Excitation and Abundance of C$_3$ in star forming cores: Herschel/HIFI * observations of the sight-lines to W31C and W49N

B. Mookerjea4,5, T. Giesen2, J. Stutzki2, J. Cernicharo3, J. R. Goicoechea2, M. De Luca4, T. A. Bell5, H. Gupta6, M. Gerin2, C. M. Persson7, P. Sonnentrucker9, Z. Maka2, J. Black7, F. Boulanger10, A. Coutens13, E. Dartois10, P. Encena4, E. Falgarone4, T. Geballe11, B. Godar6, P. F. Goldsmith5, C. G. Groenenboom12, P. Hennebelle8, E. Herbst8, P. Hily-Blant12, C. Joblin13, M. Kaźmierczak17, R. Kolos16, J. Krebs17, D. C. Lis5, J. Martin-Pintado3, K. M. Menten15, R. Monje5, J. C. Pearson6, M. Peralta4, T. G. Phillips4, R. Plume18, M. Sale4, S. Schlemmer9, M. Schmidt19, D. Teysier20, C. Vastel13, S. Yu4, P. Dieleman23, R. Güsten15, C. E. Honingh2, P. Morris21, P. Roelfsema3, R. Schieder2, A. G. G. M. Tielens22, and J. Zmuidzinas5

(Affiliations can be found after the references)

Received ... accepted ...

ABSTRACT

We present spectrally resolved observations of triatomic carbon (C$_3$) in several ro-vibrational transitions between the vibrational ground state and the low-energy v$_3$ bending mode at frequencies between 1654–1897 GHz along the sight-lines to the submillimeter continuum sources W31C and W49N, using Herschel’s HIFI instrument. We detect C$_3$ in absorption arising from the warm envelope surrounding the hot core, as indicated by the velocity peak position and shape of the line profile. The sensitivity does not allow to detect C$_3$ absorption due to diffuse foreground clouds. From the column densities of the rotational levels in the vibrational ground state probed by the absorption we derive a rotation temperature (T$_{\text{rot}}$) of ∼50–70 K, which is a good measure of the kinetic temperature of the absorbing gas, as radiative transitions within the vibrational ground state are forbidden. It is also in good agreement with the dust temperatures for W31C and W49N. Applying the partition function correction based on the derived T$_{\text{rot}}$, we get column densities N(C$_3$) ∼ 7 × 10$^{12}$ cm$^{-2}$ and abundance x(C$_3$)/H$_2$ ∼ 10$^{-8}$ with respect to H$_2$. For W31C, using a radiative transfer model including far-infrared pumping by the dust continuum and a temperature gradient within the source along the line of sight we find a model with x(C$_3$)/H$_2$ = 10$^{-7}$, T$_{\text{kin}}$ = 30–50 K, N(C$_3$) = 1.5 × 10$^{13}$ cm$^{-2}$ fits the observations reasonably well and provides parameters in very good agreement with the simple excitation analysis.

Key words. ISM: molecules – Submillimeter: ISM – ISM: lines and bands – ISM: individual (W49N, W31C) – line: identification – molecular data – Radiative transfer

1. Introduction

Small carbon chains are relevant in the chemistry of stellar and interstellar environments for several reasons: ubiquitous interstellar spatial distribution, they likely participate in the formation of long carbon chain molecules, and they are produced in photo-fragmentation processes of larger species such as PAHs. Triatomic carbon, C$_3$, was first tentatively identified in interstellar gas by [Van Orden et al. 1995] and [Haffner & Meyer 1995]. The mid-infrared spectrum of C$_3$ (ν$_3$ antisymmetric stretching mode) was measured in the circumstellar envelope of CW Leo (IRC +10216) by [Hinkle et al. 1988], and in low-resolution interstellar absorption in the far-IR (ν$_2$ bending mode) toward Sgr B2 by [Cernicharo et al. 2000]. [Giesen et al. 2001] discussed new laboratory data on the vibrational spectrum of C$_3$ in its low-frequency bending mode and re-visited the first identification of the ν$_2$ R(2) line in absorption toward Sgr B2 [Van Orden et al. 1995]. The abundance and excitation of C$_3$ in translucent clouds were determined convincingly by [Maier et al. 2001], [Roueff et al. 2002] and [Oka et al. 2003] at optical wavelengths.

