

Project VAMDC: molecular data and metadata

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Content

VAMDC

Motivation

Virtual Atomic and Molecular Center

Atomic & Molecular Databases

A&M Challenges

VAMDC End User Communities

VAMDC project organisation

Molecular data and metadata

Problem Definition

Molecular spectroscopy model

Elementary solution of spectroscopic problem

Primary information sources

Upload of energy levels

Transitions. Comparison and Download

Line Profile Root mean square deviations

Composite solution of spectroscopic problems

Validity

Properties for solution of spectroscopic problem T6

Automatically computed root-mean square deviation of solutions

Decomposition of composite data sources H₂O

Automatic semantic processing

Distributed information system on molecular spectroscopy



Motivation

The existing problems can be divided into two categories:
(1) ***data completeness and quality assessment*** and
(2) ***data interface including problem specific tools for data mining.***

Today those issues are tackled by a number of data centres but they are highly focussed on specific applications and non-flexible. Thus, there is a strong need to:

- Develop close links between the user communities, the data producers and data centres based on modern technology.
- Establish better international coordination in order to promote atomic and molecule data compilation and database activities, avoid duplication of efforts and ensure the use of the best available data.



Virtual Atomic and Molecular Center

- Name of the coordinating person:
Professor M.L. Dubernet, LPMAA/CNRS
- FP7 – e-Infrastructure Program Project
- 15 legal partners - 21 institutes or departments
- France, UK, Austria, Italia, Sweden, Germany, Serbia
- Russian Federation (ISAN, IAO, IA RAS, Institute of Technical Physics)
- Venezuela
- Duration 1 July 2009 – 31 December 2012



Atomic & Molecular Databases

- Contain Atomic and Molecular Data
 - Data from laboratory experiments & calculations
 - Spectroscopic data: linelists and their characteristics
 - Rate coefficients as a function of temperature
 - Cross-sections as function of energy, angles, ...
 - Many processes: chemical reaction, collisional excitation, photo-chemical reaction
- Very Different Chemical Species from atomic (isotopes and ions) to molecules (various isotopologues) and even to surfaces or solids



A&M Challenges

- A&M data underpins many areas of research
 - Providing access to a wide range of users (astronomy, nuclear, climatology, biology) in academia and industry
- Data is complex and increasingly large
- Handling of data (often) involves use of applications
- Issues with ensuring data completeness & quality
- Coordination and standards – organising the A&M community

Challenge: provide data access to all A&M data to all end user communities



VAMDC End User Communities

- Astrophysical, atmospheric, plasma, combustion media
- Simulations, Observations, Diagnostics
- Industrial Applications, e.g. lighting, etching, e.g. PLASIMO
- Teaching Outreach
- Range of Complexity of user requirements



VAMDC project organisation

- Networking Activities
 - Training, workshops
 - Science requirements, strategy
 - Interface to external groups (VO, Grid, etc)
- Service Activities
- Deployment of A+M services
 - Support to the service and user communities
- Research Activities
 - Standards (XML Schema, Dictionaries, Query Language, Registry)
 - Publishing and Data MiningTools



Problem Definition

Create a distribution information system on molecular spectroscopy oriented on *semantic description of molecular spectroscopy problems' solutions properties*

1. Create a distributed information system on molecular spectroscopy containing the solutions of spectroscopic problems and the solution properties.
2. Create an open computable logic theory of solution properties



Model of Atmospheric Spectroscopy

Direct Problems **(0-th approximation)** Inverse Problems

Calculations

Isolated molecule
physical characteristics task
(T1)



Isolated molecules spectral
line parameters task (T2)



Spectral line profile
parameters task (T3)



Spectral functions
calculation task (T4)

Measurements

Task on isolated molecule
energy level definition (T7)



Einstein coefficients
definition task (T6)



Task on quantum numbers
assignment to spectral lines
(T5)



Task on interacting molecule
spectral line parameters
definition (ET)



