FT spectroscopy of the comet-tail ($A^2\Pi_i - X^2\Sigma^+$) system bands in $^{12}C^{17}O^+$

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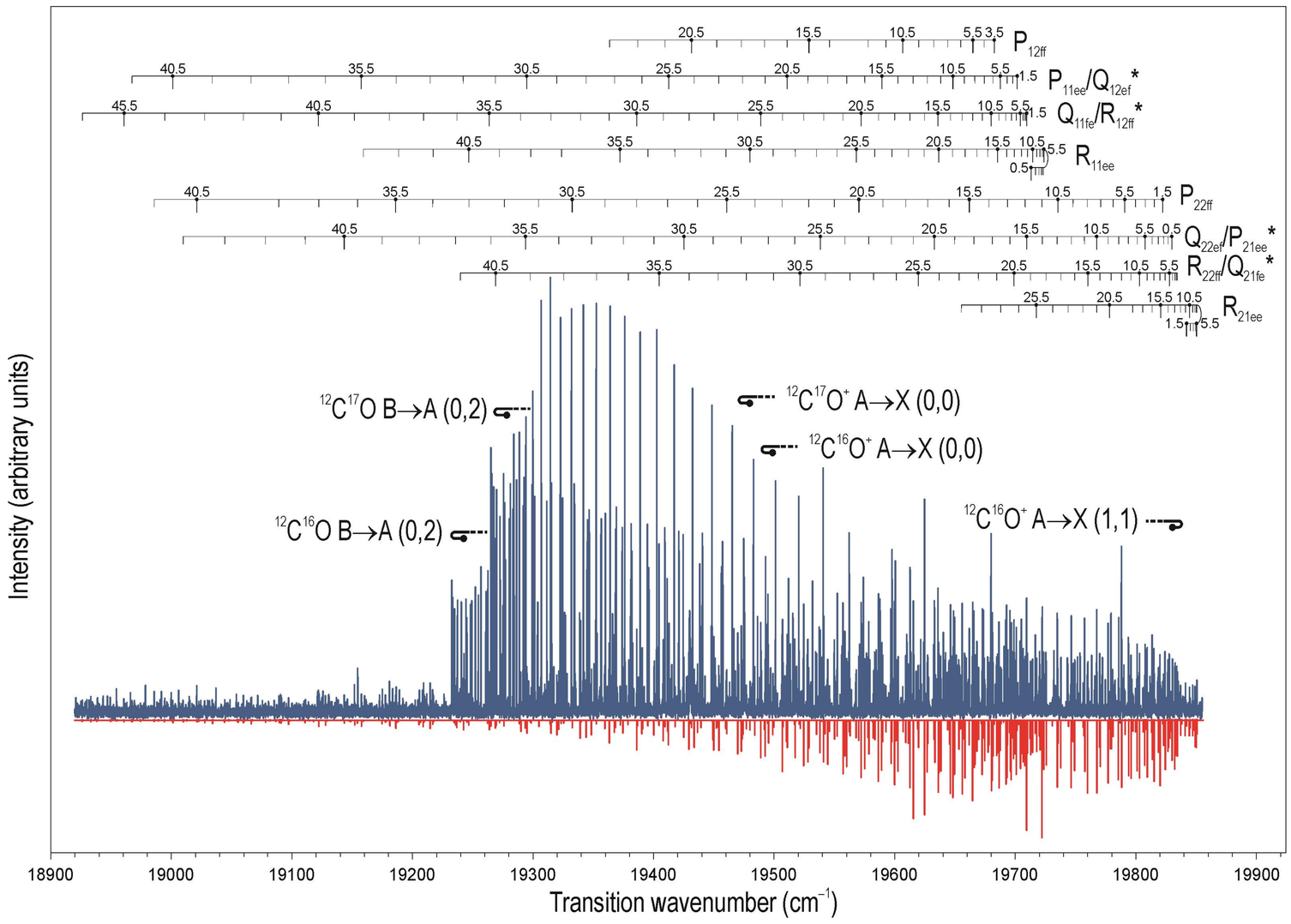
Summary

In the emission spectrum of $^{12}C^{17}O^+$ molecule new observations and analyses were performed. Two bands ((1,0) and (1,1)) of the comet-tail ($A^2\Pi_i - X^2\Sigma^+$) system in the 19850 to 15250 cm^{-1} region were recorded with the Fourier transform spectrometer (BRUKER IFS 125-HR).

