Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Potential energy and dipole moment surfaces of H_3^- molecule[1]
OLIVIER DULIEU, MEHDI AYOUZ, ROMAIN GUÉROUT, JACQUES ROBERT, Laboratoire Aimé Cotton, CNRS, Université de Paris Sud, Orsay, France, VIATCHESLAV KOKOOULINE[2], Department of Physics, University of Central Florida, Orlando, Florida 32816 — A new potential energy surface for the electronic ground state of the simplest triatomic anion H_3^- is determined for a large number of geometries. Its accuracy is improved at both short and large distances compared to previous studies. The permanent dipole moment surface of this state is also computed for the first time. Nine vibrational levels of H_3^- and fourteen levels of D_3^- are obtained, bound by at most $\sim 70\text{cm}^{-1}$ and $\sim 126\text{cm}^{-1}$ respectively. These results should guide the spectroscopic search of the H_3^- ion in cold gases (below 100K) of molecular hydrogen in the presence of H^- ions.

[1]Supported by Triangle de la Physique contract QCCM.
[2]Laboratoire Aimé Cotton, CNRS, Université de Paris Sud, Orsay, France

Olivier Dulieu
Laboratoire Aimé Cotton, CNRS, Université de Paris Sud, Orsay, France

Date submitted: 22 Jan 2010 Electronic form version 1.4