2017 Astrobiology Graduate Conference

CHARLOTTESVILLE, VA

1
00:00:00,790 --> 00:00:07,629
[Music]

2
00:00:15,530 --> 00:00:12,520
so my presentation will mostly deal with

3
00:00:17,990 --> 00:00:15,540
reactivity and all the results issue

4
00:00:19,609 --> 00:00:18,000
from theoretical computations so I won't

5
00:00:21,470 --> 00:00:19,619
give any details about the methods

6
00:00:23,529 --> 00:00:21,480
because I'm pretty sure that you don't

7
00:00:27,500 --> 00:00:23,539
care about that

8
00:00:29,870 --> 00:00:27,510
so I am working on prebiotic chemistry

9
00:00:31,999 --> 00:00:29,880
which basically aims at understanding

10
00:00:35,030 --> 00:00:32,009
how life could appear on an earth

11
00:00:36,680 --> 00:00:35,040
originally in organic planet considering

12
00:00:40,280 --> 00:00:36,690
that it is ruled mainly by organic

13
00:00:42,770 --> 00:00:40,290

chemistry to solve this issue two main

14
00:00:45,709 --> 00:00:42,780
hypotheses have been made the first one

15
00:00:50,840 --> 00:00:45,719
is based on an endogenous synthesis

16
00:00:53,569 --> 00:00:50,850
theory here in this case the building

17
00:00:56,240 --> 00:00:53,579
blocks of life that are amino acids

18
00:00:58,849 --> 00:00:56,250
nucleic acid bases or simple sugars for

19
00:01:02,330 --> 00:00:58,859
example were thought to have been

20
00:01:06,050 --> 00:01:02,340
synthesized on the atmosphere of the

21
00:01:09,080 --> 00:01:06,060
early Earth based on the compounds that

22
00:01:13,250 --> 00:01:09,090
were found at that time that are methane

23
00:01:16,100 --> 00:01:13,260
nitrogen or ammonia for example this

24
00:01:18,910 --> 00:01:16,110
theory is supported by the miller-urey

25
00:01:22,670 --> 00:01:18,920
experiment in which they simulated the

26
00:01:25,280 --> 00:01:22,680
atmosphere of early Earth and discovered

27
00:01:29,649 --> 00:01:25,290
after some time that five different

28
00:01:32,240 --> 00:01:29,659
amino acids had been synthesized this

29
00:01:35,899 --> 00:01:32,250
experiment had been have been performed

30
00:01:38,990 --> 00:01:35,909
in 1962 fifty two and a couple of years

31
00:01:42,560 --> 00:01:39,000
ago they realized the mixture and found

32
00:01:44,270 --> 00:01:42,570
20 amino acids so it's a good thing for

33
00:01:47,270 --> 00:01:44,280
this theory however they just found

34
00:01:51,710 --> 00:01:47,280
amino acid they didn't find any sugars

35
00:01:53,630 --> 00:01:51,720
or whatsoever this is also why now some

36
00:01:56,209 --> 00:01:53,640
people are looking for are looking on

37
00:01:59,870 --> 00:01:56,219
Titan's atmosphere because it is thought

38
00:02:03,950 --> 00:01:59,880

to be very similar to that atmosphere of

39
00:02:06,800 --> 00:02:03,960
early Earth the second theory is based

40
00:02:08,960 --> 00:02:06,810
on an exogenous delivery of these

41
00:02:11,059 --> 00:02:08,970
building blocks of life that would be

42
00:02:13,670 --> 00:02:11,069
synthesized in interstellar medium and

43
00:02:16,880 --> 00:02:13,680
then brought back to brought back

44
00:02:19,399 --> 00:02:16,890
to hurt thanks to comets or asteroids

45
00:02:22,039 --> 00:02:19,409
for example and this is supported by the

46
00:02:25,699 --> 00:02:22,049
fact that we actually find some building

47
00:02:30,890 --> 00:02:25,709
blocks of life on comets I will focus on

48
00:02:33,770 --> 00:02:30,900
that so so far as it was mentioned

49
00:02:35,809 --> 00:02:33,780
before around 200 compounds have been

50
00:02:41,229 --> 00:02:35,819
detected in interstellar medium they are

51
00:02:44,599 --> 00:02:41,239
mainly molecules with 2 to 12 atoms and

52
00:02:46,670 --> 00:02:44,609
