Ab Initio Studies of the Collisions Involving Lanthanide Atoms and Ions

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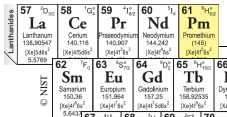
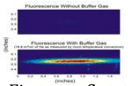


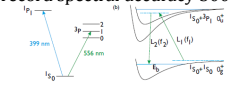
It turns out that the bare lanthanide atoms and ions has got rapid promotion their bottom obscure period to the forefront of cold atomic and molecular physics research

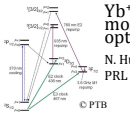


C. J. Hancox *et al.* Nature **431**, 281 (2004).

First non-S state atoms ever trapped in magnetic trap

Yb: BEC of three bosonic isotopes: record spectral accuracy 500 Hz





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Yb$^+$ ion: most precise optical clock

N. Huntemann *et al.* PRL 116, 063001 (2016)

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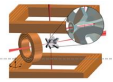
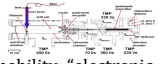
La$^-$ & Lu$^-$: first and only candidates to trapped anions

Ion-atomic collisions in a hybrid trap: single Yb$^+$ in Rb BEC



C. Zipkes *et al.* Nature **464**, 388 (2010).

M. Laatiaoui *et al.* EPJD **66** 232 (2012).



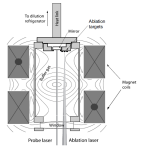
Ion mobility: "electronic state chromatography" revisited

Theoretical A&M physics perspectives: Sensitive probe for

Ab initio methods for interaction potentials, spin-orbit couplings, transition moments and non-adiabatic matrix elements: from 10^{-7} to a few cm^{-1} on energy scale

Inelastic scattering (not a single collision, but gains from perfect control of internal states and collision pair states – temperature and magnetic field projections)

Buffer gas cooling and magnetic trapping of the Tm atom

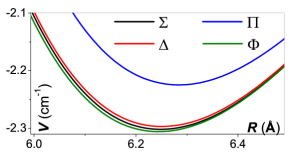


C. J. Hancox *et al.* Nature **431**, 281 (2004).

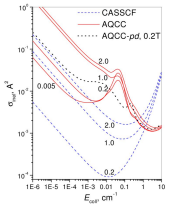
γ - ratio of elastic to *inelastic* collision rates for M + He collisions

Inelastic: transitions between Zeeman sublevels, driven by interaction anisotropy, or splitting between Λ (or Ω) projections of the electronic orbital *L* (or total *J*) angular momentum on the molecular axis

Tm(^{2}F) => Tm-He ($^2\Sigma^+$, $^2\Pi$, $^2\Delta$, $^2\Phi$): *ab initio* SC ECP CASSCF/AQCC



Splitting ~ 0.2 cm^{-1}

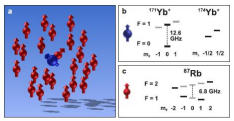


Zeeman relaxation rate, cm^3/s:	
CASSCF	1.0×10^{-15}
AQCC	1.5×10^{-15}
Exptl.	$(5\pm2)\times10^{-15}$

Interaction anisotropy is suppressed for submerged *f* shell

A. A. Buchachenko, M. M. Szczesniak, and G. Chalasinski, J. Chem. Phys. **124**, 114301 (2006); A. A. Buchachenko, G. Chalasinski, M. M. Szczesniak, and R. V. Krems, Phys. Rev. A **74**, 022705 (2006).

Yb$^+$ ion in Rb BEC: spin relaxation

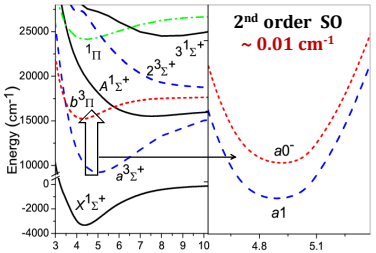


C. Zipkes et al. Nature **464**, 388 (2010).
C. Zipkes et al. PRL **105**, 133201 (2010).

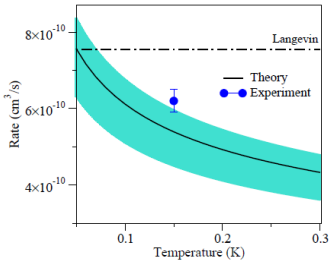
Fully spin-polarized state can be created by immersing a single ion into BEC

Measurements:
- Charge transfer rate (trap "mass spectrometry")
- Collision-induced spin relaxation (temperature and populations)