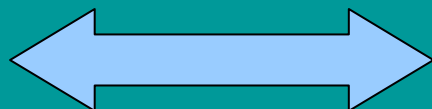
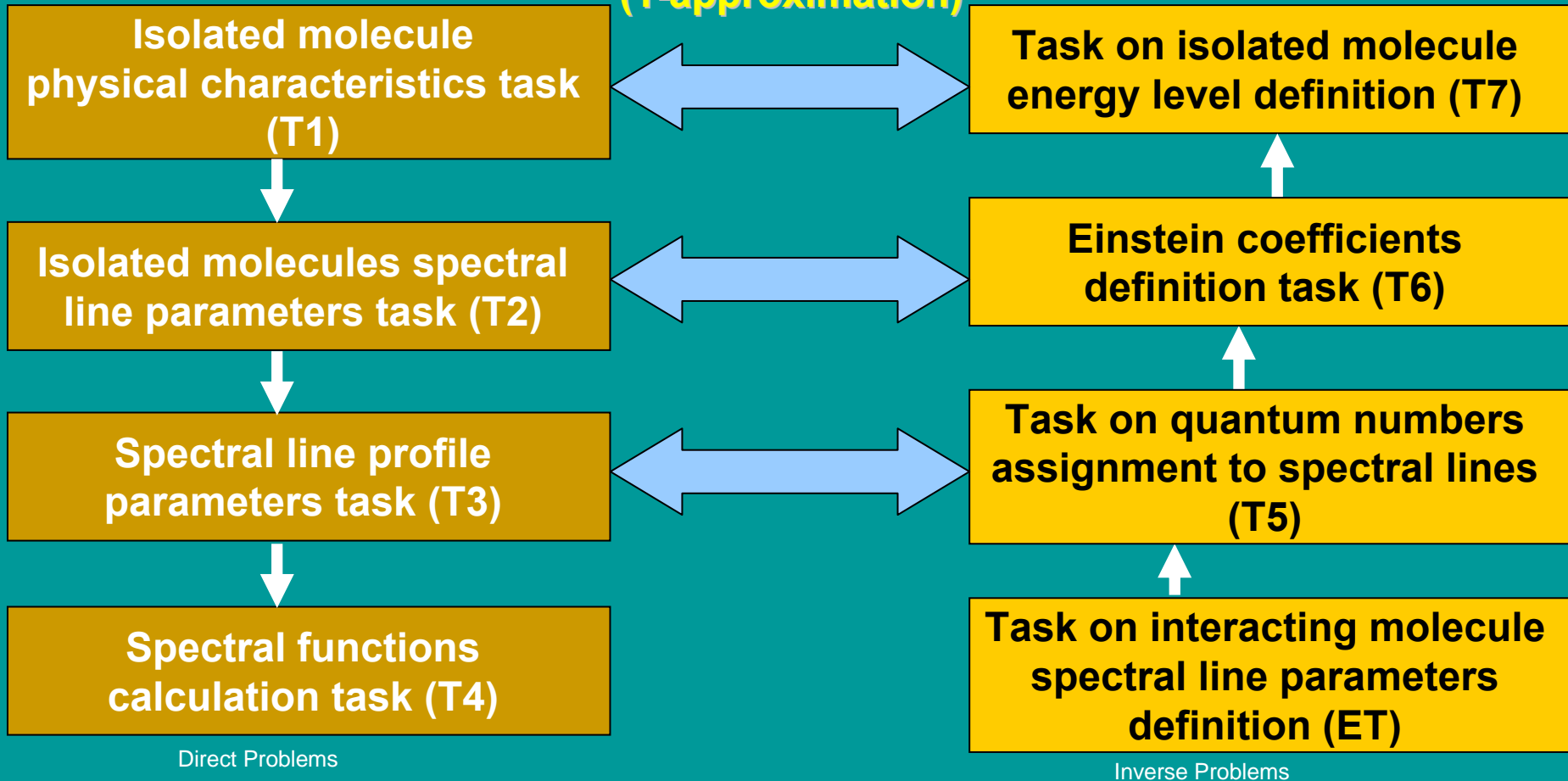
Spectral functions
measurement task (E)

Two chains of problems are selected for approximation for domain description.



Model of Atmospheric Spectroscopy

(1-approximation)



Root-mean-square deviations



Elementary solution of spectroscopic problem

| Information source (Left) Calculations/Experiments | | | | | | | | |
|--|------------------------|------------------------------|------------------------------|------------------------------|-----------------|------------------------------|------------------------------|---------------------------------------|
| 1998_Schwenke_H2O | | | | | | | | |
| Schwenke D.W., New H ₂ O Rovibrational Line Assignments. // Journal of Molecular Spectroscopy, 1998, v. 190, no. 2, p. 397-402. | | | | | | | | |
| Number of transitions | dE (cm ⁻¹) | v ₁ ^{NM} | v ₂ ^{NM} | v ₃ ^{NM} | J ^{NM} | K _a ^{NM} | K _c ^{NM} | Energy Levels (E (cm ⁻¹)) |
| 1 | 0.012 | 3 | 2 | 0 | 2 | 1 | 1 | 13738.7339 |
| 3 | 0.001197 | 2 | 4 | 0 | 5 | 4 | 1 | 14051.135061 |
| 9 | 0.001324 | 1 | 4 | 1 | 6 | 4 | 2 | 14224.050961 |
| 2 | 0.000997 | 0 | 4 | 2 | 7 | 2 | 5 | 14288.10269 |
| 5 | 0.000915 | 0 | 6 | 1 | 8 | 7 | 1 | 15204.10038 |
| 6 | 0.000858 | 3 | 0 | 1 | 9 | 5 | 5 | 15209.327197 |
| 4 | 0.000935 | 1 | 0 | 3 | 10 | 3 | 8 | 15661.812495 |

Elementary source characteristics

molecule – H₂O

the list of physical quantities – energy levels E (cm⁻¹), Quantum numbers (v₁ v₂ v₃ J K_a K_c), correction for the value of energy level dE (cm⁻¹), Number of transitions

publication - Schwenke D.W., New H₂O Rovibrational Line Assignments. // Journal of Molecular Spectroscopy, 1998, v. 190, no. 2,

p. 397-402

data -



| | | |
|---|---|---|
| Title * Title of the data source. Use only digits and latin letters | Title * Title of the data source only digits and latin lett | Title * Title of the data source. Use only digits and latin letters |
| Commentaries Description of the data source for user | Commentaries Description of the data for user | Commentaries Description of the data source for user |
| Search of Publication* Type keyword or author of the publication | Search of Publicati Type keyword or autho the publication | Search of Publication* Type keyword or author of the publication |

