



Automated knowledge processing. Applied ontologies of the information sources on water and carbon dioxide molecules

Alexey I. Privezentsev, Alexander Z. Fazliev
*Institute of Atmospheric Optics SB RAS,
Akademicheskoy av.1, Tomsk 634055, Russia*



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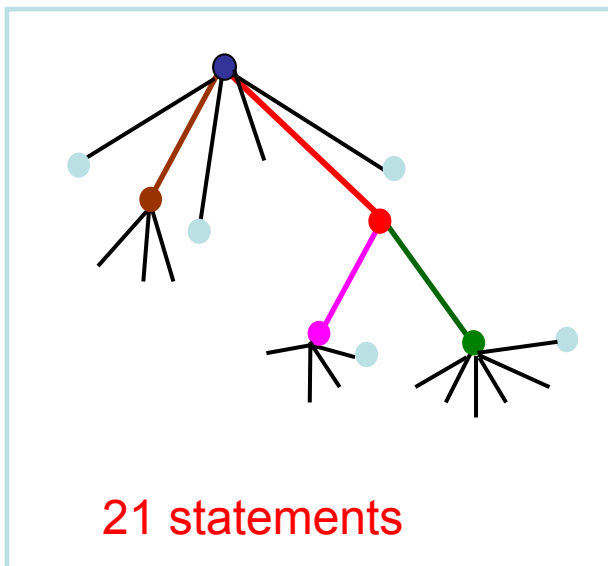


There are a lot of statements on the properties of published molecular spectroscopy problems' solutions containing the terms that characterize physical quantities. They may be either published or follow from the statements contained in publications. These statements and terms form a part of molecular spectroscopy.

Problem Definition

Create an open computable logic theory that contains most of the statements of the validity of published spectroscopic problems' solutions and based on the terms used in molecular spectroscopy dialect of natural language.

Term «information source 2006_BaTeHaTo_c_H2O»



V3_T1_102_2006_BaTeHaTo_c_H2O

hasMethod **DVR3D**
hasSubstance **H2O**
hasInputData_MD **V3_T1_102_T1-InputData_MD**
isSolutionOf **T1**
hasOutputData_MD **V3_T1_102_T1-OutputData_MD**
date 2009-03-25 18:18:00
publisher faz
comment Quantum numbers - BT2
label 2006_BaTeHaTo_c_H2O
hasReference **R.J.Barber, J. Tennyson, G.J. Harris, R.N. Tolchenov, A High Accuracy Computed Water Line List - BT2. // Mon. Not. R. Astron. Soc., 2006, v. 368, p. 1087-1094**

V3_T1_102_T1-InputData_MD

hasAtomicMass 10.1111/j.1365-2966.2006.10184.x
hasBasicWaveFunction 10.1111/j.1365-2966.2006.10184.x
hasPotentialEnergyFunction 10.1111/j.1365-2966.2006.10184.x

V3_T1_102_T1-OutputData_MD

hasQuantumNumber_MD **V3_T1_102_QuantumNumbers_MD_for_BT2**
hasEnergyLevel_MD **V3_T1_102_EnergyLevel_MD**

V3_T1_102_EnergyLevels_MD

hasUnit **cm-1**
hasNumberOfEnergyLevels 221097
hasMinEnergyLevel 0
hasMaxEnergyLevel 29999.840396

V3_T1_102_QuantumNumbers_MD_for_BT2

hasQuantumNumberType **BT2**
hasNumberOfNonuniqueQuantumNumbers 0
hasNumberOfUnlabeledQuantumNumbers 0
hasNumberOfUniqueQuantumNumbers 221091
hasTotalMaxAngularMomentum 50
hasTotalMinAngularMomentum 0

Term «information source V3_T5_279_1998_ToBr_H2_170-H2O»