The absolute accuracy of wavenumbers was about 0.005 cm^{-1}. The measurement cycle included 128 scans within 1.5 h. As a source of the studied spectrum an air-cooled, carbon hollow-cathode lamp operated at 780 V, 54 mA dc was used. The lamp was filled with a static mixture of $^{17}O_2$ (70%) and $^{16}O_2$ (30%) at a pressure of about 1 Torr. During the discharge process, the O_2 molecules react with the ^{12}C atoms ejected from the carbon filler placed inside the cathode, thus forming $^{12}C^{17}O$ and $^{12}C^{17}O^+$ molecules in the gas phase, in amounts sufficient to finally achieve a signal-to-noise ratio (SNR) of 100:1.

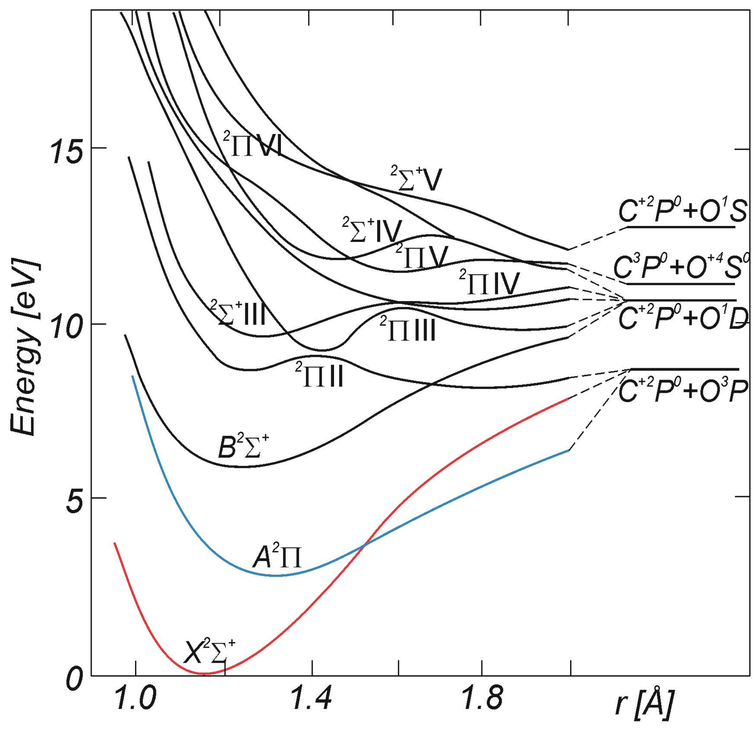
Spectra were analyzed using the OPUS™ software [1] , which finds peaks and calculates various spectral parameters (wavenumbers, FWHM, etc). As a result of a detailed spectral analysis the individual molecular constants of both $A^2\Pi_i$ and $X^2\Sigma^+$ states were obtained. For the upper $A^2\Pi_i$ state all these constants were delivered for the first time. The parameters for the lower $X^2\Sigma^+$ state were also calculated and can be compared with these determined previously [2].

