

# Atomic and Molecular Standardisation

**Interop Trieste 2008**

**ML Dubernet**

# Historical

- **Turning Besançon Observatory on-line facilities into the VO - Galactic Model Simulation, Binary Star, Molecular Collisional and TNO data bases."** B. Debray, M.L. Dubernet, A. Grosjean, E. Oblak, J.M. Petit, C. Reylé, A. Robin, Proceedings ADASS XII, 2002, Baltimore.
- "ACI/ANR Masse de Données en Astrophysique" (F. Génova – 2003-2006)
- Forum in Meudon (Use Cases), 2004, M.L. Dubernet
- Definition of general structuration of data and UCDs, 2004, ML Dubernet & E Roueff
- **Start of Collaboration with ESAC, 2004 (Pune Interop) on LINE**
- **Start of Collaboration NIST/IAEA/ORNL, 2004 (ICAMDATA, Nagoya) on GENERAL MODEL**
- Implementation of SLAP on fundamental and observed DBB from 2006 (N. Moreau, Y. Ralchenko, P. Osuna at ESAC, Astrogrid with CHIANTI)

# At. & Mol. Line DM in IVOA

- ❑ **Line: isolated, intrinsic physical properties**
- ❑ **Measured, calculated, evaluated**
  - **Theoretical At. & Mol. Physics**
- ❑ **From Observed Spectra**
  - **Modeling of the Observed Media**
    - **Link to Spectrum DM**
    - **Link to Micro-Simulations (methods to extract lines)**
    - **Context related**
- ❑ **Some provision for Line Modification**
  - **But No proper Modelisation**

# Different Draft Versions

**AMLDM version 0.5: incomplete, never fully implemented – but discussed by all parties in collaboration ESAC/Paris**

ML Dubernet, P. Osuna, M. Guainazzi, J. Salgado, E. Roueff

**AMLDM version 0.6: has been completed for**

physics, errors, quality, link to target for observations  
differentiate observed, measured, calculated,  
evaluated, semi-empirical data