| N | | Publication | Publication* |
|----|----------------------------------|--|--|
| 1 | <input type="radio"/> | O.Naumenk Cavity ring Journal of I | Article or monograph, which identify data source |
| 2 | <input type="radio"/> | P. Pyykko, K.G. Dyall, A.G. Csaszar, G. Tarczay, O.L. Polyansky, J. Tennyson, . // Physical Review, A, 2001, p. art. no. 024502. | |
| 3 | <input checked="" type="radio"/> | Coheur P.-F., P.F.Bernath, M. Carleer, R. Colin, O.L. Polyansky, N.F.Zobov, S.V.Shirin, R.J.Barber and J.Tennyson, A 3000 K laboratory emission spectrum of water. // Journal of Chemical Physics, 2005, v. 122, p. 074307 (8 pages). | |
| 29 | <input type="radio"/> | Schermaul R., A.A.D.Canas, R.C.M. Learner, J.W. Brault, O.L.Polyansky, N.F.Zobov, D.Belmiloud and J.Tennyson, Weak Line Water Vapor Spectra in the Region 13 200–15 000 cm ⁻¹ . // Journal of Molecular Spectroscopy, 2002, v. 211, B. 2, p. 169-178. | |
| 30 | <input type="radio"/> | Tolchenov R.N., J.Tennyson, J.W. Brault, A.A.D.Canas, and R.Schermaul, Weak line water vapor spectrum in the 11,787 - 13,554 cm ⁻¹ region. // Journal of Molecular Spectroscopy, 2002, v. 215, B. 2, p. 269-274. | |

Coheur P.-F., P.F.Bernath, M. Carleer, R. Colin, O.L. Polyansky, N.F.Zobov, S.V.Shirin, R.J.Barber and J.Tennyson, A 3000 K laboratory emission spectrum of water. // Journal of Chemical Physics, 2005, v. 122, p. 074307 (8 pages).

Title and link to publication



Inverse problem for energy levels of an isolated molecule
Review and making user's data sources

rows starting from

In all rows 77

| N | Title | Publication | Edit |
|----|---|--|----------------------|
| 44 | 2005PCCP_Kassi | Samir Kassi, Peter Macko, Olga Naumenko, Alain Campargue, The absorption spectrum of water near 750 nm by CW-CRDS: contribution to the search of water dimer absorption. // Physical Chemistry Chemical Physics, 2005, № 12, C. 2460-2467. | Edit |
| 45 | 2005_Coheur | Coheur P.-F., P.F.Bernath, M. Carleer, R. Colin, O.L. Polyansky, N.F.Zobov, S.V.Shirin, R.J.Barber and J.Tennyson, A 3000 K laboratory emission spectrum of water. // Journal of Chemical Physics, 2005, № 123, C. 216-227. | Edit |
| 46 | 2005_Naumenko_JMS_234_HDO | Campargue A., Vas absorption spectros cm ⁻¹ . // Journal of 2, C. 216-227. | |
| 47 | 2005_Tolchenov_2_H2_170 | Tolchenov R.N., O.M O.L.Polyansky, J.Te A.Jenouvrier and A. assignments in the Journal of Molecular 68-76. | |

Qualitative metadata

Method

List of input data URL:

Picklist (URL) :

Primary information source
Additional data (Metadata) formed by user



Choose data source in table for data upload from your file

rows starting from
In all rows 71

| N | Title | Publication |
|----|-------------------------------------|--|
| 1 | 2005JMS2_Tolchenov_ | Tolchenov R.N., O.Naumenko, N.F.Zobov, S.V.Shirin, O.L.Polyansky, J.Tennyson, M.Carleer, P.-F.Coheur, S.Fally, A.Jenouvrier and A.C.Vandaele, Water vapour line assignments in the 9250-26 000 cm ⁻¹ frequency range. // Journal of Molecular Spectroscopy, 2005, v. 233, B. 1, p. 68-76. |
| 2 | 2001JMS_Bykov | Bykov A., O.Naumenko, L.Sinitsa, B.Voronin, J.-M.Flaud, C.Camy-Peyret, and R.Lanquetin, High-Order Resonances in the Water Molecule. // Journal of Molecular Spectroscopy, 2001, T. 205, B. 1, C. 1-8. |
| 3 | 1977_CamyPeyret | Camy-Peyret C., J.-M.Flaud, J.-P. Maillard, G. Guelachvili, Higher ro-vibrational levels of H ₂ O deduced from high resolution oxygen-hydrogen flame spectra between 6200 and 9100 cm ⁻¹ . // Molecular Physics, 1977, T. 33, C. 1641-1650. |
| 70 | 1999_Camy-Peyret | C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, A. Bykov, O. Naumenko, L. Sinitsa, and B. Voronin. Fourier-transform absorption spectrum of the H ₂ ¹⁷ O |
| 71 | 2005_Coheur | Coheur P.-F., P.F.Bernath, M. Carleer, N.F.Zobov, S.V.Shirin, R.J.Barber and laboratory emission spectrum of wa |

Basic Characteristics of Elementary Data Source

| Physical Entity | Value |
|-----------------|--|
| Substance | <input type="text" value="H2O"/> <ul style="list-style-type: none"> H2C_13CH2 H2C_18O H2O H2O2 H2S H2_13CO HBr HCN HCOOH |

Loaded File Parameters

| | |
|------------------------|--|
| Type of File Structure | <input checked="" type="radio"/> Column File |
| Number of the Entities | <input type="text" value="4"/> |

