Electronic structure and reactivity of astrochemically relevant inorganic hydrides
Nathan J. DeYonker, Marco Fioroni
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High-accuracy electronic structure of FeH
- Controversial identity of ground electronic state
- Line lists used in dwarf star/gas-giant population ratios, extrasolar planetary atmospheres and cores
- Single reference theories vs. multireference theories?

“Chemical accuracy” for $T_e$ of all spin components for \( X^4\Delta, a^6\Delta, A^4\Pi, b^6\Pi \)
- Improved Bond Dissociation Energy

POSS H\(_2\) Formation
- High universal abundance of molecular hydrogen is not well-explained
- Do TM defects on siliceous grains (Fe\(^+\)-POSS) catalyze H\(_2\) formation in ISM?

- Barrier-less POSS-H, POSS-H\(_2\) formation
- Agreement between double-hybrid DFT and MP2-F12
- Chemisorption of H to Si or O centers is not thermodynamically favorable

Spectroscopic survey of electronic transitions of C₆H, ¹³C₆H and C₆D
X. Bacalla, E.J. Salumbides, H. Linnartz, W. Ubachs, D. Zhao

Department of Physics and Astronomy, VU University, De Boelelaan, 1081 HV, Amsterdam, The Netherlands
Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, The Netherlands
University of Science and Technology China, Hefei, China

- Measurement of optical absorption spectra
- \( B^2\Pi - X^2\Pi \) system 473 – 527 nm
- Isotopic substitution H/D, 12C/13C
- Renner-Teller analysis of bending modes
- Analysis of rotational structure 19 bands

Details at the poster #2
Poster 3
Inner-shell photo-excitation as probe of the molecular ions CH\(^+\), OH\(^+\), and SiH\(^+\): Measurements and theory

J.-P. Mosnier et al.
School of Physical Sciences and NCPST, Dublin City University, Dublin 9, Ireland

• Photoionization cross-sections were measured for the processes

\[
\text{AH}^+ + h\nu \rightarrow \text{A}^{2+} + \text{H}^+ + e^- \\
\text{A}^+ + h\nu \rightarrow \text{A}^{2+} / \text{A}^{3+} + e^-
\]

K-shells CH\(^+\) (290 eV), OH\(^+\) (550 eV) and L-shell SiH\(^+\) (110 eV)

• Ion-photon merged-beam technique at SOLEIL synchrotron

• Data interpreted by ab initio calculations of the core-excited molecular energy level structures and corresponding dipole transition moments

• Contributions from ground and excited valence electronic states.
Quantum calculations on diatomic hydrides for stellar atmosphere modelling

M. Guitou\textsuperscript{a,*}, A. Mitrushchenkov\textsuperscript{a}, A. Spielfiedel\textsuperscript{b}, N. Feautrier\textsuperscript{b}
S. A. Yakovleva\textsuperscript{c}, A. K. Belyaev\textsuperscript{c}

Mg + H $\rightarrow$ Mg$^+$ + H$^-$

Mg$^+$ + H$^- \rightarrow$ Mg + H

$\rightarrow$ 9 $^2\Sigma^+$; 5 $^2\Pi$; 2 $^2\Delta$;

4 $^4\Sigma^+$; 3 $^4\Pi$, 1 $^4\Delta$ states

$\rightarrow$ Potential energy functions

$\rightarrow$ Radial and rotational couplings

$\rightarrow$ inelastic collisions treatment

Mg-H internuclear distance $R$, (a.u.)
Sensitivity from frequency splittings in the molecular spectra

Florin Lucian Constantin, Laboratoire PhLAM CNRS UMR 8523 Villeneuve d'Ascq France

References

Cosmological variation of the fundamental constants
- Possible spatial and temporal variations of $\mu = m_p/m_e$
- $\alpha$, $g_N$

Sensitivity of a molecular frequency to a variation of $\mu$:
$\frac{df}{d\ln\mu}$

Comparison of astrophysical lines with different sensitivity coefficients
Address here the comparison of frequency intervals in the quasar spectra

Molecular modelisation
- Dunham expansion model of isotopic LiH, CO energy levels
- Calculations of the sensitivities of rotational transitions
- Address here the comparison of frequency intervals in the quasar spectra
- Frequency splittings with sensitivity coefficients at ±10$^{-2}$ level

Constraint on $\Delta \mu/\mu$ from the microwave spectra of B0218+357
Comparison between 14NH$_3$ inversion lines (J,K) = (1,1), (2,2), (3,3) [1] with frequency intervals between rotational lines J=0->1 of 7LiH [2] and respectively J=1->2 of 12C$^{16}$O or 13C$^{16}$O [3].

- Effective radial velocity for a frequency interval
- Constraint based on the unweighted average of $V_{NH_3} - V_{split,eff}$
$\Delta \mu/\mu = (5.06 \pm 3.67) \times 10^{-6}$ at $z=0.68466$ (6.4 Gyr look-back time)

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Formation of cationic hydrides of noble gases in the protosolar nebula

O. Ozgurel, E. Zicler, F. Pauzat, Y. Ellinger, M-C. Bacchus-Montabonel

- Non observation of HeH\(^+\) in ISM
- Deficiency of noble gases (Ar, Kr, Xe) in Titan’s atmosphere

Small HeH\(_n\)^+ clusters as a proper target?