among them around 60 can be called

53
00:02:49,159 --> 00:02:46,680
complex organic molecules they are very

54
00:02:51,259 --> 00:02:49,169
important in providing chemistry because

55
00:02:54,500 --> 00:02:51,269
they can be considered either as

56
00:02:57,559 --> 00:02:54,510
precursors or as intermediate in the

57
00:03:01,429 --> 00:02:57,569
synthesis four of the building blocks of

58
00:03:03,140 --> 00:03:01,439
life the question is how can they be

59
00:03:05,629 --> 00:03:03,150
formed in interstellar medium

60
00:03:08,809 --> 00:03:05,639
considering that the environment there

61
00:03:13,520 --> 00:03:08,819
is very harsh the temperature and the

62
00:03:15,559 --> 00:03:13,530
pressure are really low just so you know

63
00:03:17,539 --> 00:03:15,569

the two molecules I will talk about

64
00:03:20,719 --> 00:03:17,549
later have been detected there here

65
00:03:23,199 --> 00:03:20,729
there is the formamide and cyano

66
00:03:28,909 --> 00:03:26,990
so the reactivity in interstellar medium

67
00:03:32,899 --> 00:03:28,919
is very different from the one we can

68
00:03:35,330 --> 00:03:32,909
find on earth because this very low

69
00:03:37,610 --> 00:03:35,340
temperature condition will lead to the

70
00:03:39,710 --> 00:03:37,620
fact that the only energy that is

71
00:03:43,460 --> 00:03:39,720
available for a reaction comes from the

72
00:03:45,289 --> 00:03:43,470
reactants so we can we cannot have any

73
00:03:48,649 --> 00:03:45,299
reaction that would exhibit a barrier

74
00:03:51,640 --> 00:03:48,659
the very low pressure as far as it is

75
00:03:55,249 --> 00:03:51,650
concerned will lead to the fact that

76
00:03:58,789 --> 00:03:55,259
three bodies won't be able to meet there

77
00:04:03,710 --> 00:03:58,799
so we have to focus only on two body

78
00:04:05,599 --> 00:04:03,720
reactions the study of this reactivity

79
00:04:06,379 --> 00:04:05,609
in interstellar medium can be split in

80
00:04:07,849 --> 00:04:06,389
two parts

81
00:04:12,199 --> 00:04:07,859
the first one is the dust grain

82
00:04:14,439 --> 00:04:12,209
chemistry here so in that case the

83
00:04:17,499 --> 00:04:14,449
reaction would occur at the surface of

84
00:04:20,149 --> 00:04:17,509
just grain that is composed of

85
00:04:24,279 --> 00:04:20,159
carbonaceous or silicate silicate core

86
00:04:27,560 --> 00:04:24,289
surrounded by Isis of carbon monoxide

87
00:04:32,090 --> 00:04:27,570
water and so on

88
00:04:34,670 --> 00:04:32,100

in that case these reactions on surface

89
00:04:39,140 --> 00:04:34,680
can help to reduce the potential

90
00:04:42,320 --> 00:04:39,150
barriers that a reaction could see and

91
00:04:44,480 --> 00:04:42,330
it can also is the encounter between the

92
00:04:46,850 --> 00:04:44,490
reactants because they are not far from

93
00:04:52,640 --> 00:04:46,860
each other since they are all adsorbed

94
00:04:54,620 --> 00:04:52,650
on the dust however it can also involve

95
00:04:57,170 --> 00:04:54,630
some physical processes such as a

96
00:04:59,330 --> 00:04:57,180
absorption and desorption that can be

97
00:05:03,950 --> 00:04:59,340
problematic in some regions that are

98
00:05:06,200 --> 00:05:03,960
cold or dark for example the other field

99
00:05:09,410 --> 00:05:06,210
is just phase chemistry so in that case

100
00:05:11,480 --> 00:05:09,420
we again have the same conditions no

101
00:05:14,810 --> 00:05:11,490
barrier no three-body collisions but in

102
00:05:20,000 --> 00:05:14,820
addition in the case of multi slit multi

103
00:05:21,770 --> 00:05:20,010
step reactions we cannot overpass the

104
00:05:25,730 --> 00:05:21,780
energy that comes from the reactants

105
00:05:28,970 --> 00:05:25,740
