

Very accurate non-adiabatic calculations of the rovibrational levels of LiH isotopologues

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Synopsis Non-adiabatic calculations of rovibrational states are reported for the four stable isotopologues of lithium hydride. Our results are the most accurate ab initio predictions reported so far and present a dramatic improvement over previous calculations of ^7LiH isotopologue. Complete linelists of the others isotopologues are in progress.

Non-adiabatic calculations of rovibrational states are reported for the four stable isotopologues of lithium hydride, ^7LiH , ^7LiD , ^6LiH and ^6LiD . The best presently available potential curve and the most accurate dipole moment curve [1] was used to calculate the transition energies and the Einstein coefficients for the rovibrational transitions of these isotopologues. Non-adiabatic corrections to these properties were computed by means of a coordinate-dependent mass which is obtained from a multi-structure valence bond calculation [2]. For ^7LiH

transition energies, our results are the most accurate ab initio predictions reported so far (accuracy $\approx 0.2\text{ cm}^{-1}$). Not yet reported in the literature, complete linelists of the others isotopologues of lithium hydride are in progress.

References

- [1] Leonardo G. Diniz et al., J. Mol. Spect. 322, 22-28 (2016).
- [2] Leonardo G. Diniz et al., Chem. Phys. Lett. 633, 89 (2015).

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