Upload of energy levels

Choice of substance and description of data file structure



Data file structure

```
0 5 0 2 0 2 7612.724380
0 5 0 2 1 1 7683.029190
```

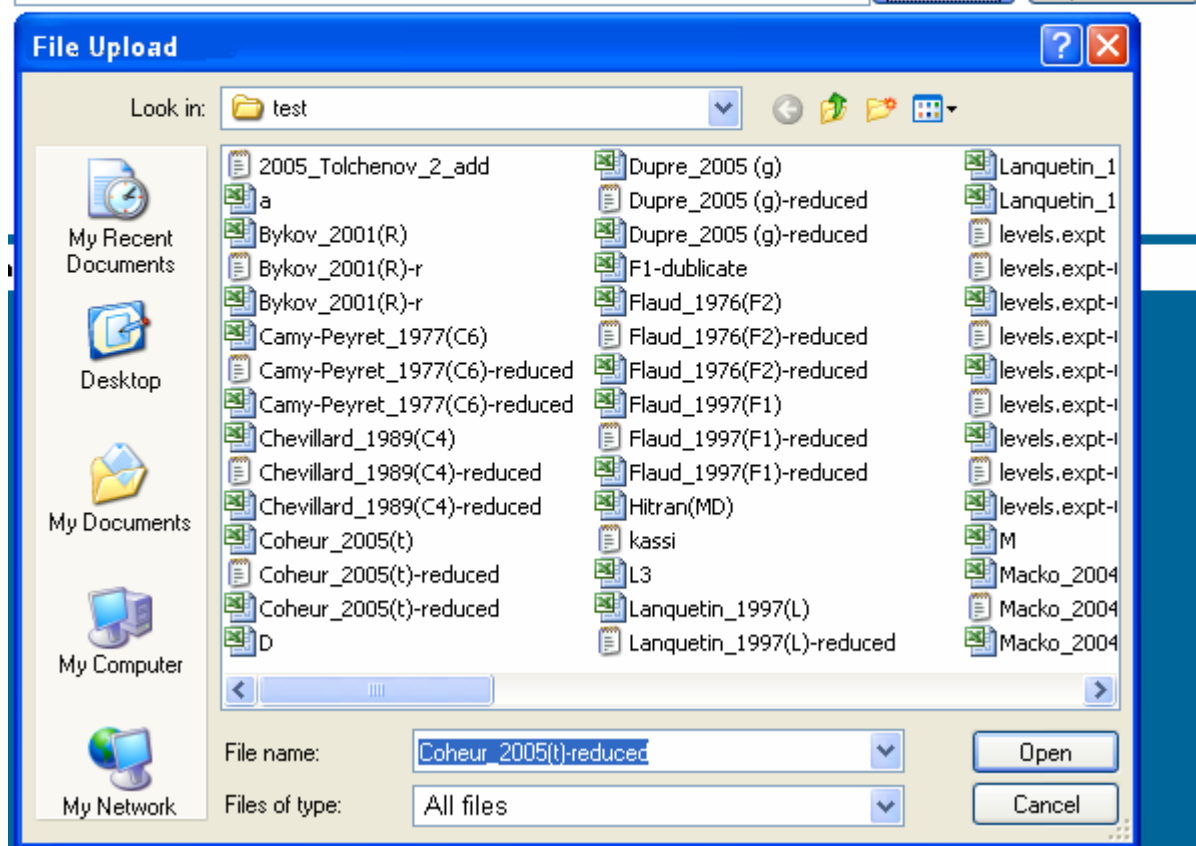
Description of file structure

Inverse problem for energy levels of an isolated molecule
Entities for uploading

Inverse problem for energy levels of an isolated molecule
2 File Uploading

E:\grants\Tennyson\Experiment\test\Coheur_2005(t)-reduced.txt

| | Beginning Position of the Column | End Position of the Column |
|---------|----------------------------------|----------------------------|
| Modes | 1 | 34 |
| | 35 | 52 |
| ^-1) | 53 | 60 |
| g level | 61 | 67 |



Data file schema and file upload



| Data source | Information | Chosen Information source |
|---------------|-------------|---------------------------|
| Substance | Substance | Title |
| Energy Levels | | |