origin of data

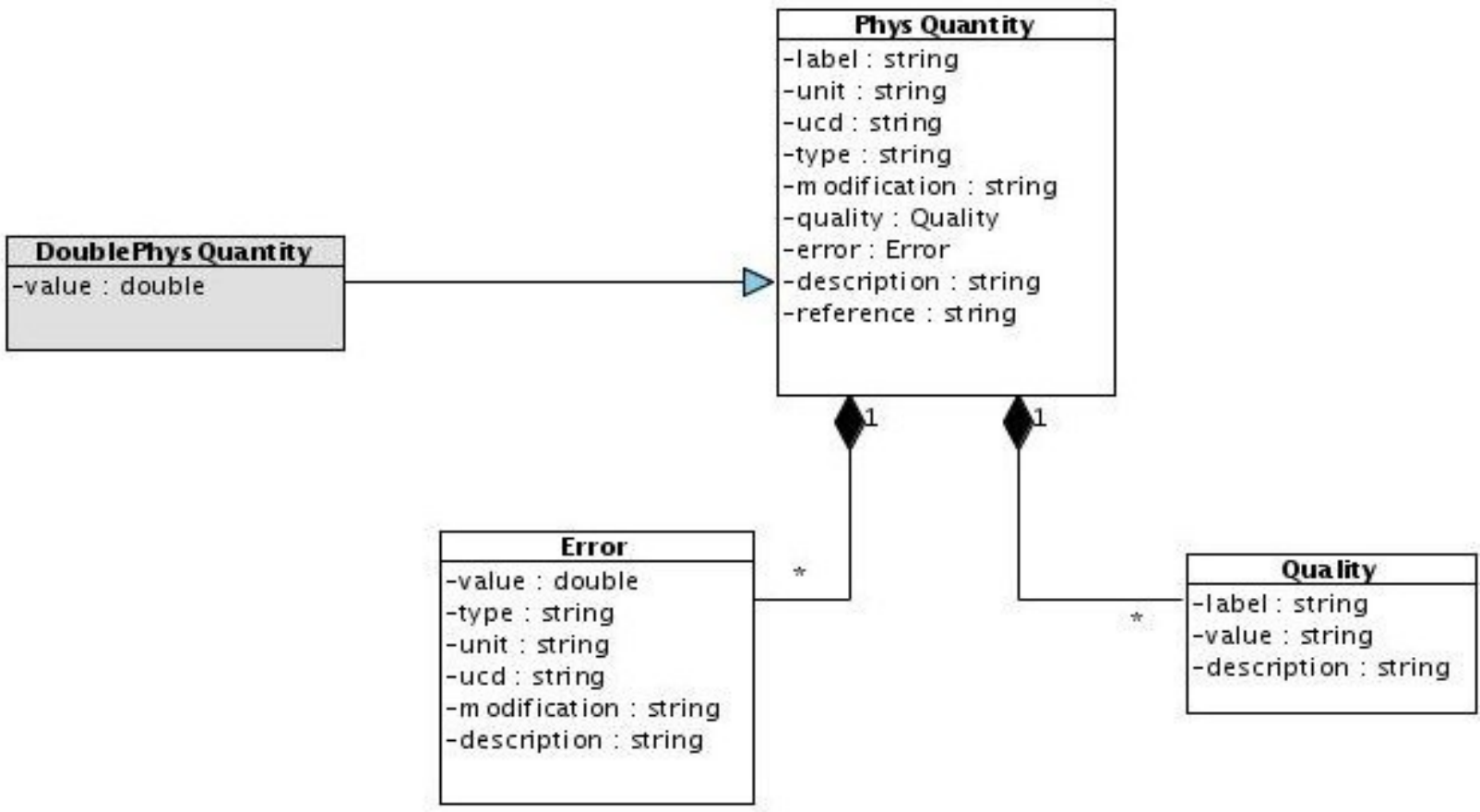
---> introduction of PhysQuantity

---> link to Spectrum DM

--> link to Curation, DataID

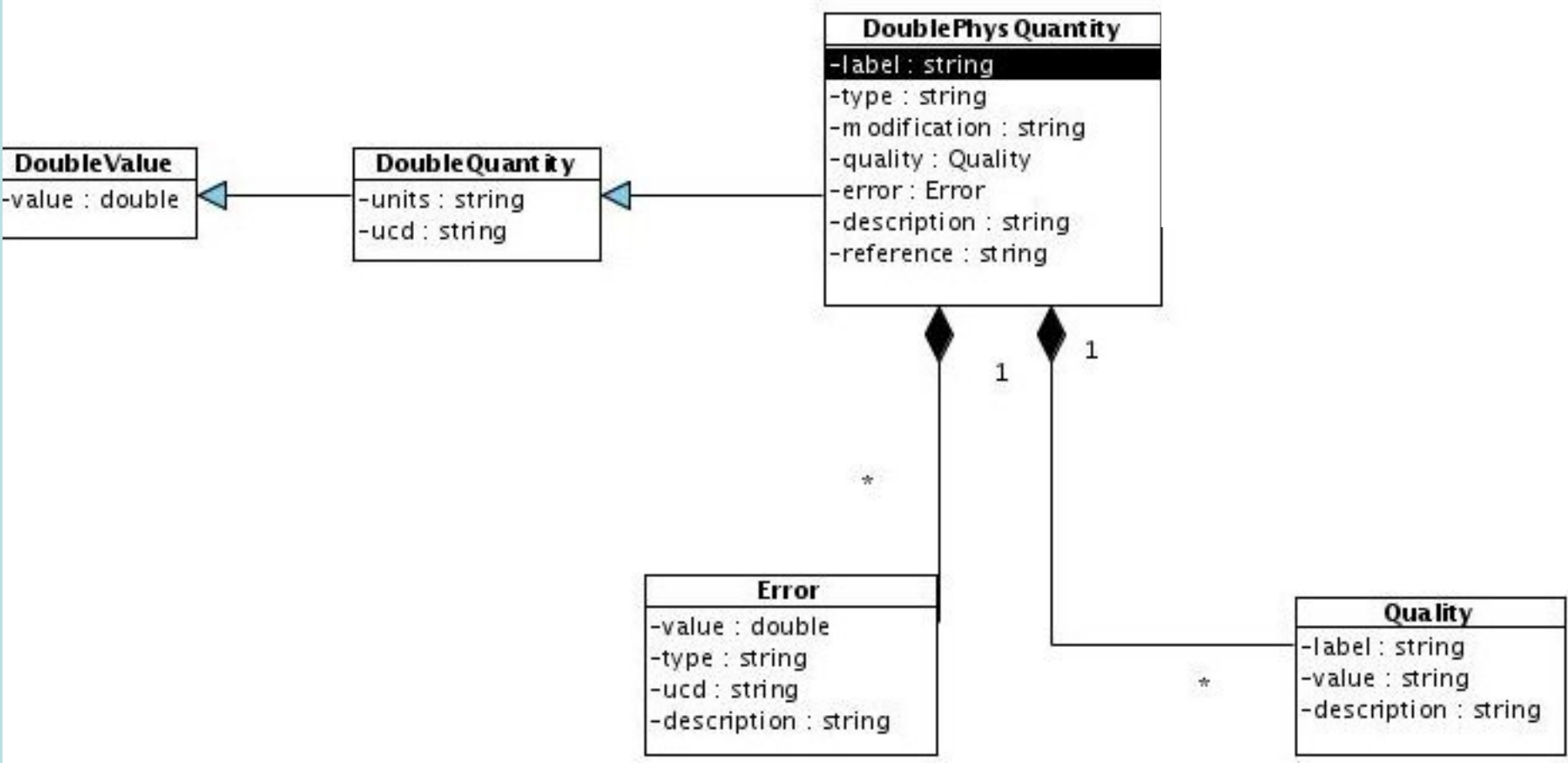
DM version 0.6 suggested by Paris team, but not yet commented among teams

# PhysQuantity version 1



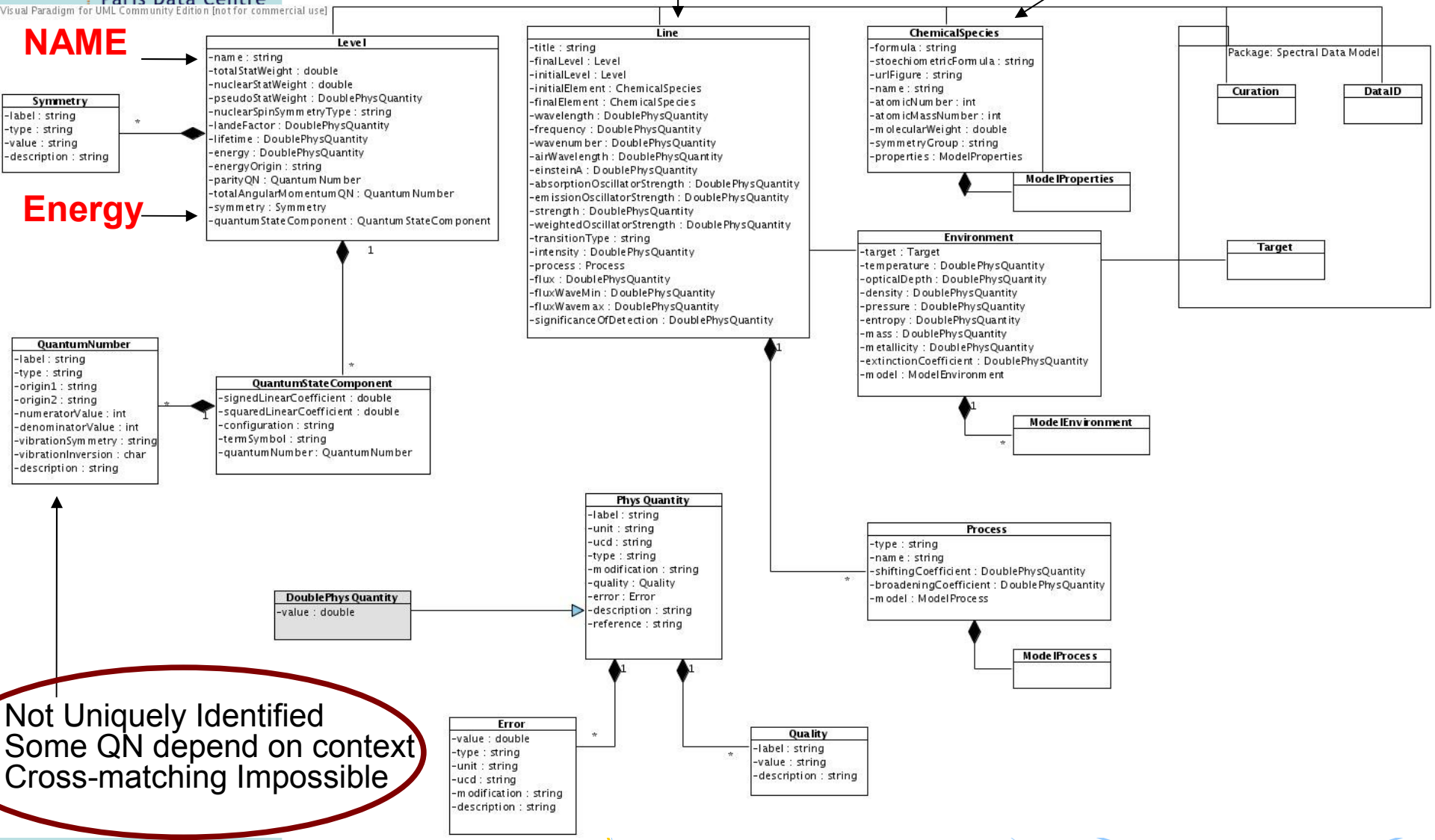
**Type: calculated, measured, semi-empirical, extrapolated**

