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► To cite this version:

Yaye Awa Ba, Christian Wenger, Romain Surleau, Vincent Boudon, Maud Rotger, et al.. MeCaSDa and ECaSDa: Methane and ethene calculated spectroscopic databases for the virtual atomic and molecular data centre. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 2013, 130, pp.62-68. 10.1016/j.jqsrt.2013.05.001 . hal-03844245

HAL Id: hal-03844245

<https://hal.science/hal-03844245v1>

Submitted on 8 Nov 2022

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MeCaSDa and ECaSDa: Methane and Ethene Calculated Spectroscopic Databases for the Virtual Atomic and Molecular Data Centre

Yaye Awa Ba^{†a}, Christian Wenger^b, Romain Surleau^b, Vincent Boudon^{b,*}, Maud Rotger^{a,**}, Ludovic Daumont^a, David A. Bonhommeau^a, Vladimir G. Tyuterev^a, Marie-Lise Dubernet^c

^a*Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA), CNRS UMR 7331, Université de Reims Champagne-Ardenne, U.F.R. Sciences Exactes et Naturelles, Moulin de la Housse B.P. 1039, 51687 Reims Cedex 2, France*

^b*Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), CNRS UMR 6303, Université de Bourgogne, 9 avenue A. Savary, BP 47870, 21078 DIJON Cedex, FRANCE*

^c*Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique (LPMAA), CNRS/INP UMR 7092, Université Pierre et Marie Curie, Case 76, 4 Place Jussieu, 75252 Paris Cedex 05, France*

Abstract

Two spectroscopic relational databases, denoted MeCaSDa and ECaSDa, have been implemented for methane and ethene, and included in VAMDC (Virtual Atomic and Molecular Data Centre, http://portal.vamdc.eu/vamdc_portal/home.seam). These databases collect calculated spectroscopic data from the accurate analyses previously performed for the electronic ground state of methane, ethene, and some of their isotopologues: ¹²CH₄, ¹³CH₄, and ¹²C₂H₄. Both infrared absorption and Raman scattering lines are included. The polyad structures are reported and the transitions are precisely described by their energy, their intensity and the full description of the lower and upper states involved in the transitions. The relational schemas of ECaSDa and MeCaSDa databases are equivalent and optimized to enable the better compromise between data retrieval and compatibility with the XSAMS (XML Schema for Atoms, Molecules, and Solids) format adopted within the VAMDC European project.

1. Introduction

Methane (CH₄) and ethene (or ethylene, C₂H₄) have been thoroughly studied by both experimental and theoretical spectroscopic techniques during the past decades.

*Principal corresponding author

**Corresponding author

Email addresses: vincent.boudon@u-bourgogne.fr (Vincent Boudon),
maud.rotger@univ-reims.fr (Maud Rotger)

[†]Present address: Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique (LPMAA), CNRS/INP UMR 7092, Université Pierre et Marie Curie, Case 76, 4 Place Jussieu, 75252 Paris Cedex 05, France

As a matter of fact, these two molecules are of great interest for various applications, among which atmospheric sciences and planetology are the most important. CH_4 is one of the most important greenhouse gases in the Earth's atmosphere and it is present in significant quantities in the atmosphere of the Solar System's giant planets, on Titan, but also on brown-dwarfs and some exoplanets. C_2H_4 is a pollutant produced by biomass fires and is also present on some astronomical objects like Jupiter, Saturn, Neptune, Titan and maybe some exoplanets. It is thus important, in order to perform remote concentration measurements or to run radiative transfer codes to model such atmospheres, to have extensive and accurate line lists for these molecules. A close collaboration between the ICB group in Dijon and the GSMA groups in Reims has allowed to perform extensive high resolution spectroscopic studies on these two species and develop specific formalisms and models helpful for fitting experimental data and producing synthetic line lists [1, 2].

Initiated mid-2009, the Virtual Atomic and Molecular Data Centre (VAMDC) European FP7 project aims to build an interoperable e-infrastructure for relating atomic and molecular databases and make them easily accessible by the scientific community [3]. The databases involved in this project cover a wide range of systems from atoms with databases such as the Vienna Atomic Line Database (VALD) [4] or the CHIANTI database [5], to molecules of interest in astrochemistry and atmospheric physics with databases such as the HIGH-resolution TRANsmission molecular absorption database (HITRAN) [6, 7], the Spectroscopic and Molecular Properties of Ozone database (S&MPO) [8] or the MeCaSDa (Methane Calculated Spectroscopic Database) and ECaSDa (Ethene Calculated Spectroscopic Database) databases described in the present paper, and also solids with the Grenoble astrophysics and planetology Solid Spectroscopy and Thermodynamics database (GhoSST) [9] or the Laboratorio di Astrofisica Sperimentale (LASp) database [10, 11]. The MeCaSDa and ECaSDa databases only collect theoretical data although the spectroscopic data included in other VAMDC databases come from both experimental studies such as Fourier transform infrared spectroscopy or Cavity ring-down spectroscopy and semi-empirical lines resulting from analyses.

