IUPAC Database of Water Transitions
from Experiment and Theory:

\[ \text{H}_2^{16}\text{O}, \text{H}_2^{18}\text{O}, \text{H}_2^{17}\text{O}, \text{HD}^{16}\text{O}, \text{HD}^{18}\text{O}, \text{HD}^{17}\text{O}, \text{D}_2^{16}\text{O}, \text{D}_2^{18}\text{O}, \text{and D}_2^{17}\text{O} \]


**A** MTA-ELTE Research Group on Complex Chemical Systems, H-1518 Budapest, 112. P.O. Box 32, Hungary

**Introduction**

Full characterization of the spectrum of water vapor from the microwave to the near ultraviolet is a prerequisite for the modeling and understanding of many fields in chemistry, physics, and engineering.

- **Atmospheric modeling and climate change**
- **Remote-sensing and communication-related fields using the Earth's atmosphere**
- **Astrophysics**, such as the atmospheres of most cool stars and brown dwarfs, where hot water is a major constituent
- **Water lasers and masers** (widespread in outer space)

- **Characteristics of selected sources, some with a large number of transitions, considered for \( \text{H}_2^{16}\text{O} \)**

**Tag** | Range | Transitions | Physical conditions
--- | --- | --- | ---
\( \text{O}_2\text{MuToMaEn} \) & 0.105 & 130/130 & 300-900/0-186 LDFS, HDPS, UV-Vis, RT, hot
\( \text{I}_2\text{UVjPdMas} \) & 10.649 & 1510/1540 & RT, hot, EES-FTS
\( \text{O}_4\text{UVjPdL} \) & 58.475 & 1708/1708 & 1550 1 EES-FTS
\( \text{O}_5\text{SjHjG} \) & 54.200 & 1140/1140 & 3000 EES-FTS
\( \text{D}_2\text{SjHjPd} \) & 72.475 & 1704/1721 & 3000 EES-FTS
\( \text{D}_2\text{SjHjPd} \) & 425.425 & 2810/2510 & 3000 EES-FTS

**References**


**Conclusions**

Our plans for the near future include:

- **Active maintenance of the IUPAC information system**
- **Extension to intensities**
- **Use of MARVEL energy levels, and the associated protocols, to provide new semianalytic assignment techniques**

**Acknowledgements**

We thank IUPAC for funding under project 2004/05-1-100 (A database of water transitions from experiment and theory). This work also received support from a large number of local and international sources, including BC, COST, FFRR, INTAS, NASA, EOS, NATO, NERC, NIKT, OTKA, QUASAAR, and RFBR.

**Dictionary**

- **Characteristics of selected sources, some with a large number of transitions, considered for \( \text{H}_2^{16}\text{O} \)**
- **Selected vibrational band origins (VBO)**

**Vibrational Band Origins**

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<th><strong>VBO</strong></th>
<th><strong>J = 0</strong></th>
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**Data Sources**

Only results from published spectroscopic measurements that include details of the experimental procedure were considered. Secondary data, such as tabulated energy levels or Hamiltonian fits, were not considered except occasionally for checking purposes.

**Vibrational Band Origins (VBO)**

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