# PhysQuantity version 2



# TITLE, WL, Einstein\_A

# NAME



Not Uniquely Identified  
 Some QN depend on context  
 Cross-matching Impossible

# Our Test Implementations

**Implementation of SLAP 0.6 on  
CDMS, H2 data of Molat, Spectro of  
BASECOL by N. Moreau (Paris)**

**Use of FORMAT = METADATA**

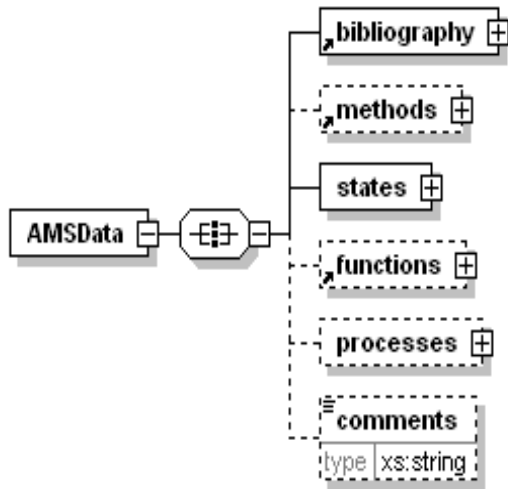
**Return VOTable with more parameters  
than required/recommended by SLAP  
0.6 (AMLDM version 0.6)**

**see <http://voparis-molecular.obspm.fr>**



# General Description of At. & Mol. Processes

**xSAMS: Schema for Atomic, Molecules and Solids**  
**NIST/ORNL/IAEA/Paris Observatory**



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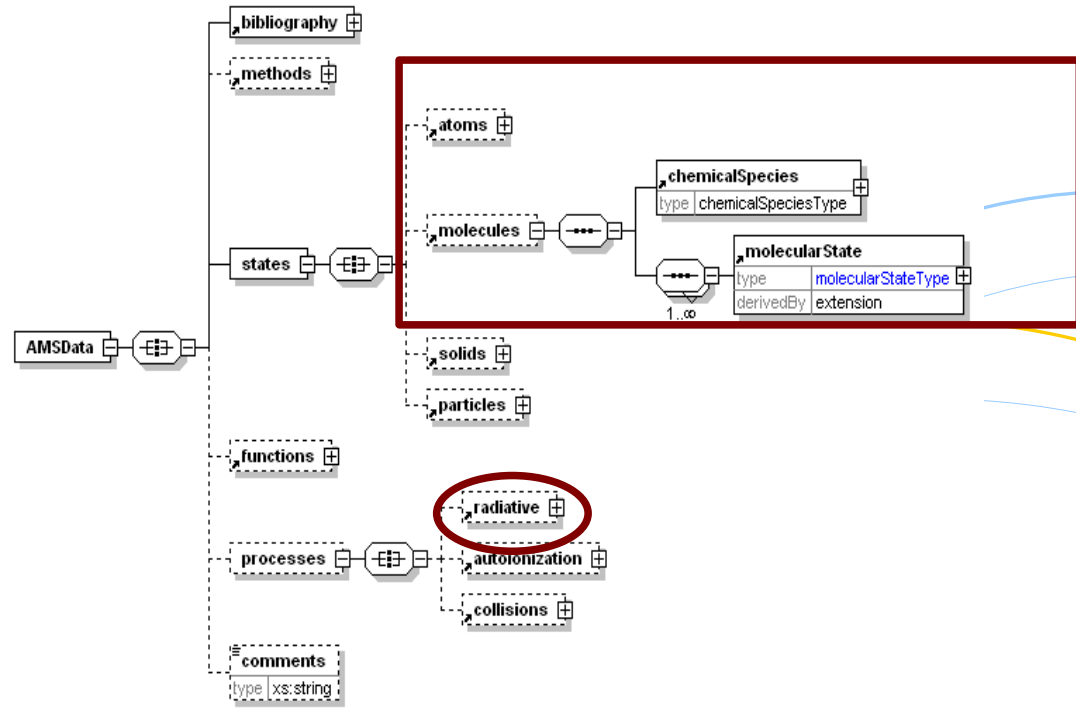
[www.altova.com](http://www.altova.com)

