Contribution ID: **170** Type: **Poster**

High-Resolution Spectroscopy of He2 and He2+ for testing ab initio calculations and metrology

Tuesday 22 October 2019 18:10 (1 minute)

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Measurements of the level energies of few-electron atoms and molecules provide reference data to test the results of quantum chemical calculations. In recent years, molecular spectroscopy has reached the level of precision at which such measurements can play a role in the context of fundamental tests of the standard model of particle physics and extensions thereof [1] and provide an alternative route to determine the values of fundamental constants. For example, the new SI definition of the Kelvin is based on the Boltzmann constant, directly linking temperature to energy [2]. The numerical value of the Boltzmann constant is determined, among other methods, by dielectric-constant gas thermometry. Such measurements [3] rely on accurate ab initio calculations of the dynamic polarizability of atomic helium [4]. The high accuracy demanded by the metrological application requires the determination of nonadiabatic, relativistic and QED corrections with reliable error control in the theory.

We have performed systematic studies [5,6] of the rovibrational structure of He2+ using MQDT-assisted Rydberg-series extrapolation in cold molecular beams of He2 in its metastable a 3Σu+ electronic state (He2*). Our measurements provide benchmark data that enable to test the polarizability calculations of atomic helium via the two-body interaction potential. In addition, our measurements revealed a discrepancy with the most recent ab initio calculations of He2+ that are available in literature [7]. This discrepancy can partially be attributed to the neglect of nonadiabatic contributions in these calculations [8].

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Session Classification: BBQ - Drinks & Posters