V3_T5_279_1998_ToBr_H2_170-H2O

isSolutionOf T5
hasMethod UNDEFINED
hasSubstance H2_170
hasOutputData_MD V3_T5_279-T5_OutputData_MD
hasReference **Toth R.A., Brown L.R., Self-broadened widths and frequency shifts of water vapor lines between 590 and 2400 cm⁻¹. // Journal of Quantitative Spectroscopy and Radiation Transfer, 1998, v.59, p.529-562.**

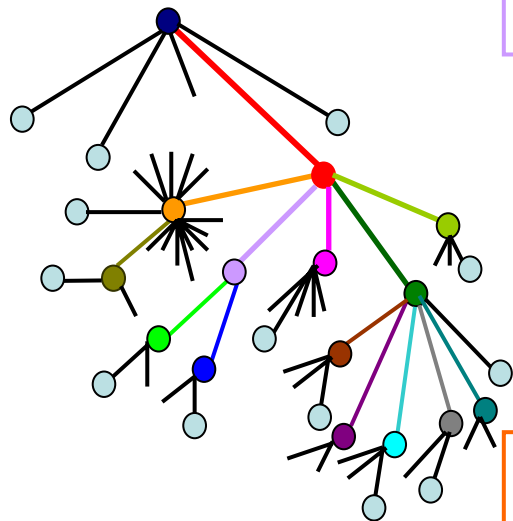
V3_T5_279-T5_OutputData_MD

hasBroadeningSubstance_MD
V3_T5_279_BroadeningSubstances_MD_for_H2O
hasWavenumbers_MD V3_T5_279_Wavenumbers_MD
hasTransitions_MD
V3_T5_279_Transitions_MD_for_NormalModes
hasPhysicalCondition_MD
V3_T5_279_PhysicalCondition_MD
hasIntensity_MD V3_T5_279_Intensity_MD

V3_T5_279_BroadeningSubstances_MD_for_H2O

hasBroadeningSubstance H2O
hasHalfwidth_MD V3_T5_279_Halfwidth_MD_for_H2O
hasPressure_MD
V3_T5_279_PressureValue_MD_for_H2O
hasPressureDependence_MD
V3_T5_279_PressureDependence_MD_for_H2O
hasShift_MD V3_T5_279_Shift_MD_for_H2O
hasTemperatureDependence_MD
V3_T5_279_TemperatureDependence_MD_for_H2O

Term structure



V3_T5_279_PhysicalCondition_MD
hasTemperature_MD
V3_T5_279_TemperatureValue_MD
hasPressure_MD
V3_T5_279_PressureValue_MD

V3_T5_279_PressureValue_MD
hasUnit atm
hasFloatValue 1

V3_T5_279_TemperatureValue_MD
hasUnit K
hasFloatValue 296

V3_T5_279_Intensity_MD
hasUnit cm-1_molecule
hasUncertainty false
isPresented false

V3_T5_279_Wavenumbers_MD
hasUnit cm-1
hasUncertainty false
hasMaxWavenumber 2010.911865
hasMinWavenumber 1315.606567
hasNumberOfWavenumbers 142

V3_T5_279_Halfwidth_MD_for_H2O
hasUnit cm-1_atm-1
hasUncertainty true
isPresented true

V3_T5_279_PressureValue_MD_for_H2O
hasUnit atm
hasFloatValue 1

V3_T5_279_PressureDependence_MD_for_H2O
hasUncertainty false
isPresented false

V3_T5_279_Shift_MD_for_H2O
hasUnit cm-1_atm-1
hasUncertainty true
isPresented true

V3_T5_279_TemperatureDependence_MD_for_H2O
hasUncertainty false
isPresented false

V3_T5_279_Transitions_MD_for_NormalModes
hasSpectralBand
V3_T5_279_for_NormalModes_v1UP_v2UP_v3UP_v1LOW_v2LOW_v3LOW_SpectralBand
hasQuantumNumbersType **NomalModes**
hasTotalMaxAngularMomentum 12 hasTotalMinAngularMomentum 0
hasNumberOfInvalidTransitions 0 hasNumberOfValidWater-C2V-Transitions 142
hasNumberOfRejectedTransitions 0 hasNumberOfUnassignedTransitions 0
hasNumberOfValidTransitions 142 hasNumberOfUniqueTransitions 142
hasNumberOfValidIdentifications 142 hasNumberOfInvalidWaterTransitions 0
hasNumberOfInvalidWater-C2V-Transitions 0 hasNumberOfInvalidIdentifications 0
hasNumberOfNonuniqueTransitions 0