In this paper, we first describe in Section 2 the data included in the MeCaSDa and ECaSDa databases and briefly recall the theoretical techniques used to derive them. The relational schema of the databases is then detailed in Section 3 and Section 4 explains how to query the databases through the VAMDC portal. Section 5 gathers concluding remarks on the interest of these databases, especially within the scope of the VAMDC European project.

2. Data included in MeCaSDa and ECaSDa

2.1. Generalities

All the line lists included in MeCaSDa and ECaSDa have been assigned using the SPVIEW software and molecular effective parameters (Hamiltonians and dipole moments) have been fitted using the XTDS software [12]. Then, XTDS was also used to generate the calculated lists (line positions and intensities).

The vibrational structure of a molecule is considered as a series of polyads which are groups of interacting vibrational levels. The theoretical model implemented in XTDS [12] is based on the tensorial formalism developed in the ICB group [13, 14, 15] in line with earlier implementations for the databases of tetrahedral molecules [16]. This model allows the construction of effective Hamiltonian and transition moment (dipole moment or polarizability) operators adapted to a given polyad scheme. We define a polyad scheme as follows. Let n be the polyad number. A vibrational level with quantum numbers (v_1, v_2, \dots, v_N) of a molecule with N normal modes of vibration belongs to polyad P_n if:

$$n = \sum_{j=1}^{j=N} i_j v_j, \quad (1)$$

where the $\{i_j\}$ is a set of integers. For example, in the case of CH_4 , since the stretching modes (ν_1, ν_3) have close harmonic wavenumbers which are approximately twice those of the bending modes (ν_2, ν_4) , we choose $(i_1, i_2, i_3, i_4) = (2, 1, 2, 1)$ and the polyad number is:

$$n(\text{CH}_4) = 2v_1 + v_2 + 2v_3 + v_4, \quad (2)$$

leading to the well-known sequence of polyads: Ground State (one level), Dyad (two levels), Pentad (five levels), Octad (eight levels), *etc* [17].

2.2. Spectroscopic data

All the calculated line lists included in the MeCaSDa and ECaSDa databases result from the most recent line by line analyses of high resolution infrared and Raman experimental spectra.

For $^{12}\text{CH}_4$, the line list mostly results from the global analysis of the first four polyads (Ground State, Dyad, Pentad and Octad) performed by Albert *et al.* [17] and recently updated by Daumont *et al.* [1]. Ground State (*i.e.* pure rotational lines) intensities have been recently revised by Boudon *et al.* [18]. Preliminary results of an ongoing analysis of the Tetradecad region are also included. Note that an accurate WKMC (Wang, Kassi, Mondelain, Campargue) experimental methane line list above 5850 cm^{-1} has been recently measured in Grenoble [19] by means of laser cavity-ring-down spectroscopy technique. However, only a small fraction of this list (945 lines in the $5\nu_4/\nu_2 + 4\nu_4$ region and 164 lines in the $\nu_2 + 2\nu_3$ region), namely lines at the beginning of the icosad range, has been theoretically assigned up to now [20]. The MeCaSDa database does not yet include these data as our approach requires a full theoretical description of the included polyad.

For $^{13}\text{CH}_4$, a global analysis of the infrared spectrum in the spectral range $0 - 3200 \text{ cm}^{-1}$ has been recently performed by Niederer *et al.* [21] and will be completed by additional results [22].

In the case of ethene, global analyses are less advanced than for methane, but are in progress. Contrary to methane, this molecule has no clear and unique polyad scheme. We thus use different polyad schemes (*i.e.* different $(i_1, i_2, \dots, i_{12})$ sets of integers for this species with 12 normal modes) for each spectral region under consideration. These polyad schemes are chosen to get a proper grouping of the vibrational levels that are considered together. Moreover, line intensities are still under investigation. At present,

only the ν_{12} band intensities have been analyzed [2]. Line positions in the 3000 and 6000 cm^{-1} C–H stretching regions have been fitted [23], but the intensity analysis is in progress. This is also the case for the $\nu_{10}/\nu_7/\nu_4/\nu_{12}$ bending tetrad.