## Bi-annual Technical Interop Meetings

Vienna, Paris  
Observatory,  
Washington

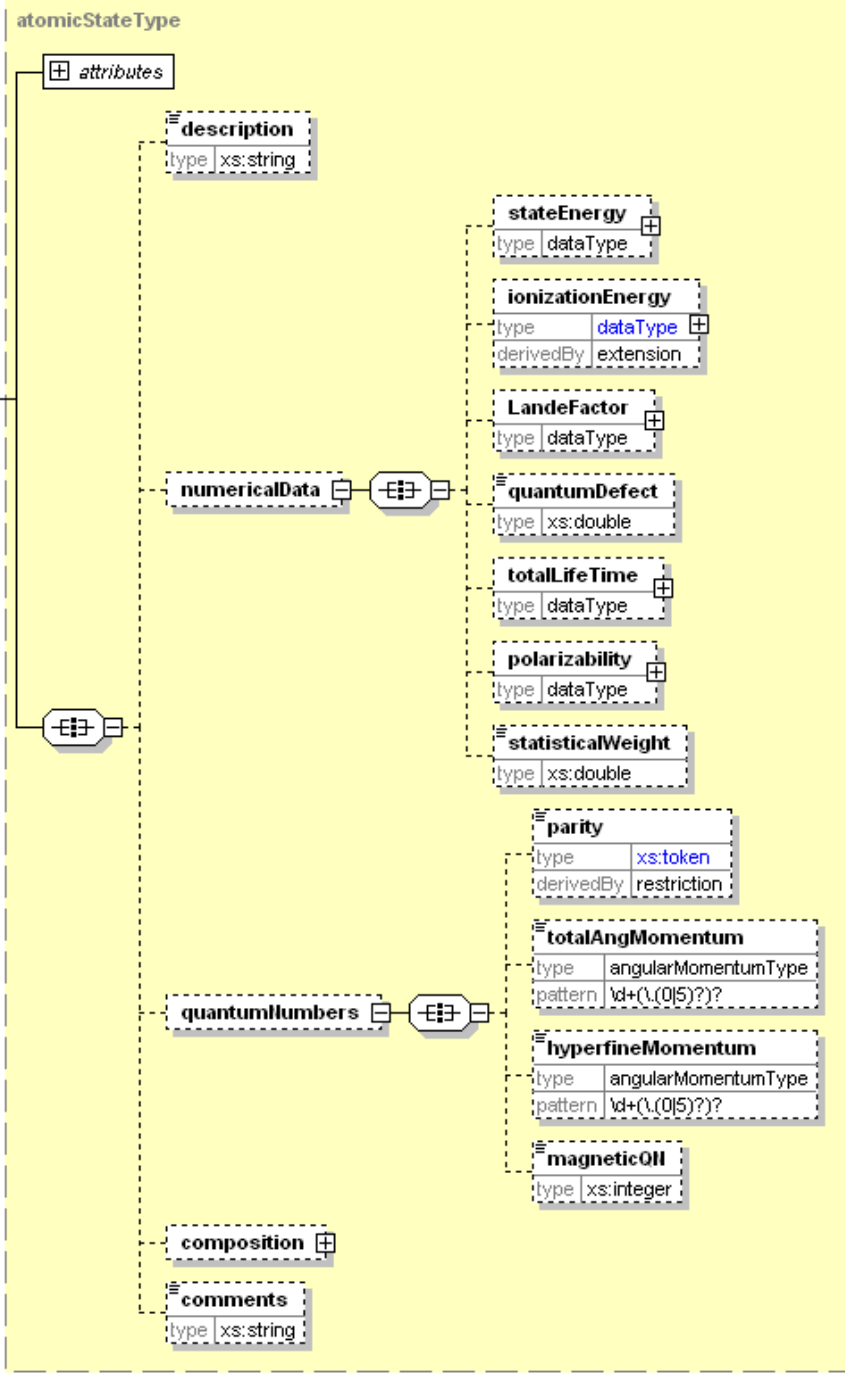
## Presentations at International Conference of Atomic and Molecular Data in 2004, 2006, 2008

- **Interest from NIFS (Japan), Kaeri (Korea), Russian Federation (VNIITF), Institute of Applied Physics and Computational Mathematics, (Beijing, China), etc ...**