V3_T5_279_for_NormalModes_v1UP_v2UP_v3UP_v1LOW_v2LOW_v3LOW_SpectralBand
hasBandType
v1UP_v2UP_v3UP_v1LOW_v2LOW_v3LOW
hasNumberOfSpectralBands 1

59 statements



Canonical information source for the solution of energy levels of water molecule determination problem

Def. (Natural language)

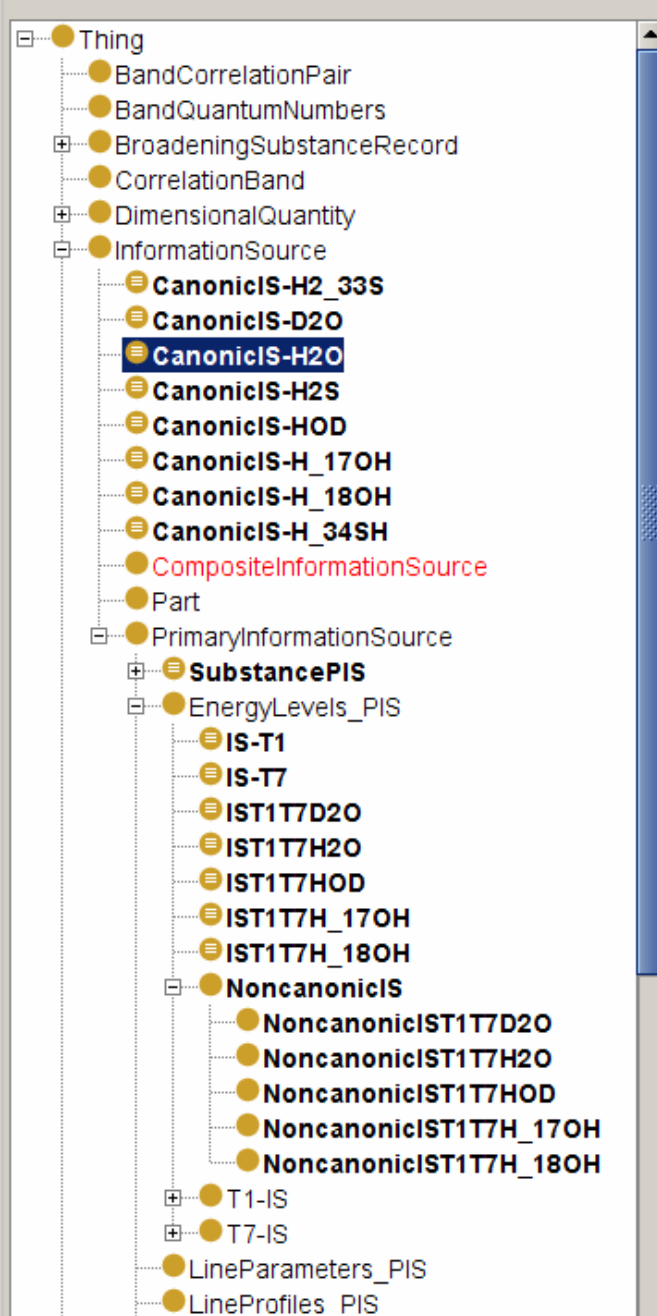
Information source is a canonical information source on determination of the energy levels of an isolated water molecule if and only if one has no errors in quantum numbers and contains only the published data.