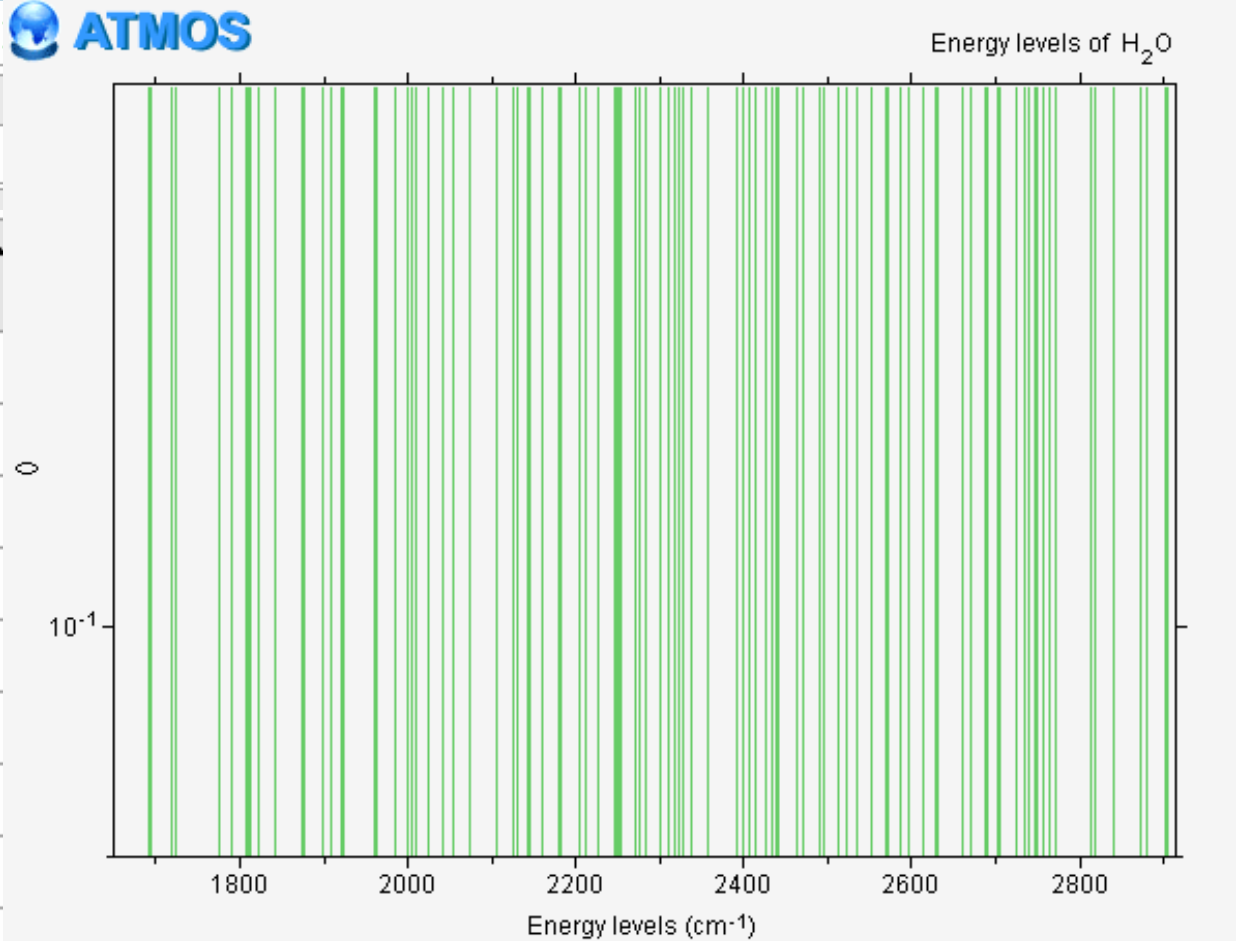
1997_PoZoViTe_H2O

O.L.Polyansky, N.F.Zobov, S.Vitia, J.Tennyson, P.F.Bernath and I. Wallace. High Temperature Rotational Transitions of Water in

[Annotation \(1997_PoZoViTe_H2O \)](#)

| Substance |
|------------------|
| H ₂ O |

| N | v_1^{NM} | v_2^{NM} | v_3^{NM} |
|---|------------|------------|------------|
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 |
| 4 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 |
| 7 | 0 | 0 | 0 |
| 8 | 0 | 0 | 0 |



Review of uploaded energy levels



Choose information source for comparison

| Substance | HOD | | | | | | | | | | | | |
|---|--|---|---|---|----------|-------|------------------------------------|----------|-------|----------|-------|----------|-------|
| Vacuum wavenumber range (cm ⁻¹) | 0 - 50000 | | | | | | | | | | | | |
| Subst Choice of spectral band (ν_1, ν_2, ν_3) ^{up} - (ν_1, ν_2, ν_3) _{low} | - ▾ - ▾ - ▾ - ▾ - ▾ - ▾ | | | | | | | | | | | | |
| Vacuum wavenumber range (cm ⁻¹) | $ w_1 - w_2 _{max}$ | | | | | | | | | | | | |
| Choice of spectral band (ν_1, ν_2, ν_3) ^{up} - (ν_1, ν_2, ν_3) _{low} | 1.455 | | | | | | | | | | | | |
| Words and numbers | > >> Control | | | | | | | | | | | | |
| Choice of information source | <table border="1"> <thead> <tr> <th>Vacuum wavenumber w_2 (cm⁻¹)</th> <th>$w_1 - w_2$ [z-a]</th> <th>Download data</th> </tr> </thead> <tbody> <tr> <td>6524.225</td> <td>1.455</td> <td rowspan="4"> Download as ASCII: whole table </td> </tr> <tr> <td>6385.969</td> <td>1.391</td> </tr> <tr> <td>6488.632</td> <td>0.858</td> </tr> <tr> <td>6462.988</td> <td>0.712</td> </tr> </tbody> </table> | Vacuum wavenumber w_2 (cm ⁻¹) | $w_1 - w_2$ [z-a] | Download data | 6524.225 | 1.455 | Download as ASCII: whole table | 6385.969 | 1.391 | 6488.632 | 0.858 | 6462.988 | 0.712 |
| Vacuum wavenumber w_2 (cm ⁻¹) | $w_1 - w_2$ [z-a] | Download data | | | | | | | | | | | |
| 6524.225 | 1.455 | Download as ASCII: whole table | | | | | | | | | | | |
| 6385.969 | 1.391 | | | | | | | | | | | | |
| 6488.632 | 0.858 | | | | | | | | | | | | |
| 6462.988 | 0.712 | | | | | | | | | | | | |
| | <table border="1"> <thead> <tr> <th>columns</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="checkbox"/> Vacuum wavenumber w_1 (cm⁻¹)</td> </tr> <tr> <td><input checked="" type="checkbox"/> ν_1^{up}</td> </tr> </tbody> </table> | columns | <input checked="" type="checkbox"/> Vacuum wavenumber w_1 (cm ⁻¹) | <input checked="" type="checkbox"/> ν_1 ^{up} | | | | | | | | | |
| columns | | | | | | | | | | | | | |
| <input checked="" type="checkbox"/> Vacuum wavenumber w_1 (cm ⁻¹) | | | | | | | | | | | | | |
| <input checked="" type="checkbox"/> ν_1 ^{up} | | | | | | | | | | | | | |

Save As

Save in: faz

- My Recent Documents
- Desktop
- My Documents
- My Computer
- My Network

File name:

Save as type:

Buttons: Save, Cancel

Benedict W.S., Gailar N., Plyler E.R., Rotational-vibration spectra of deuterated water vapor. // Journal of Chemical Physics, 1956, v. 24, no. 6, p. 1139-1165.