* Herschel is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.
Due to the ro-vibrational bending mode state of $C_3$ and 0.5 MHz respectively, which corresponds to line frequency \cite{Gendriesch2003} with frequency accuracies of 7 MHz.

2. $C_3$ energy level diagram and radiative transitions

Linear $C_3$ has an energetically unusually low $v_2$ bending mode at only ~90 K. Ro-vibrational transitions of the $v_2$ band in its $\Sigma^+_u$ electronic ground state have been reported by \cite{Gendriesch2003} and \cite{Schmuttenmaer1990}. P($J$) transitions with $J = 2, 4, 6$, R($J$) with $J = 0, 2, 4, 6$, and Q($J$) with $J = 2, 4, \ldots, 16$ have been measured in the laboratory, using high resolution Terahertz sideband spectrometers at Berkeley \cite{Schmuttenmaer1993} and Cologne \cite{Gendriesch2003} with frequency accuracies of 7 MHz and 0.5 MHz respectively, which corresponds to line frequency uncertainties of 1.1 km s$^{-1}$ and 0.08 km s$^{-1}$. All data were used in a global fit analysis to obtain most accurate molecular constants \cite{Giesen2001} which are presented as line lists for astronomical observations in the Cologne Data Base for Molecular Spectroscopy (CDMS) \cite{Muller2005}. The ground state of $C_3$ has $\Sigma^+_u$ symmetry while the vibrational excited $v_2$ is a two-fold degenerate bending state of $\Pi_u$ symmetry. Due to the $^{12}$C nuclear spin of $I = 0$ in the ground state only levels of (+) parity are present, while for the excited bending state only levels with (-) parity are allowed. As a consequence, in the ground state of $C_3$ all odd numbered $J$ rotational levels are missing, whereas in the vibrational excited state both, even and odd $J$ rotational levels are present, but the two-fold degeneracy of the vibrational state is lifted (see Fig. 1). Consequently, the statistical weights of the ro-vibrational levels is simply given by the rotational degeneracy: $g_{J'\nu'} = 2J + 1$. The $v_2$ bending mode has a perpendicular type spectrum with a calculated vibrational dipole moment of 0.437 Debye \cite{Jensen1992} which shows prominent $Q$, $P$, and $R$-branch transitions.

3. Observations and data reduction

Along the sight-lines to W31C and W49N we have observed four lines of the $v_2$ bending mode, P(4), Q(2), Q(4) and P(10) (the latter only in W31C), of trinitromethane in the upper sideband of the HIFI bands 7a, 7b and the lower sideband of band 6b of the HIFI receiver. The observations of W31C and W49N were carried out on 2010 March 8 and 2010 April 19 respectively. The P(10) line was available as a “bonus” for an LO tuning dedicated to observe the CH line at 1661 GHz and it is yet to be observed in W49N with HIFI. All observations are in dual beam switch (DBS) mode and with the Wide Band Spectrometer with its spectral resolution of 1.1 MHz, corresponding to a velocity resolution of ~0.17 km s$^{-1}$ at the frequencies of the $C_3$ lines. To identify the line origin from the lower and upper sidebands, each line was observed with three LO settings shifted by 15 km s$^{-1}$ relative to each other. The Q(2) line also shows up in the Q(4) observations from the lower sideband, and, for one of the LO tunings, partially overlap with the former. The data were first processed with HIPE \cite{Ott2010}, and subsequently exported to CLASS. At the high frequencies for these observations the $H$ and $V$ polarizations were at times found to be discrepant in the measured continuum level. Observations optimized for reliable continuum measurement were used to select the spectra with the correct continuum level, used for the subsequent analysis. All spectra were smoothed to a resolution of ~0.68 km s$^{-1}$ and the rms noise level for the spectra lie between 0.01–0.03 K. Table 2 gives the measured double sideband continuum level ($T_{CMB}$). For the remainder of this paper we discuss the line intensities normalized to the single-sideband continuum level, where we have assumed a sideband gain ratio of unity.