Def. (OWL DL language)

InformationSource and
hasOutputData_MD some ((hasQuantumNumbers_MD some (hasQuantumNumbersType value NormalModes and hasNumberOfInvalidComparedWithBT2QuantumNumbers some {"0"^^integer}) and hasQuantumNumbers_MD some (hasQuantumNumbersType value BT2)) or (hasQuantumNumbers_MD some ((hasQuantumNumbersType value BT2 and hasNumberOfInvalidQuantumNumbers some {"0"^^integer}) or (hasQuantumNumbersType value NormalModes and hasNumberOfInvalidQuantumNumbers some {"0"^^integer}))))))
and hasSubstance value H2O



Logical Inference



Description: CanonicIS-H2O

- Members +
- ◆ V3_T1_150_2007_ZoOvShPo_H2_16O
 - ◆ V3_T1_209_2007_ZoOvShPo_H2_16Opara
 - ◆ V3_T1_210_2007_ZoOvShPo_H2_16Oortho
 - ◆ V3_T7_120_2001_ByNaSiVo_H2O
 - ◆ V3_T7_121_1977_CaFIMaGu_H2O
 - ◆ V3_T7_122_1989_ChMaFICa_H2O
 - ◆ V3_T7_123_2005_CoBeCaCo_H2O
 - ◆ V3_T7_124_2005_DuGeZoTo_H2O
 - ◆ V3_T7_126_1997_FICaByNa_H2O
 - ◆ V3_T7_127_2005_KaMaNACa_H2O
 - ◆ V3_T7_129_2004_MaRoMiNa_H2O
 - ◆ V3_T7_131_1988_MaChFICa_H2O
 - ◆ V3_T7_132_2002_MiTyStWi_H2O
 - ◆ V3_T7_133_2003_NaCa_H2O
 - ◆ V3_T7_134_2001_NaUbLePo_H2O
 - ◆ V3_T7_135_2002_ScCaLeBr_H2O
 - ◆ V3_T7_136_1998_Schwenke_H2O
 - ◆ V3_T7_139_2005_ToTe_H2O
 - ◆ V3_T7_141_1994>Toth_b_H2O
 - ◆ V3_T7_142_1999>Toth_H2O
 - ◆ V3_T7_155_2002_TeBeZoSh_H2O
 - ◆ V3_T7_159_1997_Lanquetin_H2O
 - ◆ V3_T7_174_2001_TeZoWiPo_H2O
 - ◆ V3_T7_260_2004>Toth_H2O
 - ◆ V3_T7_268_1993>Toth_H2O
 - ◆ V3_T7_288_2006_MaNaKaBy_H2O
 - ◆ V3_T7_289_2007_MiLeKaCa_H2O
 - ◆ V3_T7_319_1998>Toth_H2O
 - ◆ V3_T7_367_1997_FICaByNa_H2O
 - ◆ V3_T7_87_2005_ToNaZoSh_H2O

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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)