We wish to emphasize that the present databases contain calculated lines (positions and intensities). It is thus “complete” for a given set of transitions between two polyads (up to a given rotational quantum number), but not necessarily highly accurate in all regions, depending on the quality of the fit of experimental data that led to this list. No intensity cutoff is applied. On the other hand, our lists are also combined with experimental line positions and intensities to give semi-empirical line lists that are used to update the HITRAN [6, 7] and GEISA 2009 [24] databases as described for instance by Brown et al. [25, 26]. These lists are less “complete” (in the sense defined above *i.e.* they may contain less lines in some regions) but composed of more accurate lines. In this respect, MeCaSDa and ECaSDa do not directly compete with other experimental or semi-empirical databases but bring added value to the community of spectroscopists. As a first example, Figure 1 shows a comparison between the lines included in HITRAN 2008 [6] (or GEISA 2009 [24]) and in MeCaSDa.

[Insert Figure 1 here.]

As a second example of available spectral lines in these databases Figure 2 shows the Raman scattering lines of $^{12}\text{CH}_4$ included in MeCaSDa. It is noteworthy that MeCaSD4 and ECaSDa are probably the only databases featuring Raman scattering rotation-vibration lines, which constitutes one of their specificities.

[Insert Figure 2 here.]

At present, the databases do not contain line broadening coefficients, but such data will be included in the near future, based on theoretical calculations developed by the ICB group [27, 28]. As described hereafter, the database structure has been conceived in order to allow the inclusion of pressure broadening data for various collisional partners. Tables 1 and 2 display the number of levels and transitions, respectively, for both databases at the time of the redaction of the present paper. Table 2 also show the wavenumber and intensity ranges for all transitions included in the databases.

[Insert Table 1 here.]

[Insert Table 2 here.]

3. Structure of the databases

The MeCaSDa and ECaSDa databases share the same structure since they contain the same types of data. They are compatible with the XSAMS (XML Schema for Atoms, Molecules, and Solids) [29] format adopted within the VAMDC European project [3]. Their structure is based on a set of fourteen database tables (hereafter called DB tables), as shown in Figure 3 (more detailed relational schemas for the MeCaSDa

and ECaSDa databases are supplied as Supplementary Material), that are related together through external key indices chosen to optimize both the size and query execution time of the database. Table 3 details the physical quantities (with units), main quantum numbers and chemical names used in the three main DB tables.

[Insert Figure 3 here.]

[Insert Table 3 here.]

The specificity of each database is determined by the energy level labeling which differs for methane and ethene due to the multiple choices of polyad schemes in the case of ethene. The quantum numbers and the isotopologues also differ for these molecules.

The main DB table of these databases is called “transitions”. This DB table precisely documents transitions between rovibrational states by indicating their computed wavenumber, intensity, pressure-induced line broadenings, and pressure-induced line shifts as illustrated in Figure 4. The accuracy and least-squares fit residuals of all the previous quantities and the Einstein coefficient are also provided. The remaining fields correspond to indices that refer to some other DB tables, namely “sources”, “characterisation”, “transition_types”, “molecules_isotopes”, and “molecular_states”, that enable a full description of the transition. DB table “sources” collects the references of all the publications on spectroscopic analyses (see Section 2) of methane or ethene. DB table “characterisation” specifies the physical origin of the transition (*i.e.*, electric dipole or polarizability). DB table “transition_types” indicates the spectroscopic technique corresponding to the data under consideration, such as microwave absorption, infrared absorption, or stimulated Raman spectroscopy. Each isotopologue of methane or ethene present in the MeCaSDa and ECaSDa databases are defined in DB table “molecules_isotopes” by its chemical formula in text and \TeX formats, its international chemical identifier (InChI) and corresponding InChIKey [30], and its chemical abstract service registry number. This DB table also contains an identifier for the state taken as energy reference and an identifier that refers to the molecular type (DB table “molecule_types”). For instance, the methane isotopologues currently included in MeCaSDa are of XY_4 molecular type. In ECaSDa, the ethene isotopologues have molecular type X_2Y_4 .

[Insert Figure 4 here.]

The lower and upper states involved in the transitions are described in DB table “molecular_states” by means of their term value, polyad index, total angular momentum J , irreducible symmetry group representation C of the rovibrational wavefunction, multiplicity index α , and nuclear spin statistical weight g (as mentioned above, a detailed correspondence between physical quantities and DB table labels is given in Table 3). For each wavefunction, we only provide the squared coefficients and sublevels corresponding to its decomposition on the initial normal mode basis set. Supplying both coefficients and their signs instead of squared coefficients would be feasible but requires bigger storage capacity and this would also be impractical for most users that do not need such information. In other words, we provide the most useful data on all the

Hamiltonian eigenvectors that can be used in various applications such as line-mixing calculations. The squared coefficients of the decomposition are sorted in decreasing order. The vibrational sublevels indices refer to DB table “vibrational_sublevels” that contains vibrational quantum numbers of the initial normal mode states as described in Ref. [15] for CH₄ and in Ref. [31] for C₂H₄.