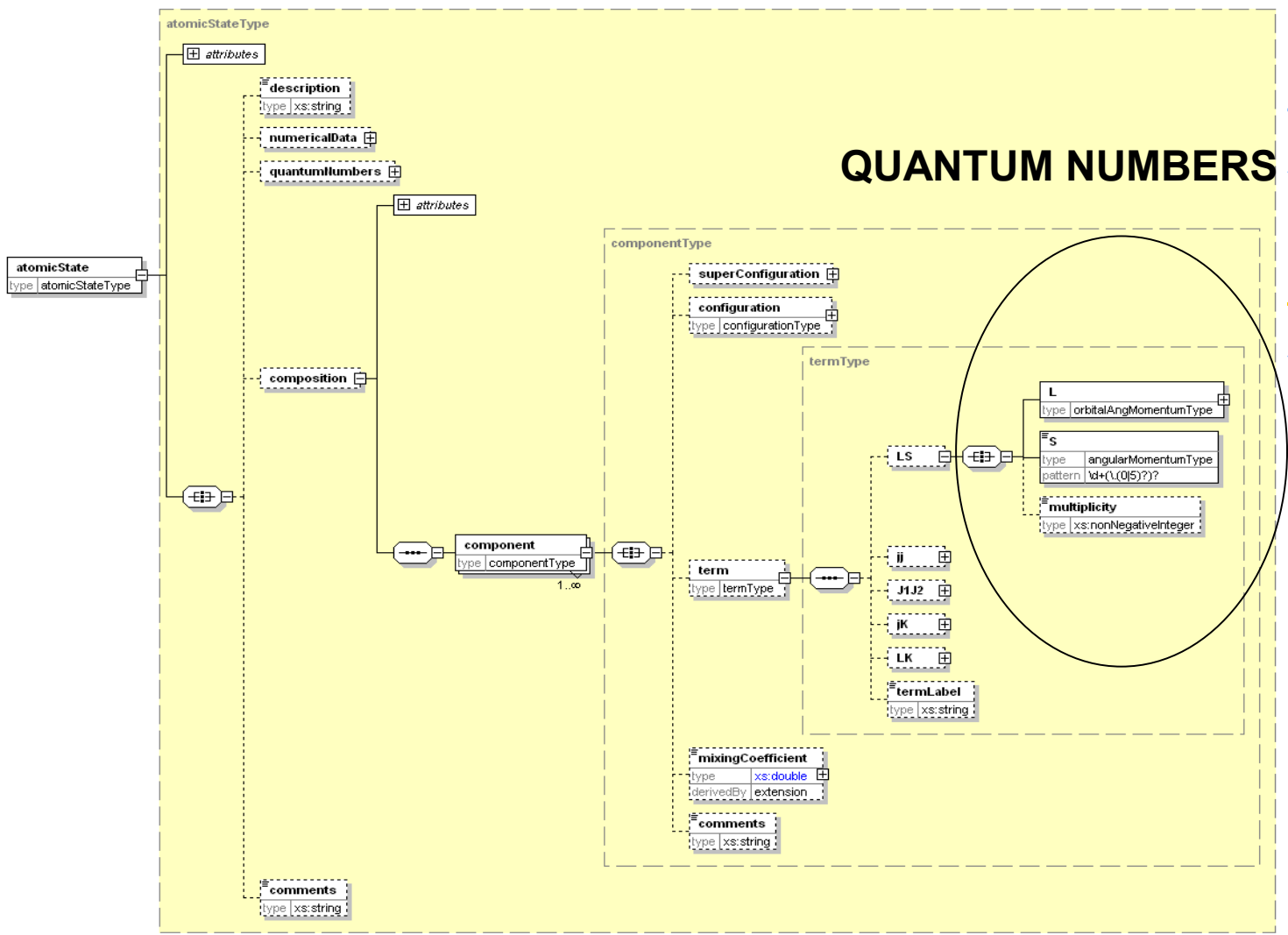


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# QUANTUM NUMBERS



MolecularState  
Quantities

ElectronicHome  
Quantities  
ElectronicQN

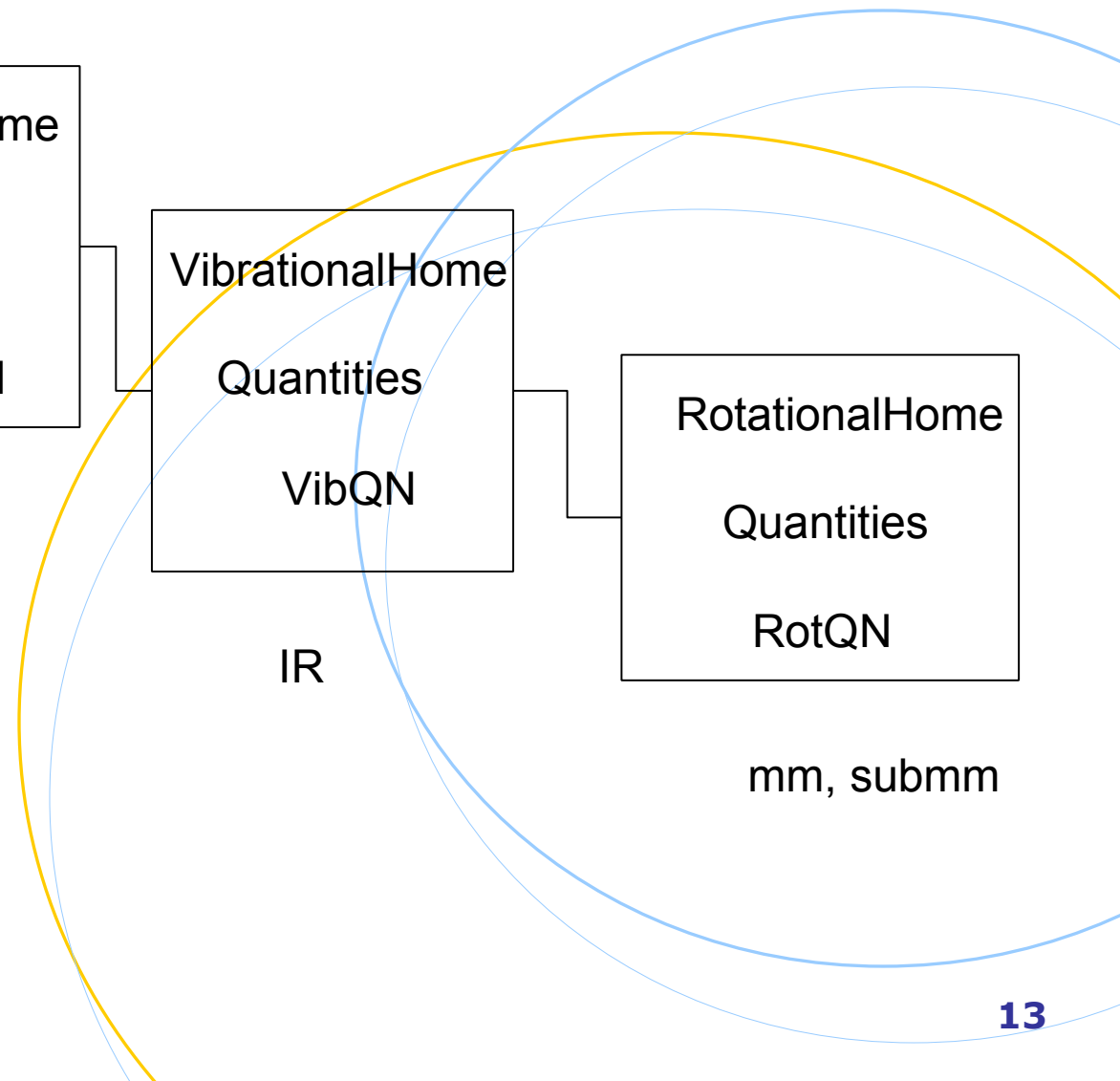
UV

VibrationalHome  
Quantities  
