Refined line list for the ions of ArH^+, KrH^+ and XeH^+

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Introduction

This poster is based on the BSc project (40 credits, run in pairs) undertaken by Sam and Ben over the course of the 2017 - 2018 academic year at Aberystwyth University.

The first detection of a noble gas molecular ion in space was in 2013, when $^{36}ArH^+$ was found in the Crab Nebula using the Herschel Space Observatory (Barlow et al. 2013).

Since then, both $^{36}ArH^+$ and $^{38}ArH^+$ have been detected in the direction of the lensed Blazar PKS 1830-211 using ALMA observations. As noted by the authors (Müller et al. 2015), future observations of this region using the GREAT (German Receiver for Astronomy at Terahertz Frequencies) receiver on board SOFIA could yield promising results.

Additionally, Argonium could potentially be used as a very specific tracer of atomic gas and as a proxy for the cosmic-ray ionization rate (Bizzocchi et al. 2016).

As far as we are aware, neither KrH^+ or XeH^+ have being detected in space.

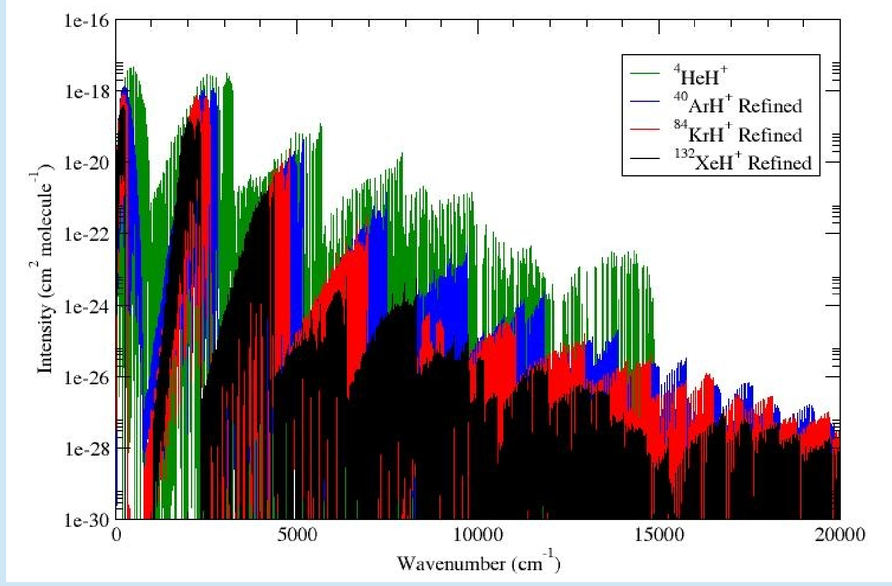


Figure 1: Spectra of various isotopologues simulated at 1500 K using a Gaussian HWHM of 1.0 . Here the existing line list of HeH^+ (Engel, Doss, Harris & Tennyson 2005) has being used.

Method

For each of the ions, *Ab initio* Potential Energy curve (PEC) and Dipole Moment Curve (DMC) calculations were performed for the ground state, $X^1\Sigma^+$. The PEC for each ion was then refined by fitting to experimental data by fitting to an Extended Morse Oscillator curve (EMO) using Duo (Yurchenko et al. 2016).

In this project, an analysis of the available experimental data was done. Experimentally derived diatomic and spectroscopic constants were used to produce energy lists via Dunham expansion and PGOPHER (Western 2016) which were then compared to outputs of MARVEL analysis of experimentally measured wavelengths.

The final experimental sources used to fit the EMO for each ion was as follows:
ArH+: Brault and Davis (1982).
KrH+: Linnartz, Zink and Evenson (1997)
XeH+: Rogers, Brazier and Bernath (1987)