because of the very low temperature this

106
00:05:31,400 --> 00:05:28,980
chemistry can involve ion ion ion

107
00:05:33,590 --> 00:05:31,410
neutral or neutral neutral reaction and

108
00:05:35,830 --> 00:05:33,600
in my case I will focus on gas phase

109
00:05:40,640 --> 00:05:35,840
chemistry involving neutral neutral

110
00:05:46,130 --> 00:05:40,650
reactions so let's start with formula

111
00:05:48,350 --> 00:05:46,140
which is here so it's very important in

112
00:05:51,590 --> 00:05:48,360
prebiotic chemistry because it is the

113
00:05:54,740 --> 00:05:51,600

simplest amide and it can be a precursor

114
00:05:57,890 --> 00:05:54,750
in via biotic amino acid synthesis and

115
00:06:01,490 --> 00:05:57,900
perhaps also in that of the nucleic acid

116
00:06:03,620 --> 00:06:01,500
bases this makes it a central compound

117
00:06:05,810 --> 00:06:03,630
that could connect both metabolism that

118
00:06:11,390 --> 00:06:05,820
is ruled by proteins and genetics that

119
00:06:13,910 --> 00:06:11,400
is ruled by DNA and RNA it was detected

120
00:06:16,070 --> 00:06:13,920
also in interstellar medium in several

121
00:06:18,380 --> 00:06:16,080
galactic central sources in an active

122
00:06:20,990 --> 00:06:18,390
site of high style of highest mass star

123
00:06:25,910 --> 00:06:21,000
formation and more recently even in a

124
00:06:30,620 --> 00:06:25,920
product in a solar type Prada store so

125
00:06:33,140 --> 00:06:30,630
the question is how did it get there the

126
00:06:35,750 --> 00:06:33,150
first thing I try to form formamide

127
00:06:38,480 --> 00:06:35,760
was using the radical OAH and

128
00:06:40,780 --> 00:06:38,490
methylamine here as pressure source and

129
00:06:43,120 --> 00:06:40,790
I got this

130
00:06:46,330 --> 00:06:43,130
reaction path which is very complicated

131
00:06:49,960 --> 00:06:46,340
I won't describe it but what we can see

132
00:06:53,530 --> 00:06:49,970
is that the first steps here are barrier

133
00:06:56,500 --> 00:06:53,540
less so we're good and all the energies

134
00:06:58,780 --> 00:06:56,510
of all the involve compounds are always

135
00:07:02,050 --> 00:06:58,790
below the energy of the reactants this

136
00:07:05,020 --> 00:07:02,060
makes it a viable path in interstellar

137
00:07:10,480 --> 00:07:05,030
medium the problem is in the case is

138
00:07:13,420 --> 00:07:10,490

that we have a lot of products including

139
00:07:16,680 --> 00:07:13,430
soap former former mine here but also

140
00:07:20,350 --> 00:07:16,690
the two isomers of metonymic acid

141
00:07:25,150 --> 00:07:20,360
formaldehyde and here H 2 Zn so we need

142
00:07:27,940 --> 00:07:25,160
to know the amount of every product and

143
00:07:31,950 --> 00:07:27,950
the relative of the proportion of them

144
00:07:35,710 --> 00:07:31,960
to do so we did some kinetic theory and

145
00:07:37,150 --> 00:07:35,720
we got these results so here we have the

146
00:07:40,080 --> 00:07:37,160
rate constant as a function of

147
00:07:43,480 --> 00:07:40,090
temperature for the formation of several

148
00:07:46,150 --> 00:07:43,490
products here we have h 2 Zn and the two

149
00:07:49,510 --> 00:07:46,160
isomers of cyano method of metonymic

150
00:07:52,350 --> 00:07:49,520
acid and the plain line represents the

151
00:07:56,500 --> 00:07:52,360
back dissociation into the reactants and

152
00:07:59,350 --> 00:07:56,510
we can see that at low temperature which

153
00:08:02,590 --> 00:07:59,360
are the temperature of interest the main

154
00:08:07,030 --> 00:08:02,600
product is H 2 Zn so it's not formamide

155
00:08:10,120 --> 00:08:07,040
we were set and when we increase the

156
00:08:14,830 --> 00:08:10,130
