UNDERSTANDING INNER-SHELL EXCITATIONS IN MOLECULES THROUGH SPECTROSCOPY OF THE 4f HOLE STATES OF YbF

STEFAN POPA, *Centre for Cold Matter, Imperial College London, London, United Kingdom*; SASCHA SCHALLER, ANDRE FIELICKE, *Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*; JONGSEOK LIM, *Centre for Cold Matter, Imperial College London, London, United Kingdom*; BORIS SARTAKOV, *Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*; MICHAEL TARBUTT, *Centre for Cold Matter, Imperial College London, London, United Kingdom*; GERARD MEIJER, *Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*.

Molecules containing a lanthanide atom have sets of electronic states arising from excitation of an inner-shell electron. These states have received little attention, but are thought to play an important role in laser cooling of such molecules and may be a useful resource for testing fundamental physics. We present a rotationally resolved study of a series of inner-shell excited states in YbF using resonance-enhanced multi-photon ionisation spectroscopy. We investigate the excited states of lowest energy, 8474, 9013 and 9090 cm^{-1} above the ground state, all corresponding to the configuration $4\mathrm{f}^{13}6\mathrm{s}^2\ ^2F_{7/2}$ of the Yb^+ ion. They are metastable, since they have no electric dipole allowed transitions to the ground state. We also characterize a state at 31050 cm^{-1} that is easily excited from both the ground and metastable states, which makes it especially useful for this spectroscopic study. Finally, we study two states at 48720 cm^{-1} and 48729 cm^{-1}, which are above the ionization limit and feature strong auto-ionizing resonances that prove useful for efficient detection of the molecules and for identifying the rotational quantum number of each line in the spectrum. We find that the rotational structure of all of these states can be described by a simple model based on Hund's case (c). Our study provides information necessary for laser slowing and magneto-optical trapping of YbF, which is an important species for testing fundamental physics. The metastable states may themselves be important for this application. They are long-lived states in a laser-coolable molecule featuring closely-spaced levels of opposite parity, all of which are desirable properties for tests of fundamental physics.