4. Results

We have for the first time detected the spectrally resolved $v_2$ band transitions P(4), P(10), Q(2) and Q(4) lines of $C_3$. Fig. 2 shows the observed spectra normalized to the (single sideband) continuum level. A multi-component Gaussian with common velocity width and spacing and individual amplitudes for each line was fitted to derive the basic parameters of the absorption spectra. Table 2 presents the fit results and their uncertainties. The P(10) spectrum is affected by the spectral lines of CH.

![Fig. 1. Energy level diagram of $\Sigma^+_u$ ground state and $\Pi_u$ lowest bending mode state of $C_3$. Due to nuclear spin statistics half of the rotational energy levels (dashed lines) are missing. Allowed ro-vibrational $P$, $Q$, and $R$-branch transitions from $\nu = 0$ to $\nu' = 1$ follow $\rightarrow \leftarrow \rightarrow$ selection rules.](image)

| Name | Transition | Frequency $^a$ | A-coeff $^b$ | $E_\nu$ |
|------|------------|----------------|--------------|--------|
| P(10) | (9,1) $\rightarrow$ (10,0) | 1654081.66(4.68) $^a$ | 2.58 | 47.3 |
| P(4)  | (3,1) $\rightarrow$ (4,0)  | 1787890.57(6.90) | 2.72 | 8.6 |
| Q(2)  | (2,1) $\rightarrow$ (2,0)  | 1899588.06(25)  | 7.51 | 2.6 |
| Q(4)  | (4,1) $\rightarrow$ (4,0)  | 1896706.56(15)  | 7.58 | 8.6 |

$^a$ Experimental rest frequencies, uncertainties are given in parentheses. $^b$ Calculated frequency and 1σ uncertainty taken from CDMS catalog.
and Q

We first consider a simple two-layer model in which a (warm) line and column density of C_3 towards W49N and W31C are estimated from the fitted intensities. The fitted values of line center and linewidth are: for W31C \( V_{\text{cen}} = -0.09 \pm 0.06 \text{ km s}^{-1} \) and \( \Delta V = 4.5 \pm 0.1 \text{ km s}^{-1} \) and for W49N \( V_{\text{cen}} = 11.0 \pm 0.1 \text{ km s}^{-1} \), and \( \Delta V = 5.3 \pm 0.2 \text{ km s}^{-1} \).

| Transition | W31C | W49N |
|------------|------|------|
| \( P(10) \) | 11.4 \( \pm \) 0.4 | 1.0 \( \times \) 10^{14} |
| \( P(4) \) | 10.5 \( \pm \) 0.3 | 1.5 \( \times \) 10^{14} |
| \( Q(2) \) | 11.8 \( \pm \) 0.2 | 7.2 \( \times \) 10^{13} |
| \( Q(4) \) | 11.8 \( \pm \) 0.2 | 1.1 \( \times \) 10^{14} |

We consider a simple two-layer model in which a (warm) line and column density of C_3 towards W49N and W31C are estimated from the fitted intensities. The fitted values of line center and linewidth are: for W31C \( V_{\text{cen}} = -0.09 \pm 0.06 \text{ km s}^{-1} \) and \( \Delta V = 4.5 \pm 0.1 \text{ km s}^{-1} \) and for W49N \( V_{\text{cen}} = 11.0 \pm 0.1 \text{ km s}^{-1} \), and \( \Delta V = 5.3 \pm 0.2 \text{ km s}^{-1} \).