T. Ohshima and H.Sasada, 1.5- μ m DFB semiconductor laser spectroscopy of deuterated water. // Journal of Molecular Spectroscopy, 1989, v. 136, no. 2, p. 250-263.

| |
|--|
| Substance |
| H ₂ O |
| Method |
| UNDEFINED |
| Reference |
| A.D. Bykov, N.N. Lavrentieva, T.P. Mishina, L. Tennyson, Water vapor line width and shift calculation functions. // Journal of Quantitative Spectroscopy, 109, p. 1834-1844. |
| Calculations of H ₂ ¹⁶ O rotation-vibration line pressure effects are performed using a semi-empirical based on impact theory modified by introducing an empirical data. These model parameters are determined by shifting coefficients to experimental data. The method uses anharmonic wavefunctions in the estimates of the present calculation is the use of a complete set of transition moments calculated for all possible transitions from variational nuclear motion calculations and an approach explicitly takes into account all scatterings of these calculations clearly demonstrate improved calculated parameters for both the line widths and |
| Output data |
| Thermodynamical conditions |
| Temperature |
| Pressure |
| Broadening substance |
| Broadening substance name |
| Parameter |
| Collisional Halfwidth |
| Temperature dependence of HW |
| Pressure-induced Shift |
| Collisional Halfwidth |
| Temperature dependence of HW |
| Pressure-induced Shift |
| Temperature dependence of shift |

| |
|---|
| Substance |
| H ₂ O |
| Method |
| UNDEFINED |
| Reference |
| Coheur P.-F., Fally S., Carleer M., Clerbaux C., Colin R., Jenouvrier A., Mouchienne M.-F., Hermans C., Vandaele A. C., New water vapor line parameters in the 26000-13000 cm ⁻¹ region. // Journal of Quantitative Spectroscopy and Radiation Transfer, 2002, v. 74, no. 4, p. 493-510. |
| Output data |
| Thermodynamical conditions |
| Temperature |
| Pressure |
| Broadening substance |
| Broadening substance name |
| Parameter |
| Unit |
| Availability |
| Uncertainty |
| Collisional Halfwidth |
| Temperature dependence of HW |
| Pressure-induced Shift |
| Temperature dependence of shift |

| |
|---|
| Output data |
| Wavenumbers |
| Unit |
| (Wavenumber) _{min} |
| (Wavenumber) _{max} |
| Number of transitions |
| Uncertainty |
| Intensity |
| Unit |
| Availability |
| Uncertainty |
| Transition quantum numbers |
| Quantum numbers type |
| Number of bands |
| Number of transitions with unique quantum numbers |
| Number of transitions with nonunique quantum numbers |
| Number of unidentified transitions |
| Number of allowed transitions (J' --> J'' or J''±1) |
| Number of forbidden transitions (J' -/-> J'' or J''±1) |
| Number of allowed transitions for water (k _c ' - k _c '' = 2n+1, n=1,2,3,..) |
| Number of forbidden transitions for water (k _c ' - k _c '' = 2n) |
| Number of allowed transitions for water (C _{2v}) (ν ₃ ' + k _a ' + ν ₃ '' + k _a '' = 2n+1) |
| Number of forbidden transitions for water (C _{2v}) (ν ₃ ' + k _a ' + ν ₃ '' + k _a '' = 2n) |



| Info | Information source left | Information source right |
|--------------------------------|--|---|
| 2006 | 2000_Toht_H2O-N2 | 2008_ByLaMisi_H2O-N2 |
| A.D. Tolchenov, Accurate Spect | Toht R.A., Air- and N ₂ -broadening parameters of water vapor: 604 to 2271 cm ⁻¹ . // Journal of Molecular Spectroscopy, 2000, v. 201, p. 218-243. | A.D. Bykov, N.N. Lavrentieva, T.P. Mishina, L.N. Sinita, R.J. Barber, R.N. Tolchenov, J. Tennyson, Water vapor line width and shift calculations with accurate vibration-rotation wave functions. // Journal of Quantitative Spectroscopy and Radiation Transfer, 2008, v. 109, p. 1834-1844. |

| Number | Number of lines with the same quantum numbers | $ w_1 - w_2 _{\max}$ (cm ⁻¹) | $ h_1 - h_2 _{\max}$ (cm ⁻¹ atm ⁻¹) | $ s_1 - s_2 _{\max}$ (cm ⁻¹ atm ⁻¹) |
|--------|---|--|--|--|
| 3447 | 724 | 0.22041 | 1.10657 | 1.00963 |

| | | | |
|---|--------------------|------|---------|
| Show <input type="text" value="2"/> rows starting from <input type="text" value="0"/> | In all rows 166341 | > >> | Control |
|---|--------------------|------|---------|

