO ice toward massive proto-stars	33
2.1	Introduction	34
2.2	Methods	37
2.2.1	Investigated sources	37
2.2.2	Observations and data reduction	40
2.2.3	Gas emission subtraction	40
2.2.4	Laboratory data collection	40
2.3	Results	41
2.3.1	CH ₃ OH ice	42
2.3.2	4 μ m region: CH ₃ OH, S-bearing species, and HDO	44
2.3.3	HDO ice	46
2.3.4	H ₂ O ice	48
2.4	Discussion	50
2.4.1	Inferred ice HDO/H ₂ O ratios	50
2.4.2	Comparing ice and gas HDO/H ₂ O ratios	51
2.4.3	Ice envelope evolution	53
2.5	Conclusions	55
2.6	Acknowledgements	55
2.A	Appendix	56
2.A.1	Laboratory data	56
2.A.2	χ^2 plots	64
2.A.3	Estimated continuum errors	64
2.A.4	Literature HDO/H ₂ O values	68
2.B	Bibliography	69

3	HDO ice detected toward an isolated low-mass protostar with JWST	73
3.1	Introduction	74
3.2	Methods	76
3.2.1	Observations	76
3.2.2	Ice fitting	78
3.3	Results and discussion	80
3.3.1	HDO ice	80
3.3.2	H ₂ O ice	81
3.3.3	HDO/H ₂ O ratio	83
3.4	Conclusions	85
3.5	Acknowledgments	86
3.A	Appendix	87
3.A.1	Observations	87
3.A.2	Continuum, silicate, and CH ₃ OH ice fitting	87
3.A.3	Comparing NIRSspec and MIRI bands of the same ice species	92
3.A.4	Ice fitting uncertainties	94
3.A.5	Comparison with AKARI results	97
3.A.6	Literature HDO/H ₂ O values	99
3.B	Bibliography	101
4	Ammonium hydrosulfide (NH₄SH) as a potentially significant sulfur sink in interstellar ices	103
4.1	Introduction	104
4.2	Methodology	107
4.2.1	Experimental	107
4.2.2	Observational	111
4.3	Spectroscopic characterization	113
4.3.1	NH ₃ :H ₂ S	113
4.3.2	H ₂ O:NH ₃ :H ₂ S	117
4.4	Comparing NH ₄ SH:H ₂ O laboratory spectra to observations	124
4.4.1	NH ₄ ⁺ ν ₄ mode	124
4.4.2	Redshift of the 6.85 μm feature	128
4.4.3	SH ⁻ stretching mode	131
4.4.4	NH ₄ ⁺ ν ₄ and SH ⁻ libration combination mode	133
4.4.5	Other anions (OCN ⁻ , CN ⁻ , HCOO ⁻ , Cl ⁻)	134
4.5	Astronomical implications	135
4.5.1	Sulfur budgets	135
4.5.2	NH ₄ SH ice desorption front	136
4.6	Conclusions	137
4.7	Acknowledgements	138
4.A	Appendix	138
4.A.1	Calibration procedure supplementary information	138
4.A.2	Beer's law plot errors	139
4.A.3	Pure NH ₄ SH supplementary laboratory data	139
4.A.4	NH ₄ SH:H ₂ O supplementary laboratory data	144
4.A.5	Observational supplementary data	154

4.B Bibliography	158
5 Laboratory infrared spectra and band strengths of carbonyl sulfide (OCS) in CH₃OH- and CO-rich ice mixtures for analyzing interstellar ice observations	161
5.1 Introduction	162
5.2 Methods	164
5.2.1 Experimental setup	164
5.2.2 Mixing ratio calibration	165
5.2.3 Apparent band strengths	166
5.3 Results	167
5.3.1 Pure OCS ice	167
5.3.2 OCS ice mixtures	169
5.4 Astronomical implications	175
5.5 Conclusions	177
5.6 Acknowledgements	178
5.A Supplemental Information	178
5.A.1 OCS ν_3 peak positions, FWHMs, and relative integrated absorbances	178
5.B Bibliography	184
6 The hunt for formamide in interstellar ices	185
6.1 Introduction	186
6.2 Formamide formation mechanism debate	189
6.3 Methodology	191
6.4 Results	193
6.4.1 C=O stretching and NH ₂ scissoring features (~ 1700 and 1630 cm^{-1})	197
6.4.2 CH bending and CN stretching features (~ 1388 and 1328 cm^{-1}) . . .	199
6.5 Astronomical implications	201
6.6 Conclusions	208
6.7 Acknowledgements	209
6.A Appendix	209
6.A.1 Peak positions and FWHMs of formamide in pure and mixed ices . .	209
6.A.2 Relative apparent band strengths of formamide in pure and mixed ices	214
6.A.3 QMS calibration of an independent tri-dosing leak valve system and mixing ratio determination	216
6.B Bibliography	221
English summary	225
Nederlandse samenvatting	233
České shrnutí	243
Publications	251
Curriculum vitae	257
Acknowledgments	259