4.1. Two-layer excitation analysis

We first consider a simple two-layer model in which a (warm) line and column density of C_3 towards W49N and W31C are estimated from the fitted intensities. The fitted values of line center and linewidth are: for W31C \( V_{\text{cen}} = -0.09 \pm 0.06 \text{ km s}^{-1} \) and \( \Delta V = 4.5 \pm 0.1 \text{ km s}^{-1} \) and for W49N \( V_{\text{cen}} = 11.0 \pm 0.1 \text{ km s}^{-1} \), and \( \Delta V = 5.3 \pm 0.2 \text{ km s}^{-1} \).

The C_3 absorption features towards W31C and W49N are centered near 0 km s\(^{-1}\) and 11 km s\(^{-1}\) respectively. The systemic velocities of W31C and W49N are at \( V_{\text{LSR}} = -1 \text{ km s}^{-1} \) and 12 km s\(^{-1}\). Thus the C_3 absorption lines detected here appear to be physically associated with the hot core itself and most likely arise in the lower density warm envelope surrounding them. We do not detect any absorption feature arising from the foreground clouds towards either of these sources (see Sec. 5).

Fig. 2. The observed absorption spectra of the \( P(4) \), \( P(10) \), \( Q(2) \) and \( Q(4) \) ro-vibrational transitions of C_3 towards W49N (left panel) and W31C (right panel), plotted along with the best-fit profiles obtained by simultaneous Gaussian fitting to all lines.

Table 2. Parameters derived from simultaneous Gaussian fitting to all the line profiles and column densities estimated from the fitted intensities. The fitted values of line center and linewidth are: for W31C \( V_{\text{cen}} = -0.09 \pm 0.06 \text{ km s}^{-1} \) and \( \Delta V = 4.5 \pm 0.1 \text{ km s}^{-1} \) and for W49N \( V_{\text{cen}} = 11.0 \pm 0.1 \text{ km s}^{-1} \), and \( \Delta V = 5.3 \pm 0.2 \text{ km s}^{-1} \).

| Transition | \( T_{\text{c}} \) [K] | \( \tau d_V \) [km/s] | \( N_{\text{rot}} \) [cm\(^{-2}\)] | \( T_{\text{c}} \) [K] | \( \tau d_V \) [km/s] | \( N_{\text{rot}} \) [cm\(^{-2}\)] |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( P(10) \) | 11.4 \( \pm \) 0.4 | 0.51 | 1.0 \( \times \) 10^{14} | ... | ... | ... |
| \( P(4) \) | 10.5 \( \pm \) 0.3 | 0.61 | 1.5 \( \times \) 10^{14} | 16.8 \( \pm \) 0.2 | 0.62 | 1.6 \( \times \) 10^{14} |
| \( Q(2) \) | 11.8 \( \pm \) 0.2 | 0.87 | 7.2 \( \times \) 10^{13} | 18.3 \( \pm \) 0.3 | 0.87 | 7.3 \( \times \) 10^{13} |
| \( Q(4) \) | 11.8 \( \pm \) 0.2 | 1.22 | 1.1 \( \times \) 10^{14} | 18.3 \( \pm \) 0.2 | 0.90 | 7.6 \( \times \) 10^{13} |

Fig. 3. Model predictions for the \( Q(2) \), \( Q(4) \), \( P(2) \) and \( P(10) \) lines of the \( v_2=1-0 \) transition of C_3 in W31C. The black lines correspond to a model with \( n(H_2)=10^9 \text{ cm}^{-3} \), \( x(C_3)=5 \times 10^{-8} \) and \( T_{\text{kin}}=50 \text{ K} \). The red lines correspond to a model with \( n(H_2)=5 \times 10^9 \text{ cm}^{-3} \), \( x(C_3)=10^{-8} \) and \( T_{\text{kin}}=50 \text{ K} \). Finally, the blue lines correspond to the same parameters as the red ones except that \( T_{\text{kin}}=30 \text{ K} \).