A polyad (DB table “polyads”) is defined by a polyad number and a polyad scheme (DB table “polyad_schemes”). As presented in Section 2 several polyad schemes can be used to describe the vibrational energy levels of a given molecule. Each polyad scheme is a set of polyads (DB table “polyad_descriptions”) composed of a limited number of vibrational levels described in DB table “vibrational_levels”.

4. Querying MeCaSDa and ECaSDa through the VAMDC portal

The MeCaSDa and ECaSDa databases can be queried from the online VAMDC portal (http://portal.vamdc.eu/vamdc_portal/home.seam). Through this interface, it is possible to retrieve lines within a given wavenumber and/or intensity range. Examples are given in Figures 5 and 6. The VAMDC portal also searches entries for methane and ethene in other databases such as HITRAN.

[Insert Figure 5 here.]

[Insert Figure 6 here.]

5. Conclusion

The approach adopted in the MeCaSDa and ECaSDa relational databases relies on good quality extrapolation properties of the underlying spectroscopic models, particularly for high J values and hot band intensities based on accurate fits of experimental data obtained for smaller sets of quantum numbers values. This approach could help interpret future observations, in particular for atmospheric and planetary applications. MeCaSDa and ECaSDa do not compete with other public databases containing either experimental or semi-empirical transitions. This is a complementary approach, giving complete line lists, but with a lower accuracy for some regions, depending on the status of line-by-line analyses of experimental spectra (see Section 2.2). These two databases will be regularly updated in the future, as soon as some new analyses are performed, leading to improved spectroscopic models. We also intend to include soon some other molecules that are studied in our groups, like CF₄ [32] or SF₆.

6. Acknowledgements

We are grateful to the VAMDC community for fruitful discussions. The ROMEO supercomputer center of Champagne-Ardenne is acknowledged for technical support and server hosting. This work was supported by the VAMDC european project within the framework of the “Research Infrastructures - INFRA-2008-1.2.2 - Scientific Data Infrastructures” initiative, and by the “Agence Nationale de la Recherche” (ANR) CH₄@Titan under grant n° BLAN08-2_321467.

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TABLE 1: Number of vibrational levels and sublevels, maximum J value (rotational quantum number) and rovibrational states included in the databases..

TABLE 2: Rovibrational transitions included in the databases (see Table 1 for polyad definitions).

TABLE 3: Correspondence between physical quantities and labels in the DB tables “transitions”, “molecule_isotopes”, and “molecular_states”. In DB table “transitions” the index i stands for the collision partner responsible for line broadenings or line shifts (ie, self, N₂, O₂, air, H₂O, CO₂, H₂, He, Ar).

Table 1: Number of vibrational levels and sublevels, maximum J value (rotational quantum number) and rovibrational states included in the databases.

| MeCaSDa | $^{12}\text{CH}_4 / ^{13}\text{CH}_4$ | Vib. levels | Vib. sublevels | Max. J | Rovib. states |
|----------|--|-------------|----------------|----------|---------------|
| | P_0 GS | 1 | 1 | 25 / 25 | 282 / 282 |
| | P_1 Dyad | 2 | 2 | 25 / 25 | 1408 / 1408 |
| | P_2 Pentad | 5 | 9 | 25 / 25 | 5352 / 5352 |
| | P_3 Octad | 8 | 24 | 22 / 12 | 12142 / 3874 |
| | P_4 Tetradecad | 14 | 60 | 17 / 0 | 18900 / 0 |
| ECaSDa | $^{12}\text{C}_2\text{H}_4$ | Vib. levels | Vib. sublevels | Max. J | Rovib. states |
| Scheme 1 | P_0 GS | 1 | 1 | 45 | 2116 |
| | P_1 $\nu_4/\nu_7/\nu_{10}/\nu_{12}$ | 4 | 4 | 45 | 8464 |
| Scheme 2 | P_0 GS | 1 | 1 | 36 | 1369 |
| | P_1 ν_5 | 1 | 1 | 35 | 1296 |
| | P_2 ν_9/ν_{11} | 2 | 2 | 35 | 2592 |
| | P_3 $\nu_5 + \nu_9/\nu_5 + \nu_{11}$ | 2 | 2 | 35 | 2592 |

Table 2: Rovibrational transitions included in the databases (see Table 1 for polyad definitions).