energies the back dissociation becomes

157
00:08:16,600 --> 00:08:14,840
prevailing so unfortunately the form of

158
00:08:21,790 --> 00:08:16,610
mod and formaldehyde rate constants were

159
00:08:24,670 --> 00:08:21,800
not shown on the figure because the rate

160
00:08:26,860 --> 00:08:24,680
constants were found negligible so

161
00:08:29,920 --> 00:08:26,870
that's not what we wanted but it can be

162
00:08:33,280 --> 00:08:29,930
understood by the fact that a lot of

163
00:08:35,050 --> 00:08:33,290

steps are required to obtain them and we

164
00:08:39,280 --> 00:08:35,060
need to overpass this very high

165
00:08:41,110 --> 00:08:39,290
transition state so since the first

166
00:08:46,570 --> 00:08:41,120
reaction you don't work in forming

167
00:08:48,730 --> 00:08:46,580
formamide we started other reactants

168
00:08:50,440 --> 00:08:48,740
that are NH 2 and formaldehyde and

169
00:08:52,870 --> 00:08:50,450
actually we took the problem the other

170
00:08:54,130 --> 00:08:52,880
way around because they are formed in

171
00:08:56,170 --> 00:08:54,140
this reaction and instead

172
00:08:59,830 --> 00:08:56,180
of considering them as products we

173
00:09:02,730 --> 00:08:59,840
consider them as reactants and in that

174
00:09:05,710 --> 00:09:02,740
case we obtain this a lot simpler

175
00:09:08,590 --> 00:09:05,720
reaction path that also doesn't have any

176
00:09:10,360 --> 00:09:08,600
barrier and has energies that are below

177
00:09:14,500 --> 00:09:10,370
the energy of the reactants so in that

178
00:09:17,550 --> 00:09:14,510
case we were happy formamide is the only

179
00:09:20,140 --> 00:09:17,560
species that is formed by that path so

180
00:09:22,510 --> 00:09:20,150
we wanted to know how much of it was

181
00:09:25,570 --> 00:09:22,520
formed this is why we did the kinetics

182
00:09:29,320 --> 00:09:25,580
Theory the kinetics study thanks to our

183
00:09:30,610 --> 00:09:29,330
KN theory and we obtained that the rate

184
00:09:33,880 --> 00:09:30,620
constant as a function of temperature

185
00:09:36,700 --> 00:09:33,890
again of the formation of formalised

186
00:09:38,890 --> 00:09:36,710
using the different methods but it's

187
00:09:41,470 --> 00:09:38,900
only the formation of formamide and in

188
00:09:43,600 --> 00:09:41,480

that case we found that at low energy

189
00:09:47,170 --> 00:09:43,610
the formamide was actually formed

190
00:09:50,070 --> 00:09:47,180
largely more than the back dissociation

191
00:09:54,040 --> 00:09:50,080
into the reactants so that's good and

192
00:09:56,530 --> 00:09:54,050
moreover when we put those reactors rate

193
00:10:01,870 --> 00:09:56,540
constants into actual chemical models we

194
00:10:05,680 --> 00:10:01,880
had matching abundances so we were happy

195
00:10:08,680 --> 00:10:05,690
in that in order to further validate

196
00:10:10,270 --> 00:10:08,690
this we studied the deuterated formamide

197
00:10:12,700 --> 00:10:10,280
so there are three types of deuterated

198
00:10:15,970 --> 00:10:12,710
formalized because there are three

199
00:10:19,450 --> 00:10:15,980
hydrogens i think i won't have time to

200
00:10:23,340 --> 00:10:19,460
talk a lot about it but let's just say

201
00:10:27,550 --> 00:10:23,350
that again the kinetic studies based on

202
00:10:32,490 --> 00:10:27,560
this reaction studying the deuterated

203
00:10:35,920 --> 00:10:32,500
formamide also gave matching observe

204
00:10:39,870 --> 00:10:35,930
also match the observed abundances so

205
00:10:44,680 --> 00:10:39,880
this means that our path seems to be

206
00:10:47,020 --> 00:10:44,690
reliable now let's move on to sino

207
00:10:52,690 --> 00:10:47,030
methylamine so it exists under the form