4.2. Radiative transfer models for C_3 excitation in W31C

In the likely scenario that the dust continuum source and its associated continuum opacity are coexistent with the gas that absorbs in the C_3 lines, the C_3 molecule will be embedded in a relatively strong continuum radiation which would contribute to the ro-vibrational excitation. In addition, the source intrinsic continuum will partially fill in the line absorption. Thus, in a more detailed approach we use a radiative transfer model, which considers FIR pumping by the dust continuum (Cernicharo et al. 2000) and a temperature gradient of the continuum source along the line of sight. For W31C we find that the C_3 column densities can be interpreted by a cloud which is twice the size of the con-
timum source, has a molecular hydrogen density $n(H_2) = 10^5$ cm$^{-3}$, $v_{\text{rot}} = 2$ km s$^{-1}$, abundance $x(C_3) = 5 	imes 10^{-8}$, kinetic temperature of 50 K and $N(C_3) = 1.5 	imes 10^{15}$ cm$^{-2}$ (see Fig. 3). The fact that the C$_3$ column density comes out larger in this more detailed model is expected, as the dust opacity partially fills-in the absorption line.

The main source of uncertainty in these models are the ro-vibrational collisional rates which are based on rather crude assumptions (Cernicharo et al. 2000). However, irrespective of the adopted collisional rates the ground state is always thermalized, even in the presence of a strong IR radiation field in our models. We find that owing to the lack of a permanent electrical dipole moment the uncertainties in the collisional rates have little effect on the emerging intensities. Fig. 3 also shows that the resulting absorption depths are almost unaffected by a change in the local density (and hence abundance) by as much as a factor of 5, as long as the column density remains constant. We find that the $v_2 = 1$ transitions are dominated by infrared pumping. The ro-vibrational excitation temperature in the inner part of the cloud is 35–37 K for the lowest rotational levels and around 20 K for the higher-J states. In the external layers $T_{\text{ex}}$ decreases by 20 and 10 K, respectively. In a second model with $n(H_2) = 5 	imes 10^3$ cm$^{-3}$ and $x(C_3)=10^{-6}$ the results are almost equally consistent with the observations. We also note, that depending on the geometrical arrangement, the FIR-pumping in the ro-vibrational transitions can result in the net effect of lowering the rotational temperature in the vibrational ground state slightly below the kinetic temperature of the gas.

We find that the major effect on the resulting absorption depths is related to the kinetic temperature adopted for the absorbing gas. In Fig. 3 the blue lines correspond to a gas with $T_{\text{kin}}=30$ K. The high-J lines of the ground state are less populated than in the previous case and the opacities for the $v_2 = 1$–0 transitions decrease. If the opacity of the ro-vibrational lines become larger than 1, and the central continuum source is optically thick at the wavelengths of the $v_2 = 1$–0 transitions, then the $T_{\text{kin}}$ level becomes thermalized to the temperature of the dust. This effect can be counterbalanced by decreasing the gas temperature in the external layers of the cloud. Clearly, a more elaborate analysis than can be presented in this letter, is needed to explore the full parameter range.

5. Discussion

In the absence of allowed radiative transitions in the ground state, the excitation of C$_3$ in the $v_2 = 0$ state can be assumed to be thermalized to the kinetic temperature: $T_{\text{rot}} = T_{\text{kin}}$. However, $T_{\text{rot}}$ can be larger than $T_{\text{dust}}$ in the presence of direct gas heating mechanism like the photoelectric heating. The $v_2$ mode on the other hand could be excited by collisional ground as well as by infrared photons. With Einstein coefficients ranging between 2 and $7 	imes 10^{-3}$ s$^{-1}$, the line opacities can be high and the infrared pumping rather efficient. As a result, the excitation temperatures of the ro-vibrational lines are much lower, typically between the beam-diluted $T_{\text{dust}}$ and $T_{\text{kin}}$ and hence the lines are seen in absorption. However, as explained above, the excitation temperature within the rotation ladder of the ground vibrational state can have values larger than $T_{\text{dust}}$.