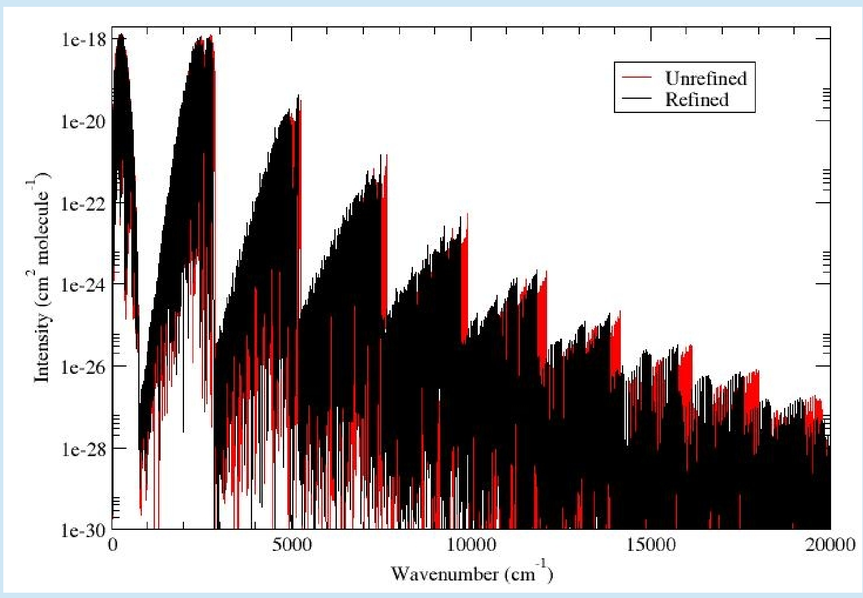


Figure 2: Simulated spectra (1500 K, Gaussian HWHM of 1.0) using the unrefined and refined PECs for the $^{40}ArH^+$ isotopologue.

Table 1: Sample fit for $^{132}XeH^+$

υ	J	Obs. (cm^{-1})	Calc. (cm^{-1})	Obs - Calc (cm^{-1})
1	4	129.2612	129.2605	0.0007
1	3	77.5777	77.5773	0.0004
1	15	1539.6293	1539.629	0.0003
1	2	38.7967	38.7965	0.0002
1	1	12.934	12.9339	0.0001
1	16	1743.0225	1743.0231	-0.0006
2	9	2750.945	2750.9457	-0.0007

Table 2: Sample fit for $^{84}KrH^+$

υ	J	Obs. (cm^{-1})	Calc. (cm^{-1})	Obs - Calc (cm^{-1})
1	18	2777.2785	2777.2788	-0.0003
1	16	2215.9021	2215.9023	-0.0002
1	15	1958.0659	1958.066	-0.0001
1	6	345.7696	345.7695	0.0001
1	9	739.3158	739.3156	0.0002
1	20	3398.5577	3398.5571	0.0006

Results

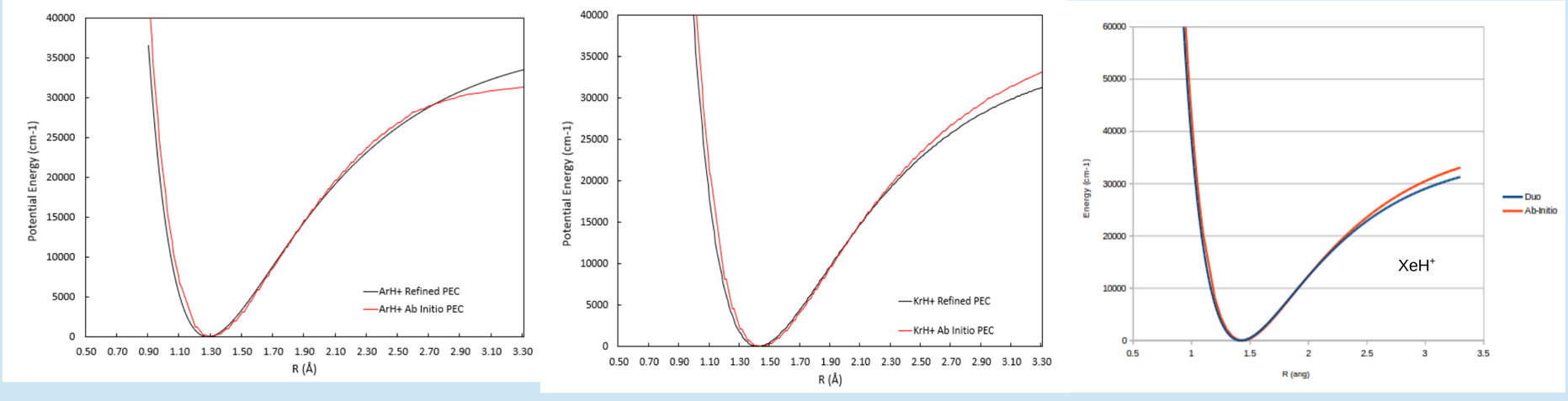
Refined ground state line lists were obtained for all three ions and their main isotopologues namely, $^{36}ArH^+$, $^{38}ArH^+$, $^{40}ArH^+$, $^{84}KrH^+$, $^{129}XeH^+$, $^{131}XeH^+$ and $^{132}XeH^+$.

A sample of the EMO fits obtained for $^{132}XeH^+$ and $^{84}KrH^+$ are presented in tables 1 and 2 respectively. For the ArH^+ isotologues, typical fits were of the order of ~0.6 cm^{-1}.

All line lists contain ~400 states and ~4000 – 7000 transitions covering appropriate vibrational and rotational states up to dissociation.

Future work

Further work will now include adapting the Dipole moment curves to take into account the difference in position between centre of mass and centre of charge for these ions.



Figures 3, 4, 5: *Ab initio* and fitted Potential Energy Curves (PEC) for ArH^+, KrH^+ and XeH^+.

Acknowledgements

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