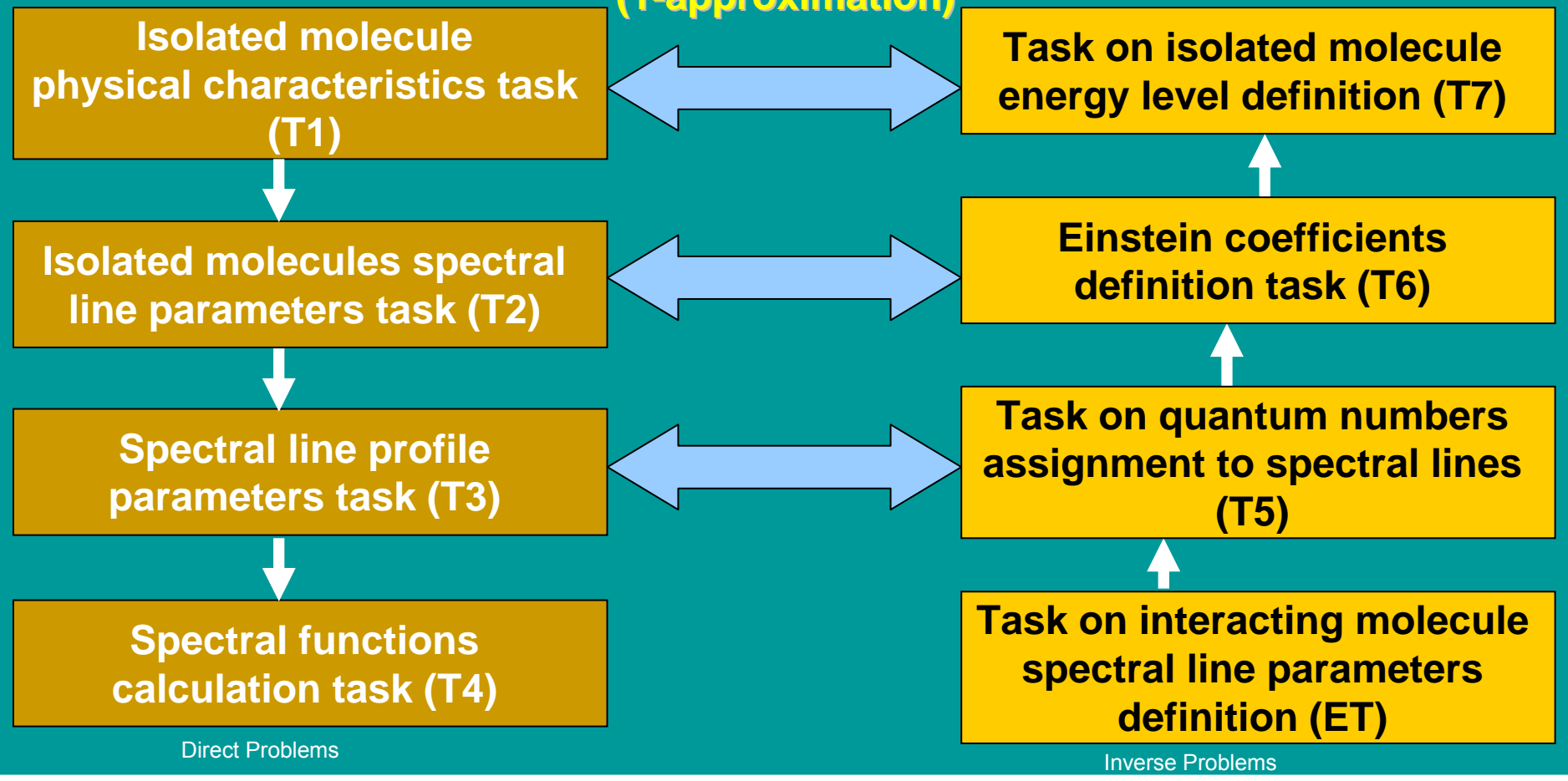
Task on interacting molecule
spectral line parameters
definition (ET)