VibQN

IR

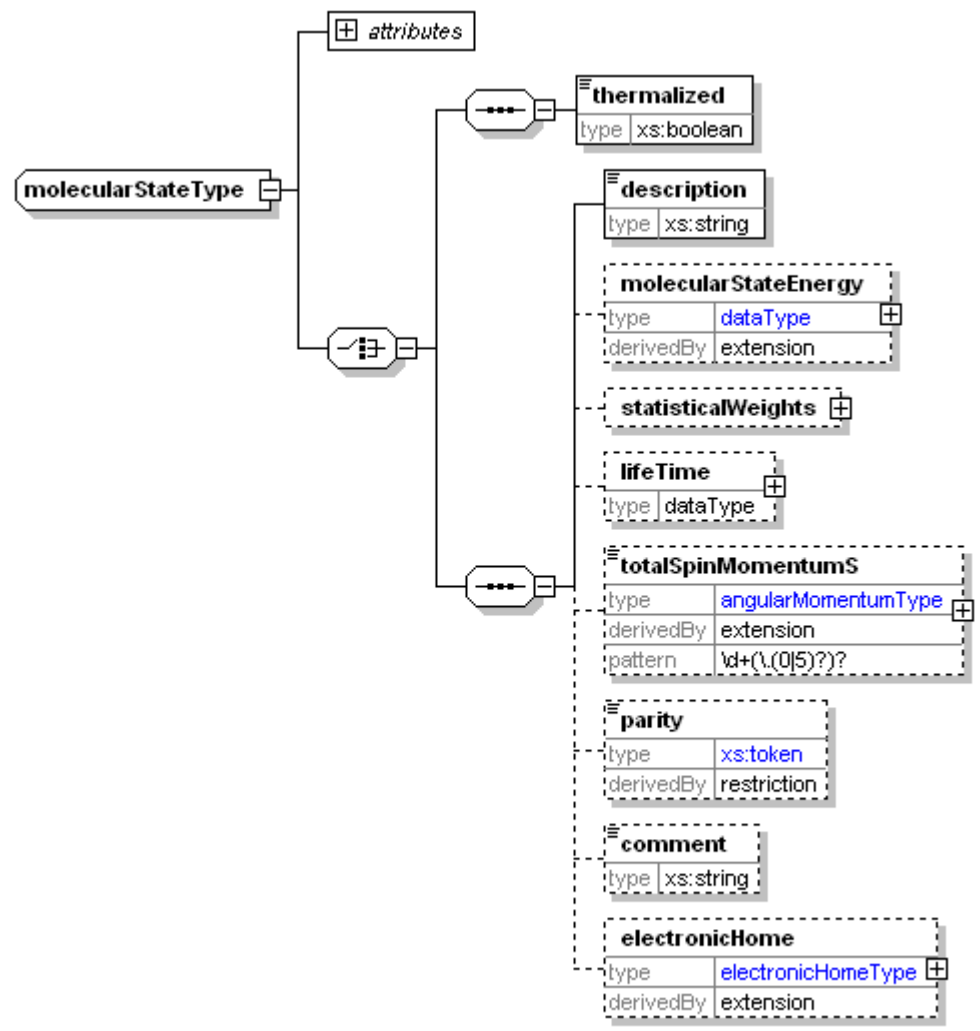
RotationalHome  
Quantities  
RotQN

mm, submm



# MolecularState

## Quantities



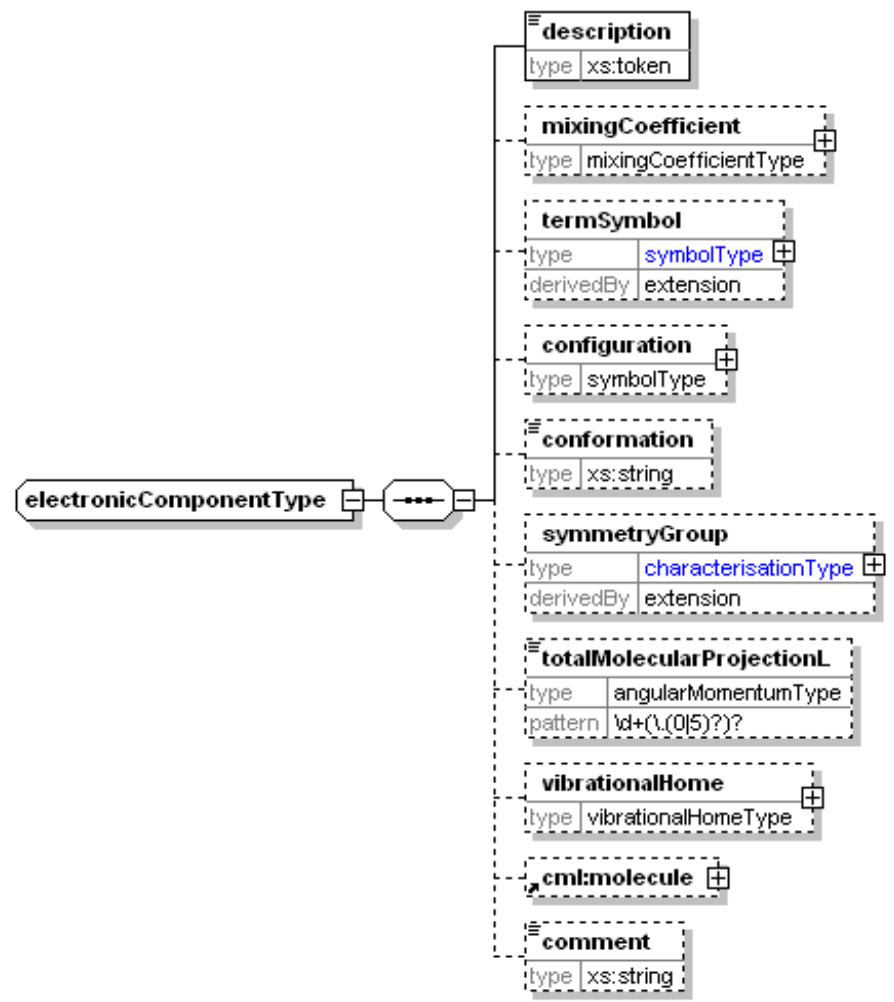
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**MolecularState**  
**Quantities**