208
00:10:55,240 --> 00:10:52,700
of three isomers the e Z and n here in

209
00:10:58,480 --> 00:10:55,250
prebiotic chemistry it's important

210
00:11:01,420 --> 00:10:58,490
because it's an i n h ZN dimer while

211
00:11:05,950 --> 00:11:01,430
adenine which is one of bases of eight

212
00:11:07,480 --> 00:11:05,960
of the GNA is the pentamer so maybe this

213
00:11:12,070 --> 00:11:07,490

compound can be an

214
00:11:14,800 --> 00:11:12,080
remediate in its formation surprisingly

215
00:11:16,570 --> 00:11:14,810
only the e isomer has been detected in

216
00:11:19,060 --> 00:11:16,580
interstellar medium thanks to microwave

217
00:11:24,010 --> 00:11:19,070
spike spectroscopy so the question is

218
00:11:27,130 --> 00:11:24,020
how is informed in is M and are also the

219
00:11:32,670 --> 00:11:27,140
other isomers formed and if they are why

220
00:11:35,769 --> 00:11:32,680
can't we detect them so the reactivity I

221
00:11:38,079 --> 00:11:35,779
started from those two precursors the

222
00:11:42,519 --> 00:11:38,089
radical CN and methylamine here

223
00:11:44,920 --> 00:11:42,529
if the CN adds to the carbon atom here

224
00:11:48,579 --> 00:11:44,930
it goes to the C isomers that are in NZ

225
00:11:54,100 --> 00:11:48,589
and if it adds on the nitrogen atom here

226
00:11:56,410 --> 00:11:54,110
it goes through the N is over here is

227
00:12:00,220 --> 00:11:56,420
the full reaction path starting so from

228
00:12:02,769 --> 00:12:00,230
the precursors that are here so again I

229
00:12:06,340 --> 00:12:02,779
don't just describe it so much but still

230
00:12:08,440 --> 00:12:06,350
still no barrier here and everything is

231
00:12:10,360 --> 00:12:08,450
below the energy of the reactants so

232
00:12:13,720 --> 00:12:10,370
again this can occur in interstellar

233
00:12:15,040 --> 00:12:13,730
medium now the question is how much of n

234
00:12:19,750 --> 00:12:15,050
is formed

235
00:12:25,090 --> 00:12:19,760
regarding the C and the Z so kinetics

236
00:12:28,060 --> 00:12:25,100
study and we got that so in red here we

237
00:12:31,360 --> 00:12:28,070
have the formation of Z in a black of e

238
00:12:34,180 --> 00:12:31,370

in green of N and in blue of the back

239
00:12:39,760 --> 00:12:34,190
dissociation into the reactants we can

240
00:12:41,740 --> 00:12:39,770
see that here at every temperature the Z

241
00:12:45,490 --> 00:12:41,750
isomer should be formed more than the

242
00:12:48,100 --> 00:12:45,500
and the N here should be formed only as

243
00:12:50,350 --> 00:12:48,110
traces this can be explained by the fact

244
00:12:54,579 --> 00:12:50,360
that the transition states that lead to

245
00:13:00,250 --> 00:12:54,589
Z are always a bit lower in energy than

246
00:13:02,440 --> 00:13:00,260
the one leading to so now thanks to that

247
00:13:05,740 --> 00:13:02,450
we said that all the three isomers

248
00:13:09,639 --> 00:13:05,750
should be formed more on Z more than E

249
00:13:14,440 --> 00:13:09,649
and everything more than n a lot more

250
00:13:16,930 --> 00:13:14,450
than n so why only the e isomers has

251
00:13:18,940 --> 00:13:16,940
been detected the first thing I tried

252
00:13:21,970 --> 00:13:18,950
was to investigate decay

253
00:13:24,220 --> 00:13:21,980
path that only Z and n could undergo but

254
00:13:26,350 --> 00:13:24,230
they were all find energy energetically

255
00:13:29,980 --> 00:13:26,360
too high so they cannot occur in

256
00:13:33,280 --> 00:13:29,990
interstellar medium the second thing I

257
00:13:34,960 --> 00:13:33,290
thought of was to question the means of

258
00:13:38,530 --> 00:13:34,970
detection because the microwave

259
00:13:40,360 --> 00:13:38,540