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



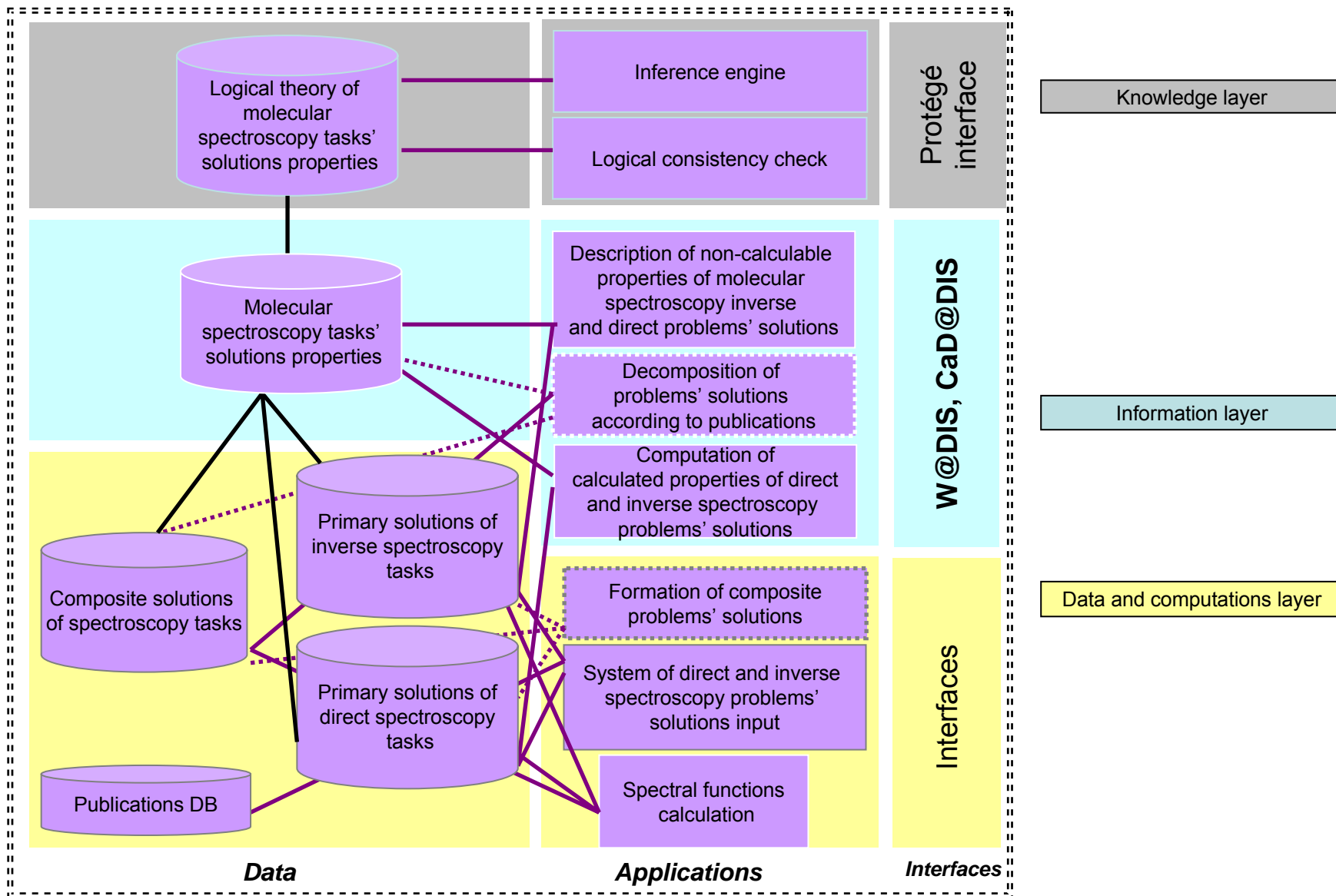
Details about the numbers of triads in the logical theory

Task	Information sources (H ₂ O)	Information sources (CO ₂)	Statements or triads (A-box)	Statements on Correlation (A-box)	Statements (T- and R-Box)
T1	26	0	1082	110740	
T7	156	0	5568		
T2	30	23	2937	467205	
T6	351	6	16033		
T3	27	7	2510	280742	
T5	254	1	19537		
Total	844	37	47667	858 687	1943
Total	881		908 297		



Information System for Atmospheric Molecular Spectroscopy

Semantic Web approach





Summary

- ▶ A full set of original experimental and calculation data on water molecules has been gathered in **W@DIS**. All data sources have detailed description of their properties.
Number of elementary data sources ~ 850
- ▶ A knowledgebase of water molecule information sources has been created. There are about 900 000 statements in the one. Basis of logical theory of solution properties is formed.
- ▶ IS **W@DIS** – <http://wadis.saga.iao.ru>,
<http://atmos.appl.sci-nnov.ru>
- ▶ IS **CaD@DIS** – <http://wadis.saga.iao.ru>,
<http://http://saga.molsp.phys.spbu.ru/>