THE BENDING VIBRATIONS OF THE C$_3$-ISOTOPOLOGUES IN THE 1.9 TERAHERTZ REGION

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15 min, Tuesday, 2016-06-21
01:47 PM - 02:02 PM
Medical Sciences Building 274
Abstract:
Short carbon chains are fundamental for the chemistry of stellar and interstellar ambiences. The linear carbon chain molecule C$_3$ has been found in various interstellar and circumstellar environments, encompassing diffuse interstellar clouds, star forming regions, shells of late type stars, as well as cometary tails. Due to the lack of a permanent dipole moment C$_3$ can only be detected by electronic transitions in the visible spectral range or by vibrational bands in the mid and far-infrared region. We performed experiments where C$_3$ was produced via laser-ablation of a graphite rod with a 3 bar He purge and a subsequent adiabatic expansion into a vacuum resulting in a supersonic jet. We report laboratory measurements of the lowest bending mode transitions of six $^{13}$C-isotopologues of the linear C$_3$ molecule. Fifty-eight transitions have been measured between 1.8-1.9 THz with an accuracy of better than 1 MHz. Molecular parameters have been derived to give accurate line frequency positions of all $^{13}$C isotopologues to ease their future interstellar detection. A dedicated observation for singly substituted $^{13}$CCC is projected within the SOFIA airborne observatory mission.
Previous work: $C_3$ @ optical & IR

Optical transitions @ 405nm
- Huggins 1882
- Herzberg 1942
- Douglas 1951
- Gausset 1965

$\nu_1$ symmetric stretching
- @ 1226 cm$^{-1}$ (not IR-active)
  - Rohlfing 1989

$\nu_3$ anti-symmetric stretching
- @ 2040 cm$^{-1}$ (IR-active)
  - Matsumura 1988
  - Moazzen-Ahmadi 1993
  - Krieg 2013

$\nu_2$ bending
- @ 63 cm$^{-1}$ = 1.9 THz (IR-active)
  - Hinkle 1988
  - Schmuttenmaer 1990
  - Gendriesch 2003

vanOrden 1995
- Cernicharo 2000
- Giesen 2001
- Maier 2001
- Haddad 2014
Excitation and Abundance of $C_3$ in star forming cores around 1.8 THz

Herschel/HIFI observations towards W31C and W49N

Two previously unsolved aspects:

- Mookerjea et al. noticed frequency shift of \( ^{12}\text{C}^{12}\text{C}^{12}\text{C} \) astrophysical lines relative to laboratory data; e.g. P(6) has already 6 MHz offset (i.e. > linewidth)

Possible reasons:
- Dynamics in source (Doppler shift), e.g. outflows
- Imprecise laboratory data

- Galactic \([^{12}\text{C}]/[^{13}\text{C}] = 20 - 30\)

\( ^{13}\text{C} \)\(^{13}\text{C} \)\(^{12}\text{C} \)\(^{13}\text{C} \)\(^{12}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)\(^{12}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)\(^{12}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)\(^{13}\text{C} \)

\( \Rightarrow \) Need of laboratory data
Experimental setup in Kassel

See talk on Thursday RH01 at Medical Sciences Building 274 01:30 PM
P1899: THE KASSEL LABORATORY ASTROPHYSICS THZ SPECTROMETERS (talk has been moved from Friday to Thursday !!!)

THz spectrometer & laser ablation supersonic jet
Measurements of the main isotopologue $^{12}\text{C}^{12}\text{C}^{12}\text{C}$
low bending vibration $\nu_2$

• Already data available [1] $\Rightarrow$ $B''$ and $B'$ from combination differences

• Until now: Critical entries in molecular database (CDMS) not precise enough to analyse astrophysical observations [2].

$\Rightarrow$ New measurements necessary

[2] B. Mookerjea (private comm.)
The problem...

\[ \Delta \nu_{B-K} \approx 2 \text{ MHz} \]

\[ \Delta B_{B-K} \approx 0.5 \text{ MHz} \]
Comparison of reduced exp. and calc. molecular parameterset (in MHz) of $^{12}$C$^{12}$C$^{12}$C

<table>
<thead>
<tr>
<th>isotopologue</th>
<th>parameter</th>
<th>This work</th>
<th>Previous exp. work [1]</th>
<th>Theor. Calc. [2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$C$^{12}$C$^{12}$C</td>
<td>$B_{0000}$</td>
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<tr>
<td></td>
<td>$\nu_{0010}$</td>
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<td>$B_{0010}$</td>
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<td>$q_{0010}$</td>
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</tbody>
</table>


$\Rightarrow \Delta B''_{B-K} \approx 0.55 \text{ MHz}$

For higher J transitions deviation between predicted line positions from previous and new experimental data significant (> line width for J=6, e.g. P(6))
Bending mode transitions of $^{13}\text{C}$-isotopologues of CCC
Bending mode transitions of $^{13}$C-isotopologues of CCC
Sample: $^{13}C/^{12}C = 2/1$

Sample: $^{13}C/^{12}C = 1/2$

with 1:3 spin statistic
Spin statistics and line intensities of $^{12}C\,^{12}C$ isotopologues

Bose-Einstein statistic of two identical carbon nuclei ($I_{12} = 0$)

Fermionic behaviour of outer C atoms ⇒ 3:1 statistical weights ($I_{13} = \frac{1}{2}$)
Similarity let to misassignment ⇒ failed astrophysical observation

Rot. Parameter $B' = 0.414$ cm$^{-1}$
Spin stat. Weights: $g_e/g_o = 1:1$

Rot. Parameter $B'' = 0.431$ cm$^{-1}$
Spin stat. Weights: $g_e/g_o = 1:0$

Rot. Parameter $B'' = 0.393$ cm$^{-1}$
Spin stat. Weights: $g_e/g_o = 1:3$
Fortrat diagram

$^{13}$C in center  scaled bandcenter-isotop-shift $\Delta v_{121212}^{0110}$  $^{12}$C in center

Rotational quantenumber J

Frequency $\nu$ (GHz)

$^{13}$C$^{13}$C$^{13}$C
$^{13}$C$^{13}$C$^{12}$C
$^{13}$C$^{13}$C$^{12}$C
$^{13}$C$^{12}$C$^{13}$C
$^{13}$C$^{12}$C$^{12}$C
$^{12}$C$^{12}$C$^{13}$C
$^{12}$C$^{12}$C$^{12}$C
Results

To be published soon...

Line predictions for astrophysical observations
SOFIA far –IR observatory
Summary

- Measurement on C₃ isotopologues and $^{12}$C$^{12}$C$^{12}$C were performed

- Molecular parameters of $^{12}$C$^{12}$C$^{12}$C could be improved
  ⇒ better match with astrophysical observations

- Molecular parameters of $^{13}$C isotopologues of C₃ could be determined
  ⇒ explanation of failed astrophysical search
  ⇒ new searches under way
Thank you for your attention!

Acknowledgment

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DFG GI 319/3-1, DFG GI 319/3-2, DFG SFB 956, Uni Kassel
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