$A^2\Pi_i - X^2\Sigma^+$ (1,1) band of $^{12}C^{17}O^+$

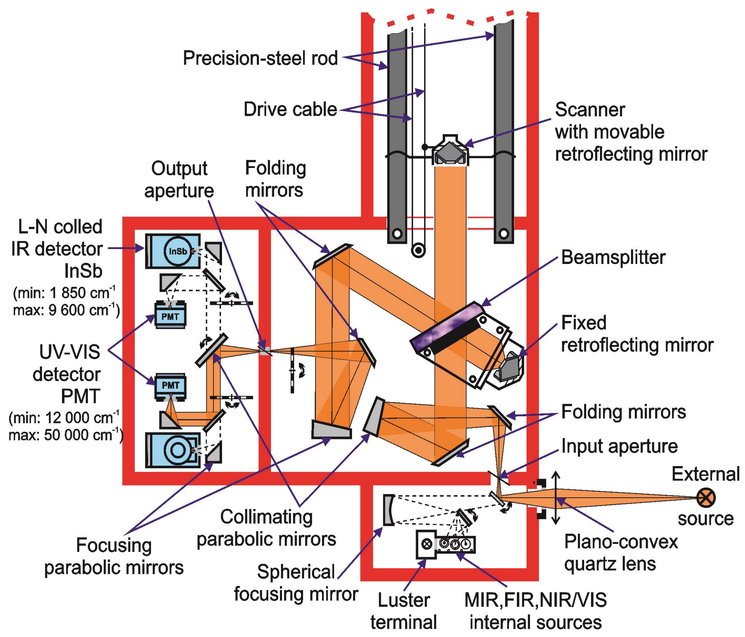


High-resolution emission spectrum (upper trace) of the (1,1) band of the comet – tail ($A^2\Pi_i$ - $X^2\Sigma^+$) system in the rare $^{12}C^{17}O^+$ isotopologue together with the simulated spectrum [4] (lower trace) of this band. During analyses the influence of the other bands was taken into consideration: $^{12}C^{16}O$ and $^{12}C^{17}O$ B-A system (0,2) bands [5,6] as well as $^{12}C^{16}O^+$ and $^{12}C^{17}O^+$ A-X system (0,0) bands and $^{12}C^{16}O^+$ A-X system (1,1) band, simulated on the basis of constants from [7]. In case of P_{11}/Q_{12}, Q_{11}/R_{12}, Q_{22}/P_{21} and R_{22}/Q_{21} main/satellite branches (denoted by an asterisk) the values of the rotational quantum number J are provided only for the main branches.

PECs of CO^+ [3]



1,71 m spectrometer (Bruker IFS 125HR)



- Spectral range: 1 850 - 50 000 cm^{-1} (5 400 - 200 nm)
- Maximum Optical Path Difference: $(OPD)_{max}$ = 258 cm
- Maximum spectral resolution: $(\Delta\upsilon)_{max}$ = 0.0035 cm^{-1}
- Resolving power: > 10^6
- Vacuum conditions: p ≈ 0.002 hPa
- Aperture: 0.5 - 12.5 mm
- Instrumental function: sinc
- Detector: PMT in integration pulse mode
  - Interferometer: modified Michelson's system
    - ✓ permanently aligned
    - ✓ *v* of mirror: 0.16 - 2.5 cm/s
    - ✓ control the scanner position: 1.2 mW He-Ne laser

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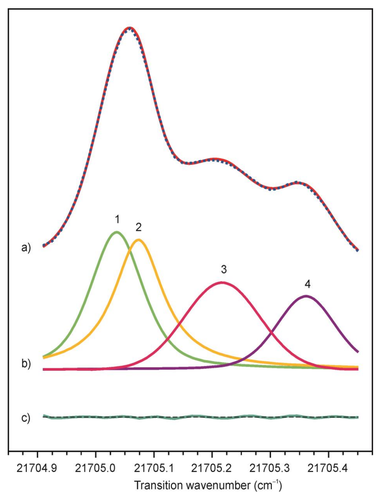
Decomposition of the overlapped lines

The part of the observed spectrum of $^{12}C^{17}O^+$ A-X (1,0) band.

Traces (a) show the experimental (red solid) and the fitted (blue dashed) lines, traces (b) present the four decomposed lines and trace (c) displays the residuals between the experimental and fitted contour.

Line identifications:

- 1 – Q_{11}(21.5) and 3 – R_{12}(20.5) of the $^{12}C^{17}O^+$ A-X (1,0) band
- 2 – P_{11}(18.5) and 4 – Q_{12}(17.5) of the $^{12}C^{16}O^+$ A-X (1,0) band



Observations and analysis of the comet - tail system in $^{12}C^{17}O^+$ [a]

Band	Number of lines	Band origin (cm^{-1})	J_{max}	$\sigma\times10^3$ [b] (cm^{-1})
(1,0)	419	21926.0028 (11)	44.5	2.73
(1,1)	441	19769.5307 (13)	46.5	

[a] Uncertainties in parentheses are one standard deviation in units of the last quoted digit.

[b] The root mean square error (rmse) value of the weighted residuals of the wavenumbers used in the global fit [4].

Rotational structure constants (in cm^{-1}) of the $A^2\Pi_i$ state in the $^{12}C^{17}O^+$ molecule [a]

Constant	$A^2\Pi_i$ (v=1)
B_v	1.5209591 (25)
$D_v \times 10^6$	6.2499 (17)
$-A_v$	121.97710 (64)
$p_v \times 10^2$	1.2567 (46)
$-q_v \times 10^4$	2.089 (17)

[a] Uncertainties in parentheses are one standard deviation in units of the last quoted digit.

Rotational structure constants (in cm^{-1}) of the $X^2\Sigma$ state in the $^{12}C^{17}O^+$ molecule [a]

Constant	$X^2\Sigma^+$ (v=0)
B_v	1.9177060 (45)
$D_v \times 10^6$	5.9588 (33)
$\Upsilon_v \times 10^3$	8.842 (44)

[a] Uncertainties in parentheses are one standard deviation in units of the last quoted digit.

References

[1] Computer program by Bruker Optik GmbH; 2014. v.7.5.18.

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