Were the building blocks already poor in noble gases?

\[
\text{H}_3^+ + X \rightarrow \text{XH}_3^+
\]

Stationary points on the XH\(_3\)^+ potential energy surface

The rate constant for the radiative association (X + H\(_3\)^+) as a function of the temperature

Ar
Kr
Xe
Temperature dependence of $\text{H}_2\text{D}^+$ and $\text{HD}_2^+$ recombination with electrons

Overtone spectroscopy of $\text{N}_2\text{H}^+$ (2$\nu_1$ band)

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<th>$\nu_{\text{exp}}$ (cm$^{-1}$)</th>
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Small-scale physical and chemical structure of diffuse molecular clouds along the line of sight of Sgr B2

V. Thiel, A. Belloche, K. M. Menten (MPIfR)

c-$C_3H_2$ in absorption along the line of sight to Sgr B2 as probed with ALMA

continuum map at 85 GHz, black contour: region selected for analysis

c-$C_3H_2$ column density map integrated from 27.0 to 33.9 km s$^{-1}$ (yellow range in spectrum)
Exploring Molecular-Cloud Formation with OH 18 cm Transition

Y. Ebisawa, H. Inokuma, Y. Watanabe (University of Tokyo), N. Sakai (RIKEN) H. Maezawa (Osaka Prefecture University), K. M. Menten (MPIfR), S. Yamamoto (University of Tokyo)

Observed spectra toward HCL2 East

Absorption against CMB

Model

Insensitive to $n$(H$_2$)

Sensitive to $T_k$

fitting

$T_k = 60 \pm 3$ K, $N$(OH) = $(4.4 \pm 0.3) \times 10^{14}$ cm$^{-2}$, o/p of H$_2$ = $3.5 \pm 0.9$

OH 18 cm transition as a thermometer for warm molecular cloud over wide range of H$_2$ density ($10^2$ - $10^6$ cm$^{-3}$)
The circum-nuclear regions of obscured AGN combine large molecular columns with intense infrared, ultra-violet, and X radiation and represent ideal laboratories for the study of the chemistry of the interstellar medium under extreme conditions.

- > 300 lines
- 45 molecules
- U-lines

Costagliola et al., 2015 ; Costagliola et al., in prep.
The circum-nuclear regions of obscured AGN combine large molecular columns with intense infrared, ultra-violet, and X radiation and represent ideal laboratories for the study of the chemistry of the interstellar medium under extreme conditions.

ALMA multi-band spectral scan of NGC4418

- > 300 lines
- 45 molecules
- U-lines!

Yes, we got a hydride!

Spatially resolved chemistry in Circinus

- Multi-band, beam matched obs at 40 pc resolution
- Spatially resolved excitation and abundance
Chemistry of Hydroxyl (OH) Radicals in the ISM Molecular Clouds: Gas-phase Reaction with H$_2$CO between 22 and 107 K

CRESU
French acronym for Cinétique de Réaction en Écoulement Supersonique Uniforme or Reaction Kinetics in a Uniform Supersonic Flow
HIFI spectral scan in the Orion Bar

Figure: M. Van der Wiel

Nagy et al. (2016)
Low energy electron induced processes in pure ammonia ice
Leo Albert Sala, Lionel Amiaud, Céline Dablemont, Anne Lafosse

Dust Grain
Ice Mantle
Non-thermal desorption

Control of Ice Morphology
Desorption of $\text{N}_2$, $\text{NH}_2$, and $\text{NH}_3$

Experiment in UHV

1. $\text{NH}_3$ 5ML ($10^{-8}$ torr, 500 s)
2. Optional Annealing 28-84 K

Gold
$T = 28 \text{ K}$

6 eV $e^-$ ($E_i$)

$e^-$ ($E_i$)

HREELS (morphology)

2-12 eV $e^-$ ($E_i$)

ESD Desorbing neutral species ($\text{NH}_2$, $\text{NH}_3$, $\text{N}_2$)
Scaling the Collisional Rate Coefficients of C₆H⁻

Kyle M. Walker
LOMC UMR 6294, CNRS - Universite du Havre, France
Fabien Dumouchel, François Lique, Richard Dawes

- Anions in the ISM: molecular clouds, circumstellar envelopes
- Collisional rate coefficients needed to model non-thermal emission
- C₆H⁻ potential energy surface & scattering calculations
- Use hydride relationship to scale anion rate coefficients

\[
\begin{align*}
\text{HF} & \rightarrow \text{HCl} \\
\text{C}_6\text{H}^- & \rightarrow \text{C}_x\text{H}^-
\end{align*}
\]
Theoretical ab-initio calculations of photoabsorption spectra of \( \text{XH}_2^+ \) (X= C, O, Si) molecular ions: comparison with experimental data

X-Ray spectroscopy provides a powerful tool to study astrophysical and laboratory plasma.

Synchrotron facilities and theoretical/computational approaches are developed to probe the chemical composition of the plasma.

Most results have already been obtained on atomic ions and molecules.

Hydride Molecular ions