Crude estimates based on the “two-layer” approach derive a $T_{\text{rot}}$ consistent with the dust temperature of the continuum source and give column densities of C$_3$ in W31C and W49N to be between $7–9 	imes 10^{14}$ cm$^{-2}$. Using the more elaborate radiative transfer model we derived a column density of $1.5 	imes 10^{15}$ cm$^{-2}$ for W31C for $T_{\text{kin}}$ of 30 K. Based on the discussion above we further argue that the thus derived column density of C$_3$ is likely to be a lower limit. Implicit assumptions like a source filling factor of unity, $T_{\text{ex}} < T_{\text{c}}$ etc. in the two-layer approach translate to an underestimate of $T_{\text{rot}}$. Moreover the source intrinsic continuum opacity at 1.9 THz partially re-fills the absorption (as shown in the radiative transfer model), and hence the column densities derived from the radiative transfer model are higher than those derived in the two-layer model. Thus taking all uncertainties into account we conclude that for both W31C and W49N the C$_3$ column densities are $\sim 10^{15}$ cm$^{-2}$, correct to within a factor of 2 or so. The H$_2$ column densities in W31C and W49N are $2.5 \times 10^{22}$ cm$^{-2}$ (Miettinen et al. 2006) and $\sim 10^{15}$ cm$^{-2}$ respectively, so that the abundances of C$_3$ are $\sim 10^3$. It is interesting to note that warm-up chemical models of the environment around hot cores similar to the models by Hassel et al. (2008), with $n=2 	imes 10^3$ cm$^{-3}$ and $A_V = 10$ yield an abundance of 4–6$\times 10^{-8}$.

Based on absorption studies of C$_3$ in optical wavelengths the C$_3$ column densities in diffuse and translucent clouds are found to range between $10^{12}$–$10^{13}$ cm$^{-2}$ (Maier et al. 2001, Roueff et al. 2003, Oka et al. 2003). The C$_3$ column density observed in the present study is larger by about a factor of 100 or more than those from the optical studies. Thus, the non-detection of C$_3$ in the foreground diffuse gas in the direction of our sources is consistent with the sensitivity of our observations.

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Appendix A: Formulae used for the excitation analysis

In the approximation of weak absorption ($\tau \ll 1$) and a negligible population in the upper, $\nu_2 = 1$, state, the lower state column density is given by:

$$N_l = \frac{8\pi\nu^3}{3c} \frac{g_l}{A_{ul}} \int \tau dv$$  \hspace{1cm} (A.1)

The rotational temperature, $T_{\text{rot}}$, is calculated from the state specific column densities by

$$T_{\text{rot}}(J, J') = \frac{E_J - E_{J'}}{k} \ln \left( \frac{N_{J'(2J'+1)}}{N_J(2J+1)} \right)^{-1}$$  \hspace{1cm} (A.2)

where the energy of the levels is given by $E_J = hBJ(J + 1)$ and the rotational constant for the lower vibrational state ($\nu_2 = 0$) is $B = 12908.242$ MHz.

Note that a ratio of level populations close to unity, $(N_{J'(2J'+1)}/N_J(2J+1)) \approx 1$, implies high values of $T_{\text{rot}}$ in comparison to the rotational energy scale defined by $hB/k_B$, i.e. 0.62 K in the case of C$_3$. The formal errors derived for the $T_{\text{rot}}$ are correspondingly very large.