**ElectronicHome**  
**Quantities**  
**ElectronicQN**

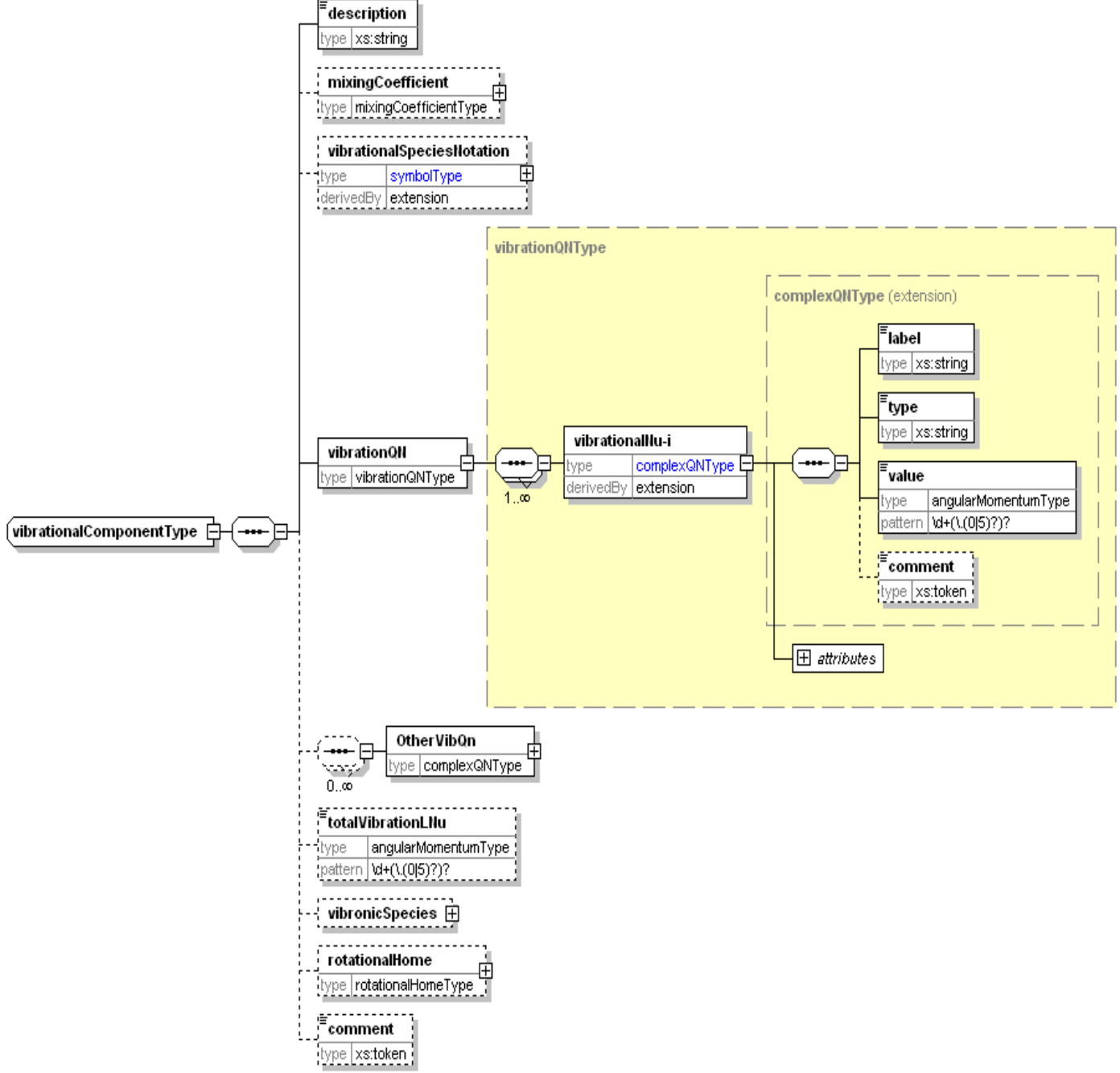
UV



Generated by XmlSpy

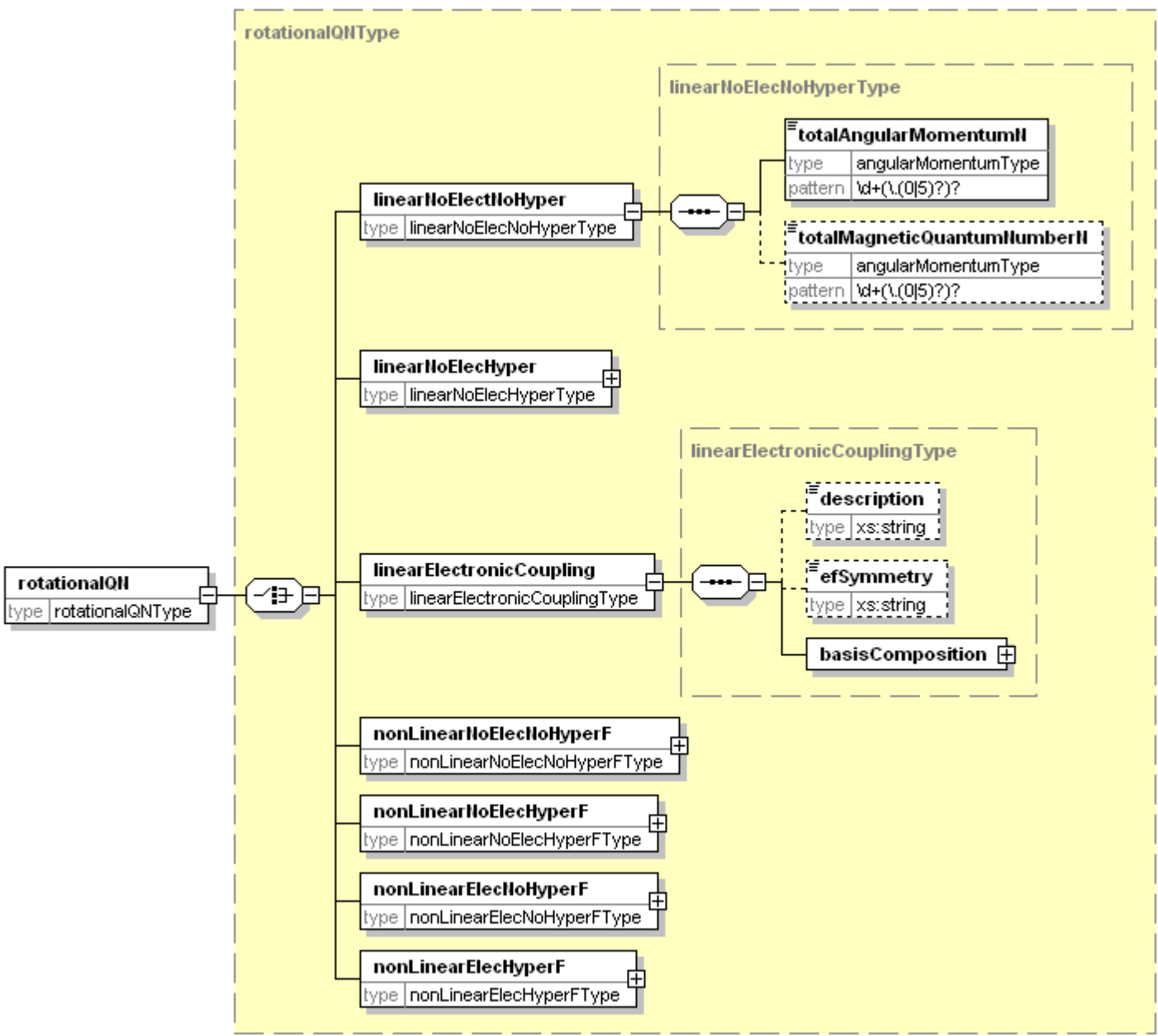
[www.altova.com](http://www.altova.com)