Ab initio SC ECP CCSD(T), EOM-CCSD(T), MRCI, SI-SOCI



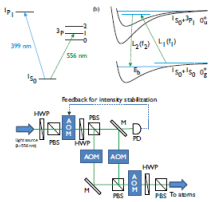
Fully spin-polarized state is immune to relaxation ... except hf and **SO**



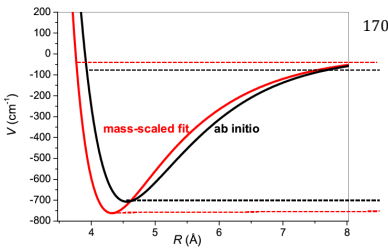
E. R. Sayfutyarova, A. A. Buchachenko, S. A. Yakovleva, and A. K. Belyaev, Phys. Rev. A **87**, 052717 (2013);
T. V. Tscherbul, P. Brumer, and A. A. Buchachenko, Phys. Rev. Lett. **117**, 143201 (2016).

Lanthanide dimers

Yb$_2$ photoassociation in BEC



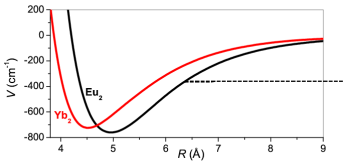
Ab initio SC ECP CCSD(T) + energy differences, MRCI & AQCC



^{170}Yb$_2$ last bound level
-0.000924 cm^{-1}
-0.000923 cm^{-1} (exptl)
-0.05 cm^{-1}

ΔD_e = 40 cm^{-1}

Eu$_2$ in magnetic trap



Heisenberg spin coupling:

$s = 7/2$, $S = 0 - 7$:

$E(S) = -(J/2)[S(S+1) - s(s+1)]$

$J = 0.3$ cm^{-1}

Zeeman relaxation rate, cm^3/s:	
Heisenberg	8.6×10^{-13}
Exptl.	$(2.5\pm1.5)\times10^{-13}$

Y. Suleimanov, PRA 81, 0227011 (2010)

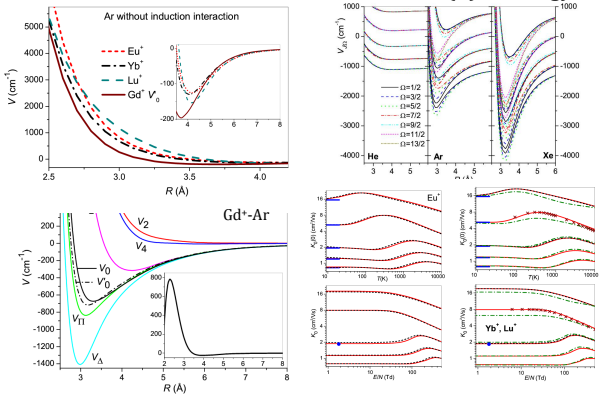
A. A. Buchachenko, G. Chalasinski, and M. M. Szczesniak, Eur. Phys. J. D **45**, 147 (2007); A. A. Buchachenko, G. Chalasinski, and M. M. Szczesniak, J. Chem. Phys. **131**, 241102 (2009);
M. Borkowski, A. A. Buchachenko, R. Ciuryło, P. S. Julienne, H. Yamada, K. Yuu, K. Takahashi, Y. Takasu, and Y. Takahashi, in preparation.

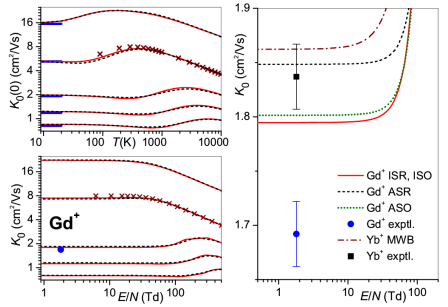
Ion mobility: sensitivity to electronic configuration

Electronic state chromatography [P. R. Kemper& M. T. Bowers, J. Am. Chem. Soc. **112**, 3231 (1990)]

Gd$^+$ ($4f^75d6s$, ^{10}D°), Eu$^+$ ($4f^76s$, ^{9}S°), Yb$^+$ ($4f^{14}6s$, ^{2}S), Lu$^+$ ($4f^{14}6s^2$, ^{1}S°)

Ab initio SC ECP CCSD(T) + energy differences & SO MRCI





A. A. Buchachenko and L. A. Viehland, J. Chem. Phys. **140**, 114309 (2014).

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