Assuming a thermalized population across the rotational ladder with a unique value of $T_{\text{rot}}$ for all levels, a measured single state column density can be converted to the total column density $N(C_3)$ using:

$$N(C_3) = P(T_{\text{rot}}) \frac{N_J}{2J + 1} \exp \left( \frac{hB}{k_BT_{\text{rot}}} J(J + 1) \right)$$  \hspace{1cm} (A.3)

$$\approx \frac{T_{\text{rot}}}{2hB/k_B} \frac{N_J}{2J + 1} \exp \left( \frac{hB}{k_BT_{\text{rot}}} J(J + 1) \right)$$  \hspace{1cm} (A.4)

where the approximation $T_{\text{rot}} \gg hB/k$ has been applied for the partition function

$$P(T_{\text{rot}}) = \sum_{J=0,2,4,...} (2J + 1) \exp (-E_J/kT_{\text{rot}}) \approx \frac{k_BT_{\text{rot}}}{2hB},$$  \hspace{1cm} (A.5)

which is half of the usual value for a linear rotor due to the symmetry not allowing odd-J states.

Acknowledgements. HIFI has been designed and built by a consortium of institutes and university departments from across Europe, Canada and the United States under the leadership of SRON Netherlands Institute for Space Research, Groningen, The Netherlands and with major contributions from Germany, France and the US. Consortium members are: Canada: CSA, U. Waterloo; France: CESR, LAB, LERMA, IRAM; Germany: KOSMA, MPIfR, MPA; Ireland: NUI Maynooth; Italy: ASI, IFSI-INAF; Osservatorio Astrofisico di Arcetri-INAF; Netherlands: SRON, TUD; Poland: CAMK, CBK; Spain: Observatorio Astronómico Nacional (IGN), Centro de Astrobiología (CSIC-INTA); Sweden: Chalmers University of Technology - MC2, RSS & GARD; Onsala Space Observatory; Swedish National Space Board, Stockholm University - Stockholm Observatory; Switzerland: ETH Zurich, FHNW; USA: Caltech, JPL, NHSC. JC and JRG thanks spanish MICINN for funding support under projects AYA2009-07304 and CSD2009-00038. M.S. acknowledge support from grant N 203 39334 from Polish MNiSW.

1. Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400005, India e-mail: bhaswati@tifr.res.in
2. J. Physikalisches Institut, University of Cologne, Germany
3. Centro de Astrobiología, CSIC-INTA, 28850, Madrid, Spain
4. LERMA, CNRS, Observatoire de Paris and ENS, France
5. California Institute of Technology, Pasadena, CA 91125, USA
6. JPL, California Institute of Technology, Pasadena, USA
7. Onsala Space Observatory, Chalmers University of Technology, SE-43992 Onsala, Sweden
8. Depts. of Physics, Astronomy & Chemistry, Ohio State Univ. USA.
9. The Johns Hopkins University, Baltimore, MD 21218, USA
10. Institut d’Astrophysique Spatiale (IAS), Orsay, France.
11. Laboratoire d’Astrophysique de Marseille (LAM), France.
12. Laboratoire d’Astrophysique de Grenoble, France.
13. Université Toulouse; UPS ; CESR ; and CNRS ; UMR5187, 9 avenue du colonel Roche, F-31028 Toulouse cedex 4, France
14. Gemini telescope, Hilo, Hawaii, USA.
15. MPI für Radioastronomie, Bonn, Germany.
16. Institute of Physical Chemistry, PAS, Warsaw, Poland
17. Nicolaus Copernicus University, Toruń, Poland
18. Dept. of Physics & Astronomy, University of Calgary, Canada
19. Nicolaus Copernicus Astronomical Centre (CAMK), Toruń, Poland
20. European Space Astronomy Centre, ESA, Madrid, Spain
21. Infrared Processing and Analysis Center, California Institute of Technology, MS 100-22, Pasadena, CA 91125
22. Sterrewacht Leiden, University of Leiden, Leiden, The Netherlands
23. SRON Netherlands Institute for Space Research, Landleven 12, 9747 AD Groningen, The Netherlands