**VibrationalHome**  
**Quantities**  
**VibQN**





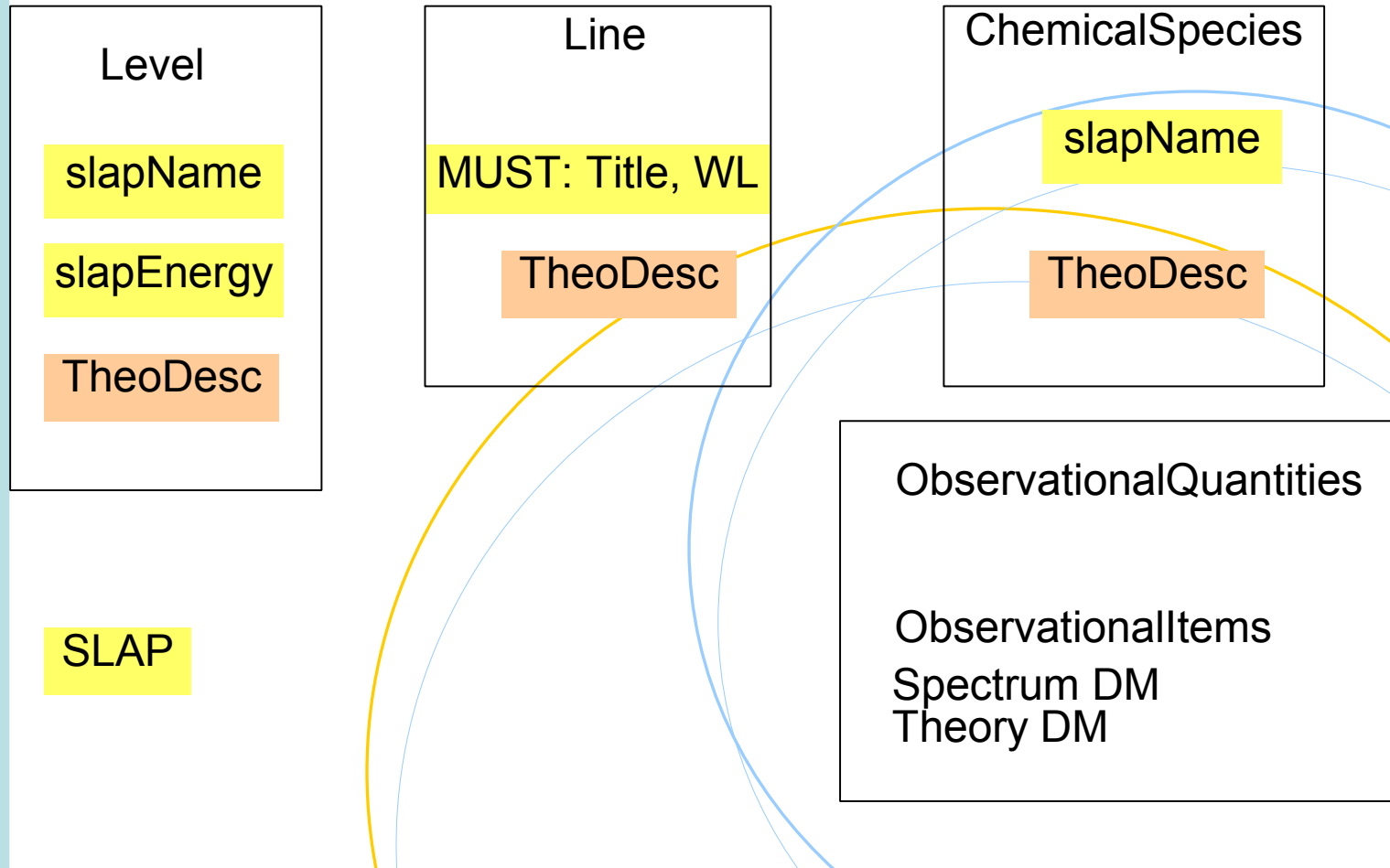
RotationalHome  
 Quantities  
 RotQN



# Suggestion to get to PR

- ❑ **Separate Objects related to Observations from those related to Theory**
- ❑ **Agree on minimal common interface in relation with SLAP requirements**  
MUST, SHOULD, MAY
- ❑ **Description of ChemicalSpecies and Level, non observational Line attributes from the Model designed and maintained by the physicists community**
- ❑ **AML DM points to observational quantities designed and maintained by another group.**

# Suggestion For Evolution



# Next Deadlines

- ❑ **StatesMolecules stable at 15/06/08**
- ❑ **Implementations of xSAMS on NIST (atom spectroscopy), ALADDIN (atoms & molecules reactions) already existing**
- ❑ **Implementation of xSAMS on ALADDIN (solids), CDMS (molecular spectro.) for end of July -**
- ❑ **Next technical Meeting on xSAMS: End of August**
- ❑ **Release of xSAMS Version 1.0: September (no lineModification)**
- ❑ **Presentation at ICAMDATA & Interop: same week in October**

# From 2009

- ❑ **DM of line Modification from the point of view of theoretical/experimental physicists**
- ❑ **Query Language/General Access Protocol**
- ❑ **DM of Line in Astrophysical Medium**
  - > to be done by another team
  - > is related to every specific modelisation: should be related to micro-simulations