



Universiteit
Leiden
The Netherlands

Molecular inheritance from cloud to disk: a story of complex organics and accretion shocks

Gelder, M.L. van

Citation

Gelder, M. L. van. (2022, November 24). *Molecular inheritance from cloud to disk: a story of complex organics and accretion shocks*. Retrieved from <https://hdl.handle.net/1887/3487189>

Version: Publisher's Version

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

License: <https://hdl.handle.net/1887/3487189>

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

Molecular inheritance from cloud to disk

- *A story of complex organics and accretion shocks* -

Proefschrift

ter verkrijging van
de graad van doctor aan de Universiteit Leiden,
op gezag van rector magnificus prof. dr. ir. H. Bijl,
volgens besluit van het college voor promoties
te verdedigen op donderdag 24 november 2022
klokke 12:30 uur
door

Martijn Lucas van Gelder

geboren te 's-Gravenhage, Nederland
in 1994

Promotores:

Prof. dr. E. F. van Dishoeck

Prof. dr. M. R. Hogerheijde Universiteit Leiden
Universiteit van Amsterdam

Co-promotor:

Dr. B. Tabone Université Paris-Saclay

Promotiecommissie:

Prof. dr. H. J. A. Röttgering

Prof. dr. S. Viti

Prof. dr. J. K. Jørgensen University of Copenhagen

Dr. B. Nisini INAF, Osservatorio Astronomico di Roma

Dr. B. A. McGuire MIT, Cambridge

ISBN: 978-94-6419-632-0

Cover design: Marta Paula Tychoniec

If the truth is worth telling,
it is worth making a fool of yourself to tell it.
- *Frederick Buechner*

Table of contents

1	Introduction	1
1.1	How do stars form?	2
1.1.1	Prestellar phases and start of collapse	2
1.1.2	Low-mass star formation	3
1.1.3	High-mass star formation	6
1.2	Chemistry during protostellar evolution	7
1.2.1	Prestellar cores	7
1.2.2	Hot cores	10
1.2.3	Shocks	10
1.3	Astronomical observatories	14
1.3.1	ALMA	14
1.3.2	JWST	15
1.4	Complex organic molecules in protostars	16
1.4.1	Ices	17
1.4.2	Gas phase	18
1.5	Inheritance versus reset: accretion shocks	23
1.6	This thesis	25
PART I	Chemical complexity in young protostars	29
2	Complex organic molecules in low-mass protostars on Solar System scales. I. Oxygen-bearing species	31
2.1	Introduction	33
2.2	Observations	35
2.3	Spectral modeling and results	37
2.3.1	Methodology	37
2.3.2	Column densities and excitation temperatures	39
2.3.3	Relative abundances	42
2.4	Discussion	43
2.4.1	Occurrence of COMs in young protostars	43
2.4.2	Dependence on source size	44
2.4.3	From cold (Band 3) to hot (Band 6) COMs	45
2.4.4	Comparison to other sources	48

2.4.5 Comparison with ices	50
2.4.6 Temperature dependence of deuterated methanol	50
2.5 Summary	51
Appendices	53
2.A Laboratory spectroscopic data	53
2.B CASSIS modeling results	54
2.C Full ALMA Band 6 spectra	61
2.D B1-c Band 3 spectrum	67
2.E Additional tables	71
3 Importance of source structure on complex organics emission.	
I. Observations of CH₃OH from low-mass to high-mass protostars	95
3.1 Introduction	97
3.2 Methodology	98
3.2.1 Observations and archival data	98
3.2.2 Deriving the column density	100
3.2.3 Calculating the warm methanol mass	102
3.3 Results	103
3.3.1 Amount of warm methanol from low to high mass	103
3.3.2 Comparison to spherically symmetric infalling envelope . .	105
3.4 Discussion	107
3.4.1 Importance of source structure	107
3.4.2 Continuum optical depth	110
3.5 Conclusion	112
Appendices	114
3.A Observational details	114
3.B Transitions of CH ₃ OH and isotopologues	126
3.C Toy model of infalling envelope	128
3.D Calculating the reference dust mass	129
4 Methanol deuteration in high-mass protostars	131
4.1 Introduction	133
4.2 Methodology	134
4.2.1 Observations	134
4.2.2 Deriving the column densities	136
4.3 Results	138
4.4 Discussion	140
4.4.1 Methanol deuteration from low to high mass	140
4.4.2 Singly vs doubly deuterated methanol	142
4.4.3 Linking the methanol D/H to the physical conditions during formation	143
4.5 Conclusion	146
Appendices	149
4.A Transitions of CH ₃ OH and isotopologues	149
4.B Observational details	150
4.C Methanol D/H ratios of sources in the literature	154

4.D	CHD ₂ OH in B1-c, Serpens S68N, and B1-bS	156
4.E	Additional figures	157
PART II	Inheritance versus reset: accretion shocks	159
5	Modeling accretion shocks at the disk-envelope interface. Sul-	
	fur chemistry	161
5.1	Introduction	163
5.2	Accretion shock model	165
5.2.1	Shock model	165
5.2.2	Input parameters	168
5.3	Results	169
5.3.1	Temperature and density	169
5.3.2	Chemistry of SO and SO ₂	171
5.3.3	Effect of grain size and PAHs	176
5.3.4	Other molecular shock tracers: SiO, H ₂ O, H ₂ S, CH ₃ OH, and H ₂	176
5.4	Discussion	178
5.4.1	Comparison to SO and SO ₂ with ALMA	178
5.4.2	Predicting H ₂ , H ₂ O, and [S I] with JWST	179
5.5	Summary	180
	Appendices	182
5.A	Updated cooling of NH ₃	182
5.B	Input abundances	183
5.C	Changing the preshock conditions	183
5.D	Abundance grids	187
5.D.1	H ₂ S, H ₂ O, SiO, and CH ₃ OH for $G_0 = 1$	187
5.D.2	SO and SO ₂ for various G_0	188
5.E	Higher magnetized environments	190
5.E.1	C-type shocks	190
5.E.2	CJ-type shocks	191
6	Observing accretion shocks with ALMA. Searching for SO and SO₂ in Class I disks	193
6.1	Introduction	195
6.2	Observations	197
6.3	Results	198
6.3.1	Dust continuum	198
6.3.2	SO and SO ₂	199
6.4	Discussion	202
6.4.1	Inheritance vs reset: constraining the shock strength	202
6.4.2	Relation between warm SO ₂ and source properties	203
6.5	Conclusions	205
	Appendices	207
6.A	Maps of c-C ₃ H ₂ and CH ₃ OH	207

6.B Spectra of SO and SO ₂ for IRS 4 and IRS 6	208
6.C Additional tables	209
Bibliography	210
Nederlandse samenvatting	233
Publications	241
Curriculum Vitae	243
Acknowledgements	245