| Vacuum wave | Vacuum wavenumber w_1 (cm ⁻¹) | v_1^{up} | v_2^{up} | v_3^{up} | j^{up} | K_a^{up} | K_c^{up} | v_1^{low} | v_2^{low} | v_3^{low} | j^{low} | K_a^{low} | K_c^{low} | Vacuum wavenumber w_2 (cm ⁻¹) | $w_1 - w_2$ | $h_1 - h_2$ [z-a] | $s_1 - s_2$ |
|-------------|---|------------|------------|------------|----------|------------|------------|-------------|-------------|-------------|-----------|-------------|-------------|---|-------------|-------------------|-------------|
| 15036 | 2145.67848 | 1 | 0 | 0 | 4 | 1 | 4 | 0 | 1 | 0 | 3 | 0 | 3 | 2145.64858 | 0.0299 | 1.10657 | 4e-05 |
| 15089 | 2067.77907 | 0 | 0 | 1 | 2 | 2 | 0 | 0 | 1 | 0 | 3 | 2 | 1 | 2067.62817 | 0.1509 | 1.1032 | 0.0088 |

| | | | |
|---|--------------------|------|---------|
| Show <input type="text" value="2"/> rows starting from <input type="text" value="0"/> | In all rows 166341 | > >> | Control |
|---|--------------------|------|---------|

| Spect (v ₁ , v ₂ , v ₃) | Spectral band (v ₁ , v ₂ , v ₃) ^{up} - (v ₁ , v ₂ , v ₃) _{low} | (Vacuum wavenumber) _{rmsd} (cm ⁻¹) | (Halfwidth) _{rmsd} (cm ⁻¹ atm ⁻¹) | (Shift) _{rmsd} (cm ⁻¹ atm ⁻¹) |
|---|--|---|---|---|
| 0 3 3 | All bands | 0.13479042068 | 0.12069794565 | 0.12310932571 |
| 0 3 4 | 0 0 0 - 0 0 0 | 0.02343605894 | 0.14535336298 | 0.00663786949 |
| 0 4 3 | 0 0 1 - 0 1 0 | 0.14784050262 | 0.2088244857 | 0.00669400158 |
| 0 5 3 | 0 1 0 - 0 0 0 | 0.15000562581 | 0.11346870902 | 0.06100063852 |
| 0 6 3 | 0 1 0 - 0 1 0 | 0.02424 | 0.03588 | 0.00894 |
| 1 0 4 | 0 2 0 - 0 1 0 | 0.06111599836 | 0.01237110514 | 0.32458413781 |
| 1 1 3 | 1 0 0 - 0 1 0 | 0.03654837291 | 0.27689112293 | 0.00766361941 |

Line Profile

Root mean square deviations



Composite solution of spectroscopic problems

1. HITRAN, GEISA,

2. Implicit solutions, unknown solutions or unpublished solutions



Validity

Formal constraints

Data type –

quantum numbers – natural numbers,
intensity, half-width, frequency, energy levels – positive real numbers,

Variation interval –

$0 < \text{frequency} < 45000 \text{ cm}^{-1}$, $10^{-16} \text{ cm/mol} < \text{intensity} < 10^{-30}$

Selection rules -

normal modes - $k_a + k_c = J$ or $J+1$,

precise quantum numbers – $J < 60$, $0 < s < 5$,

Publication constraints

Whether a result is published or not

Non-formal constraints. **Experts' opinion**



Non-formal constraints

J. Tennyson, P.F. Bernath, L.R. Brown, A. Campargue, M.R. Carleer, A.G. Császár, R.R. Gamache, J.T. Hodges, A. Jenouvrier, O.V. Naumenko, O.L. Polyansky, L.S. Rothman, R.A. Toth, A.C. Vandaele, N. Zobov, L. Daumont, A.Z. Fazliev, T. Furtenbacher, I.F. Gordon, S.N. Mikhailenko, S.V. Shirin,

IUPAC Critical Evaluation of the Rotational-Vibrational Spectra of Water Vapor. Part I. Energy Levels and Transition Wavenumbers for H₂¹⁷O and H₂¹⁸O

Journal of Quantitative Spectroscopy and Radiative Transfer, July 2009, V.110, no.9-10, P.573-596.



Annotation (1983_PiCoCaFI_H2O of 2009)

Substance

H₂O

Method

UNDEFINED

Reference

A.S.Pine, S.J.Coulombe, C.Camy-Peyret, and J.-M. temperature water spectrum in the 3000 to 4000 cm⁻¹ and Chemical Reference Data, 1983, v. 12, no. 3, p. .

An atlas of the high-temperature (1200°K) absorption vapor in the 3000 to 4000 cm⁻¹ region is presented was recorded at Doppler-limited resolution using frequency laser spectrometer. The spectral region the strong OH stretching fundamentals, ν₁ and overtone, 2ν₂, as well as associated hot bands. been assigned using a model Hamiltonian which agreement between calculated and observed line K_a up to 14. The calculated eigenvectors applied operator predict the measured line intensities should serve as a reference for analyzing spectral sources such as combustion exhausts and cool

T=1200+/-30 K; P=0.8 to 2.0 Torr; L=252 cm

Root-mean square deviations

Type: NormalModes

Number of informa

Transition quantum numbers

| Quantum numbers type | NormalModes |
|---|-------------|
| J _{min} | 0 |
| J _{max} | 27 |
| Number of transitions with unique quantum numbers | 2163 [T] |
| Number of transitions with nonunique quantum numbers | 0 [T] |
| Number of unassigned transitions | 0 [T] |
| Number of allowed transitions for water (k _a +k _c = J or J+1) | 2163 [T] |
| Number of forbidden transitions for water (k _a +k _c ≠ J or J+1) | 0 [T] |
| Number of allowed transitions (J' --> J'' or J''±1) | 2163 [T] |
| Number of forbidden transitions (J' -/> J'' or J''±1) | 0 [T] |
| Number of allowed transitions for water (k _c ' - k _c '' = 2n+1, n=1,2,3,..) | 2163 [T] |
| Number of forbidden transitions for water (k _c ' - k _c '' = 2n) | 0 [T] |
| Number of allowed transitions for water (C _{2v}) (ν ₃ ' + k _a ' + ν ₃ '' + k _a '' = 2n+1) | 2162 [T] |
| Number of forbidden transitions for water (C _{2v}) (ν ₃ ' + k _a ' + ν ₃ '' + k _a '' = 2n) | 1 [T] |
| Number of transitions rejected by experts | 0 [T] |