spectroscopy is highly depends on the

260
00:13:43,600 --> 00:13:40,370
mode of the dipole moment value of the

261
00:13:45,940 --> 00:13:43,610
investigated compound so to check that I

262
00:13:48,730 --> 00:13:45,950
looked at the dipole moment values of

263
00:13:54,040 --> 00:13:48,740

all the three isomers and we can see

264
00:13:56,650 --> 00:13:54,050
here that e has a larger dipole moment

265
00:14:00,730 --> 00:13:56,660
than the Z which could explain why she

266
00:14:02,980 --> 00:14:00,740
was not detected there and has a large

267
00:14:07,060 --> 00:14:02,990
enough dipole moment value but we saw

268
00:14:09,910 --> 00:14:07,070
that it was it should be formed only as

269
00:14:14,710 --> 00:14:09,920
traces and some transitions that were

270
00:14:17,460 --> 00:14:14,720
that were found could match with n but

271
00:14:23,350 --> 00:14:17,470
it wasn't enough to make a definitive

272
00:14:26,560 --> 00:14:23,360
detection so to conclude gas phase

273
00:14:30,250 --> 00:14:26,570
chemistry can also explain some comes

274
00:14:33,610 --> 00:14:30,260
formations but there are still a lot of

275
00:14:34,380 --> 00:14:33,620
compounds to try in the case of

276
00:14:39,030 --> 00:14:34,390
formamide

277
00:14:43,540 --> 00:14:39,040
to formation paths were proposed and

278
00:14:47,130 --> 00:14:43,550
while the the second I shown was effect

279
00:14:49,960 --> 00:14:47,140
was shown to be effective the first one

280
00:14:52,240 --> 00:14:49,970
didn't lead to form a body it led more

281
00:14:55,720 --> 00:14:52,250
to other compounds of prebiotic

282
00:14:59,470 --> 00:14:55,730
interests and in the case of sino

283
00:15:02,980 --> 00:14:59,480
methylamine isomers we showed a path

284
00:15:06,190 --> 00:15:02,990
that seemed to work we also considered

285
00:15:11,080 --> 00:15:06,200
the ISO cyano methylamine which is

286
00:15:12,940 --> 00:15:11,090
exactly the same but the CN moiety here

287
00:15:15,460 --> 00:15:12,950
is linked through the nitrogen atom

288
00:15:17,470 --> 00:15:15,470

instead of the carbon atom but in that

289
00:15:20,890 --> 00:15:17,480
case it was too energetic so we gave up

290
00:15:23,440 --> 00:15:20,900
on that and the conclusion of that is

291
00:15:26,500 --> 00:15:23,450
that Z should before more than E and a

292
00:15:30,280 --> 00:15:26,510
lot more than n but maybe the detection

293
00:15:32,440 --> 00:15:30,290
tool was not efficient not efficient as

294
00:15:35,650 --> 00:15:32,450
efficient enough to detect them

295
00:15:50,620 --> 00:15:35,660
I would like to thank all of those

296
00:15:55,050 --> 00:15:50,630
people and you for your attention very

297
00:16:00,790 --> 00:15:57,550
first how did you calculate the dipole

298
00:16:03,790 --> 00:16:00,800
moment dipole moment yeah yeah with the

299
00:16:07,180 --> 00:16:03,800
the frequency calculations it is the

300
00:16:09,189 --> 00:16:07,190
Indians put of the it's in out in the

301
00:16:12,790 --> 00:16:09,199
output of the frequency calculation the

302
00:16:14,829 --> 00:16:12,800
informations are inside variations and

303
00:16:20,050 --> 00:16:14,839
could you please go back to slide number

304
00:16:30,240 --> 00:16:20,060
three number three number two loss so

305
00:16:38,290 --> 00:16:34,180
and before you go back to that how did

306
00:16:41,980 --> 00:16:38,300
you match abundances but you say when

307
00:16:43,930 --> 00:16:41,990
you calculate our or our km rate

308
00:16:46,389 --> 00:16:43,940
constant then you match it with

309
00:16:49,199 --> 00:16:46,399
abundances of them yes actually the the

310
00:16:52,470 --> 00:16:49,209
rate constants that are obtained are

311