| MeCaSDa | | Nb. dipolar | | Nb. Raman | | Dipolar wavenumber | | Dipolar intensity | | Raman wavenumber | | Raman intensity | |
|---------------------------------------|--|-------------|---------|-----------|--------------------|---|---|--------------------------|---------------------------------------|------------------|--|-----------------|--|
| $^{12}\text{CH}_4 / ^{13}\text{CH}_4$ | | Transitions | | Nb. Raman | Dipolar wavenumber | range / cm^{-1} | range / $\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^{-2})$ | range / cm^{-1} | range / arbitrary unit | | | | |
| | | $P_0 - P_0$ | 1222 | 0 | 0-253 | $8 \times 10^{-49} - 8 \times 10^{-25}$ | | | | | | | |
| | | $P_1 - P_0$ | 13025 | 19207 | 911-1868 | $1 \times 10^{-39} - 2 \times 10^{-19}$ | | 671-2076 | $4 \times 10^{-1} - 4 \times 10^{18}$ | | | | |
| | | $P_1 - P_1$ | 31510 | 0 | 0-688 | $3 \times 10^{-61} - 8 \times 10^{-25}$ | | | | | | | |
| | | $P_2 - P_0$ | 49475 | 72954 | 2075-3483 | $2 \times 10^{-41} - 4 \times 10^{-20}$ | | 1842-3685 | $6 \times 10^3 - 2 \times 10^{20}$ | | | | |
| | | $P_2 - P_1$ | 247325 | 0 | 456-2303 | $8 \times 10^{-49} - 4 \times 10^{-22}$ | | | | | | | |
| | | $P_2 - P_2$ | 459276 | 0 | 0-1132 | $4 \times 10^{-61} - 2 \times 10^{-27}$ | | | | | | | |
| | | $P_3 - P_0$ | 97581 | 141446 | 3322-5011 | $3 \times 10^{-37} - 8 \times 10^{-21}$ | | 3123-5179 | $2 \times 10^{-2} - 2 \times 10^{17}$ | | | | |
| | | $P_3 - P_1$ | 267105 | 375012 | 1854-3685 | $1 \times 10^{-39} - 2 \times 10^{-22}$ | | 1696-3804 | $3 \times 10^{-1} - 2 \times 10^{17}$ | | | | |
| | | $P_3 - P_2$ | 1015053 | 0 | 274-2473 | $8 \times 10^{-45} - 1 \times 10^{-24}$ | | | | | | | |
| | | $P_4 - P_0$ | 114580 | 0 | 4670-6446 | $2 \times 10^{-36} - 2 \times 10^{-21}$ | | | | | | | |
| | | $P_4 - P_1$ | 572747 | 0 | 3095-5223 | $8 \times 10^{-46} - 2 \times 10^{-23}$ | | | | | | | |
| | | $P_4 - P_2$ | 2176493 | 3024031 | 1520-4005 | $1 \times 10^{-45} - 8 \times 10^{-25}$ | | 1378-4097 | $6 \times 10^{-7} - 9 \times 10^{14}$ | | | | |
| ECaSDa | | Nb. dipolar | | Nb. Raman | | | | | | | | | |
| $^{12}\text{C}_2\text{H}_4$ | | Transitions | | | | | | | | | | | |
| Scheme 1 | | $P_1 - P_0$ | 123205 | 0 | 500-1750 | $3 \times 10^{-45} - 8 \times 10^{-18}$ | | | | | | | |
| Scheme 2 | | $P_1 - P_0$ | 0 | 6791 | | | | 3000-3150 | $2 \times 10^6 - 2 \times 10^{20}$ | | | | |
| | | $P_2 - P_0$ | 68549 | 0 | 1500-5500 | $3 \times 10^{-38} - 8 \times 10^{-18}$ | | | | | | | |
| | | $P_3 - P_0$ | 59440 | 0 | 5000-7499 | $4 \times 10^{-39} - 4 \times 10^{-17}$ | | | | | | | |

Table 3: Correspondence between physical quantities and labels in the DB tables “transitions”, “molecule_isotopes”, and “molecular_states”. In DB table “transitions” the index i stands for the collision partner responsible for line broadenings or line shifts (ie, self, N₂, O₂, air, H₂O, CO₂, H₂, He, Ar).

| DB Table name | Physical quantity | Label in the databases | Unit (if relevant) |
|------------------|--|------------------------|--|
| transitions | Wavenumber, $\tilde{\nu}$ | wavenumber | cm ⁻¹ |
| | Wavenumber accuracy, $\delta\tilde{\nu}$ | wavenumber_prec | cm ⁻¹ |
| | Wavenumber residual, $\Delta\tilde{\nu}$ | wavenumber_residual | cm ⁻¹ |
| | Intensity, I | intensity | cm ⁻² .atm ⁻¹ at 296 K |
| | HITRAN intensity (see for instance Ref. [7]) | intHITRAN | cm ⁻¹ /(molecule.cm ⁻²) |
| | Intensity accuracy, δI | intensity_prec | % |
| | Intensity residual, ΔI | intensity_residual | % |
| | Einstein coefficient, A | einstein | s ⁻¹ |
| | Pressure-induced line broadening, γ_i | gamma | cm ⁻¹ .atm ⁻¹ |
| | Pressure-induced line broadening accuracy, $\delta\gamma_i$ | gamma_prec | cm ⁻¹ .atm ⁻¹ |
| | Pressure-induced line shift, δ_i | deltai | cm ⁻¹ .atm ⁻¹ |
| | Pressure-induced line shift accuracy, $\delta\delta_i$ | deltai_prec | cm ⁻¹ .atm ⁻¹ |
| | Coefficients for temperature dependence of γ_i , n_i | nexpi | unitless |
| | Accuracy on coefficients for temperature dependence of γ_i , δn_i | nexpi_prec | unitless |
| | molecule_isotopes | Isotope name | isotope_name |
| | InChi number | inchi | |
| | InChi key | inchikey | |
| | Chemical formula in TeX format | formtex | |
| | Chemical abstract service registry number | casregnum | |
| | Energy reference | eostateid | |
| molecular_states | Term value, F | position | cm ⁻¹ |
| | Total angular momentum, J | j | |
| | Irreducible representation, C | symname | |
| | Multiplicity index, α | alpha | |
| | Nuclear spin statistical weight, g | weight | |