(|k_c' - k_c''| = 2n)

Number of allowed transitions for water (C_{2v}) (ν₃' + k_a' + ν₃'' + k_a'' = 2n+1)

2162 [T]

Number of forbidden transitions for water (C_{2v})

Properties for solution of spectroscopic problem T6

| N | Vacuum wavenumber (cm ⁻¹) | ν ₁ ^{up} NM | ν ₂ ^{up} NM | ν ₃ ^{up} NM | j ^{up} NM | k _a ^{up} NM | k _c ^{up} NM | ν ₁ ^{low} NM | ν ₂ ^{low} NM | ν ₃ ^{low} NM | j ^{low} NM | k _a ^{low} NM | k _c ^{low} NM |
|---|---------------------------------------|---------------------------------|---------------------------------|---------------------------------|--------------------|---------------------------------|---------------------------------|----------------------------------|----------------------------------|----------------------------------|---------------------|----------------------------------|----------------------------------|
| 1 | 3036.0024 | 0 | 2 | 0 | 8 | 8 | 1 | 0 | 0 | 0 | 9 | 8 | 2 |



Automatically computed root-mean square deviation of solutions

| Root-mean square deviations | | | |
|-----------------------------|-------------------------------------|--|-------------------------------------|
| Type: NormalModes | Number of information source [19] | | |
| Data Source | Wavenumbers | | |
| 2007_ZoOvShPo_H2O | 1.595e+3 6.050e+1 [1427] [11] | 1999_ToTh_H2O_UCL | 8.080e-3 9.566e-4 [1221] [3] |
| 2004_Hitran_H2O | 2.199e-1 5.380e-3 [1750] [7] | 1993_ToTh_b_H2O_UCL | 2.000e+1 6.467e-1 [985] [2] |
| 1983_PiCoCaFl_H2O | 2.059e-1 5.774e-3 [2162] [12] | 2.199e-1 Maximal value of wavenumbers' difference 5.380e-3 Total value of RMSD [1750] Number of transition used for RMSD calculation [7] Number of spectral bands | |
| 2005_ToTh_H2O | 4.020e-3 1.063e-3 [141] [3] | 2005_ToTh_H2O_ucl | 1.063e-3 [141] [3] |
| 1973_PuRa_H2O | 2.000e-4 2.000e-4 [1] [1] | 2007_ScPaTa_a_H2O | 5.404e+1 1.203e+0 [2022] [10] |
| 1973_CaFlGuAm_H2O | 3.000e+2 1.187e+1 [935] [3] | 2006_BaTeHaTo_H2O | 4.854e+0 1.828e-1 [2145] [11] |
| 1997_MiTyKeWi_H2O | 2.205e-1 1.380e-2 [257] [1] | 2007_ScPaTa_b_H2O | 5.404e+1 1.165e+0 [2156] [12] |
| 2008_FuCsTe_H2O | 5.002e-1 4.519e-2 [153] [6] | 2009_RoGoBaBe_H2O | 2.199e-1 5.380e-3 [1750] [7] |
| 1993_ToTh_a_H2O_UCL | 4.000e-3 1.022e-3 [250] [1] | 1999_JaArBaBa_H2O | 6.343e+0 2.627e-1 [1748] [7] |
| | | 2005_JaScChGa_H2O | 6.343e+0 2.627e-1 [1748] [7] |



Decomposition of composite data sources H₂¹⁶O

Residual

L.S. Rothman, I.E. Gordon, A. Barbe, D.Chris Benner,
P.F. Bernath, M. Birk, V. Boudon, L.R. Brown,
A. Campargue, J.-P. Champion, K. Chance, L.H. Coudert,
V. Dana, V.M. Devi, S. Fally, J.-M. Flaud, R.R. Gamache,
A. Goldman, etc,
The HITRAN 2008 molecular spectroscopic database.
Journal of Quantitative Spectroscopy and Radiation Transfer,
2009, v. 110, Issue 9, p. 533-572.

181 data sources
(including
HITRAN 2004,
GEISA 1997)

~ 25 lines
WN -11000-25000
Intensity 10⁻²⁵ – 10⁻²⁸

N. Jacquinet-Husson, E. Arié, J. Ballard,
A. Barbe, G. Bjoraker, B. Bonnet, L. R. Brown,
C. Camy-Peyret, J. P. Champion, A. Chédin,
A. Chursin, C. Clerbaux, G. Duxbury, J. -M. Flaud,
N. Fourrié, A. Fayt, G. Graner, et al,
The 1997 spectroscopic GEISA databank.
Journal of Quantitative Spectroscopy and
Radiation Transfer, 1999, v. 62, Issue 2, p. 205-254

183 data sources
(including
HITRAN 2004,
HITRAN 2008)

~ 4000 lines
WN – 0.4012 -19000
Intensity 10⁻²⁰ – 10⁻³²

Total number of data sources ~ 250

T_{decomposition} ~ 10 min



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The End