00:16:55,240 --> 00:16:52,480
implemented in a stroke Emma Cole model

312
00:16:57,280 --> 00:16:55,250
that calculates the abundances that we

313
00:17:01,120 --> 00:16:57,290

should have depending on the temperature

314
00:17:03,490 --> 00:17:01,130
and the environment that's what why we

315
00:17:05,079 --> 00:17:03,500
could say that they match the observed

316
00:17:09,370 --> 00:17:05,089
want but I didn't do that

317
00:17:11,799 --> 00:17:09,380
oh you didn't okay all right and the

318
00:17:17,049 --> 00:17:11,809
last question sorry I'm being selfish

319
00:17:20,350 --> 00:17:17,059
and the second option for decade you say

320
00:17:22,210 --> 00:17:20,360
involves physical processes that can be

321
00:17:25,090 --> 00:17:22,220
problematic what's the problem again I

322
00:17:26,829 --> 00:17:25,100
didn't understand that part because for

323
00:17:28,900 --> 00:17:26,839
example methanol we talked about that

324
00:17:33,460 --> 00:17:28,910
earlier with a note remember who

325
00:17:37,150 --> 00:17:33,470
methanol was we can find the reaction

326
00:17:40,060 --> 00:17:37,160
process it's found but it's also

327
00:17:45,039 --> 00:17:40,070
detected in very cold and dark places

328
00:17:47,980 --> 00:17:45,049
and we don't know yet how it can go from

329
00:17:50,500 --> 00:17:47,990
the dust grain to the gas phase because

330
00:17:53,049 --> 00:17:50,510
it's it's very cold and very dark so

331
00:17:55,270 --> 00:17:53,059
there is no UV there is no energy and

332
00:18:06,780 --> 00:17:55,280
it's not known yet so it can be a

333
00:18:13,630 --> 00:18:10,600
um thank you for your talk I'm quite

334
00:18:16,420 --> 00:18:13,640
curious about your methods yeah okay so

335
00:18:21,520 --> 00:18:16,430
for formamide

336
00:18:25,570 --> 00:18:21,530
all the optimizations were done with b2

337
00:18:27,850 --> 00:18:25,580
Pullip g3 and ml/cc pivot is did you

338
00:18:30,130 --> 00:18:27,860

know them or do you want me to so it's a

339
00:18:33,510 --> 00:18:30,140
double hits a double hybrid functional

340
00:18:37,270 --> 00:18:33,520
with dispersion effects in addition to a

341
00:18:40,810 --> 00:18:37,280
triple databases stats and all the

342
00:18:43,600 --> 00:18:40,820
energies are revaluated using CCS DT and

343
00:18:46,090 --> 00:18:43,610
a complete basis set extrapolation in

344
00:18:49,240 --> 00:18:46,100
that case so it's very precise in the

345
00:18:54,520 --> 00:18:49,250
case of cyano autonomy is just CBS QB 3

346
00:18:56,640 --> 00:18:54,530
it's a hybrid methods using a complete

347
00:19:02,140 --> 00:18:56,650
basis set extrapolation but based on

348
00:19:05,590 --> 00:19:02,150
not-so-good geometries but in this case

349
00:19:08,770 --> 00:19:05,600
we have a lot of borderline compounds

350
00:19:10,780 --> 00:19:08,780
that are in the limits of the reactants

351
00:19:13,120 --> 00:19:10,790
energy so we needed something very

352
00:19:15,610 --> 00:19:13,130
precise in the case of cyano methylamine

353
00:19:29,610 --> 00:19:15,620
everything was below so we just thought

354
00:19:36,640 --> 00:19:33,730
hello nice dog and on a curiosity do you

355
00:19:39,400 --> 00:19:36,650
know in what kind of environment they

356
00:19:42,490 --> 00:19:39,410
calculated abundances from your motto

357
00:19:43,740 --> 00:19:42,500
agree with the observed nope yeah it's

358
00:19:46,930 --> 00:19:43,750
in the paper

359
00:19:47,920 --> 00:19:46,940
their papers about that it's inside but

360
00:19:55,000 --> 00:19:47,930
I don't remember

361
00:19:58,570 --> 00:19:55,010
frankly it's alright anybody else with a

362
00:19:59,490 --> 00:19:58,580
quick question okay then let's thank our