FIG. 1: $^{12}\text{CH}_4$ lines included in MeCaSDa (red points) and corresponding lines included in HITRAN 2008 [6] and GEISA 2009 [24] (blue points) at $T = 296\text{ K}$. Polyad names are indicated.

FIG. 2: $^{12}\text{CH}_4$ Raman lines included in MeCaSDa at $T = 296\text{ K}$. Polyad names are indicated.

FIG. 3: Simplified relational schema of the MeCaSDa and ECaSDa databases. A complete relational schema of the MeCaSDa and ECaSDa databases is provided in Figs 1 and 2 of supplementary materials.

FIG. 4: Definition of line parameters: intensity I , wavenumber $\tilde{\nu}$, pressure-induced line broadening γ_i , and pressure-induced line shift δ_i where i represents the collision partner (ie, self, N_2 , O_2 , air, H_2O , CO_2 , H_2 , He, Ar). The exponent $^\circ$ is added on top of some symbols to remind that they are obtained for standard pressure conditions.

FIG. 5: Simple example of methane lines query through the VAMDC portal.

FIG. 6: VAMDC portal response to the query shown on Figure 5. Methane lines can be retrieved from either the HITRAN database (experimental and semi-empirical lines) or from the MeCaSDa database (calculated lines).

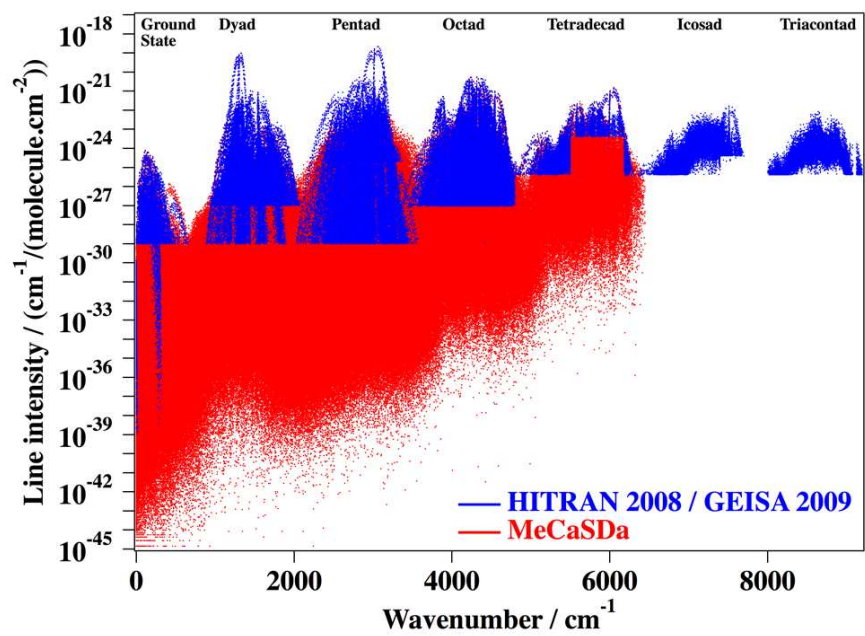


Figure 1: $^{12}\text{CH}_4$ lines included in MeCaSDa (red points) and corresponding lines included in HITRAN 2008 [6] and GEISA 2009 [24] (blue points) at $T = 296 \text{ K}$. Polyad names are indicated.

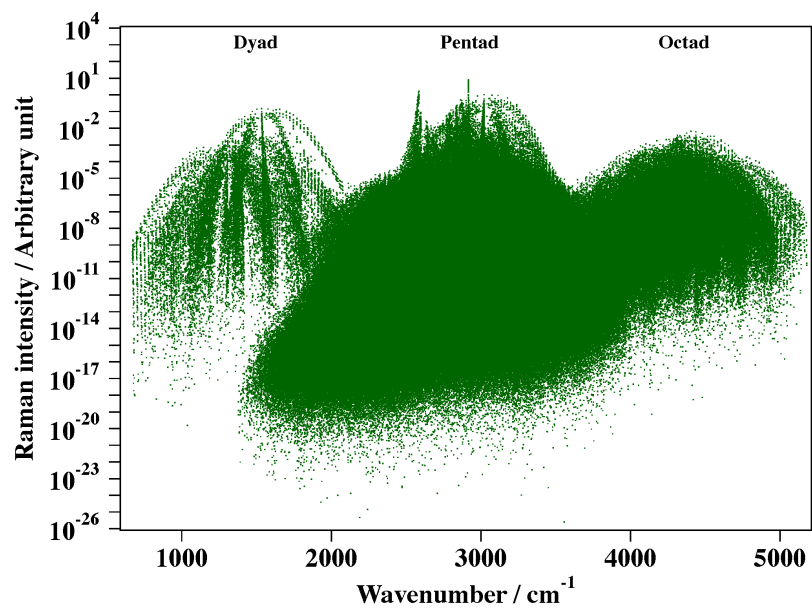


Figure 2: $^{12}\text{CH}_4$ Raman lines included in MeCaSDa at $T = 296$ K. Polyad names are indicated.

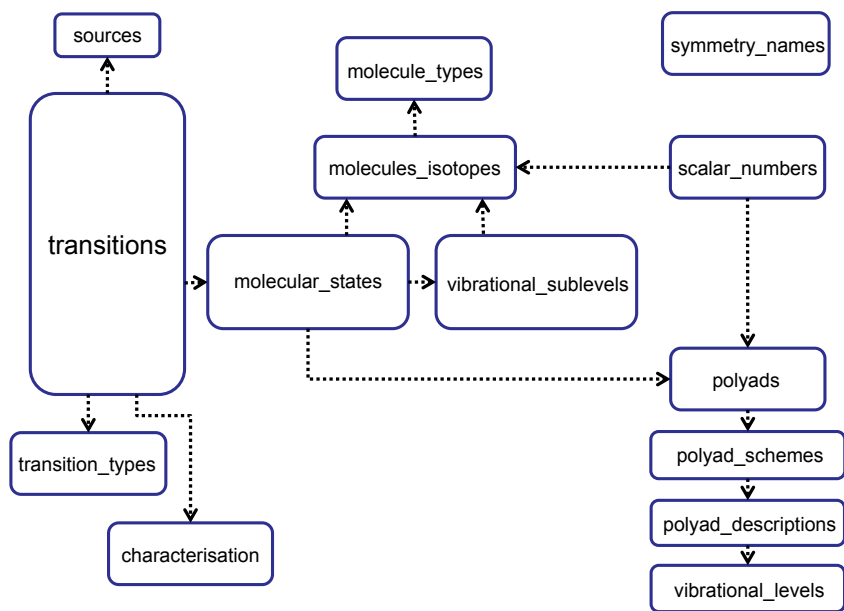


Figure 3: Simplified relational schema of the MeCaSDa and ECaSDa databases. A complete relational schema of the MeCaSDa and ECaSDa databases is provided in Figures 1 and 2 of supplementary materials.

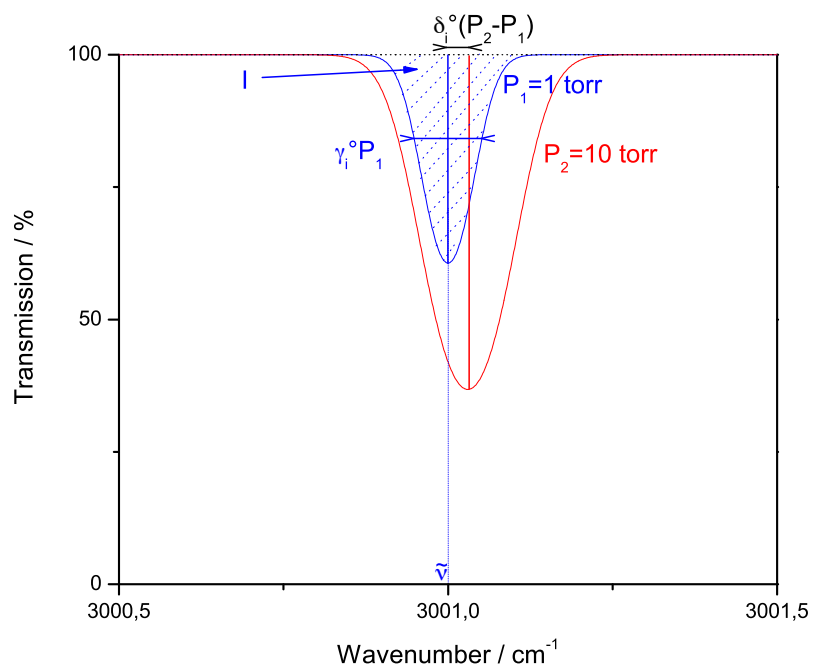


Figure 4: Definition of line parameters: intensity I , wavenumber $\bar{\nu}$, pressure-induced line broadening γ_i , and pressure-induced line shift δ_i where i represents the collision partner (ie, self, N_2 , O_2 , air, H_2O , CO_2 , H_2 , He, Ar). The exponent $^\circ$ is added on top of some symbols to remind that they are given for standard pressure conditions.

Molecules Clear Remove <

Chemical name

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

[Select All](#) [None](#) Search by stoichiometric formula if no isotopologue is selected.

Isotopologue

Methane ¹²CH₄

Methane ¹³CH₄

Methane ¹²CH₃D

Methane ¹³CH₃D

Radiative Clear Remove <

Wavenumber to cm-1

Equivalent Wavelength to Wavelength from to 76923.07692307692A

Upper state energy to 1/cm

Equivalent to 1/cm

Lower state energy to 1/cm

Equivalent to 1/cm

Probability, A to 1/s

Find data Save query

Legend

available, can answer

available, don't support query

unsupported keyword

- » Theoretical spectral database of polycyclic aromatic hydrocarbons
- » Chianti
- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- » GSMA Reims S&MPO
- » ECaSDa - Ethene Calculated Spectroscopic Database
- » GhoSST
- » Lund laboratory spectroscopy database
- » Stark-b
- » HITRAN-UCL resource
- » VALD sub-set in Moscow (obs)
- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- » MeCaSDa - Methane Calculated Spectroscopic Database
- » VALD (atoms)
- » Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
- » VAMDC species-DB
- » OACT - LASP Database
- » TOPbase : VAMDC-TAP interface
- » DESIRE database (Moscow mirror)
- » BASECOL: VAMDC-TAP interface
- » TIPbase : VAMDC-TAP interface
- » Carbon Dioxide Spectroscopic Databank 296K (VAMDC-TAP)
- » SpEctroScopy of Atoms and Molecules
- » Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP)
- » Spectr-W3
- » Water internet Accessible Distributed Information System
- » KIDA: VAMDC-TAP interface

Figure 5: Simple example of methane lines query through the VAMDC portal.

Done

Modify query Stop waiting Save query

select * where (RadTransWavelength >= 71428.37142857143 AND RadTransWavelength <= 76923.07692307692) AND ((InchiKey IN ('VNWKTOKETHGBQD-UHFFFAOYSA-N','VNWKTOKETHGBQD-OUBTZVSYSA-N')))

Comments

XSAMS processors

BibTex from XSAMS
 Table views of XSAMS
 Xsams2SME

Process

| Name | Response | Download | Species | States | Processes | Radiative | Collisions | Non Radiative |
|---|-----------------------|-----------------------|---------|--------|-----------|-----------|------------|---------------|
| <input type="checkbox"/> GheSST | OK | XSAMS | 1 | 0 | 1 | 1 | 0 | 0 |
| <input type="checkbox"/> Cologne Database for Molecular Spectroscopy: VAMDC-TAP service | OK (15/04/2013 16:18) | XSAMS | 0 | 0 | 0 | 0 | 0 | 0 |
| <input type="checkbox"/> Cologne Database for Molecular Spectroscopy: VAMDC-TAP service | OK (15/04/2013 16:18) | XSAMS | 0 | 0 | 0 | 0 | 0 | 0 |
| <input type="checkbox"/> Water internet Accessible Distributed Information System | OK (06/12/2012 18:00) | XSAMS | 0 | 0 | 0 | 0 | 0 | 0 |
| <input type="checkbox"/> McCaSda - Methane Calculated Spectroscopic Database | TRUNCATED (53%) | XSAMS | 2 | 18493 | 100000 | 100000 | 0 | 0 |
| <input type="checkbox"/> HITRAN-LJCL resource | TRUNCATED (76%) | XSAMS | 2 | 4350 | 10000 | 10000 | 0 | 0 |
| DESIRE database (Moscow mirror) | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP) | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| Carbon Dioxide Spectroscopic Databank 298K (VAMDC-TAP) | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| ECaSda - Ethene Calculated Spectroscopic Database | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| VALD sub-set in Moscow (obs) | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| VALD (atoms) | EMPTY | | 0 | 0 | 0 | 0 | 0 | 0 |
| Carbon Dioxide Spectroscopic Databank (VAMDC-TAP) | FAIL | | 0 | 0 | 0 | 0 | 0 | 0 |

Figure 6: VAMDC portal response to the query shown on Figure 5. Methane lines can be retrieved from either the HITRAN database (experimental and semi-empirical lines) or from the McCaSda database (calculated lines).