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Theoretical study of spectroscopic constants and molecular properties of rare gas hydride ions HeH^+, NeH^+, ArH^+, KrH^+, XeH^+ and RnH^+

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Abstract: Theoretical calculations have been performed to investigate spectroscopic constants and various molecular properties of rare gas hydride ions HeH^+, NeH^+, ArH^+, KrH^+, XeH^+ and RnH^+ in their ground $^1\Sigma^+$ state using different basis sets at the QCISD(T)//MP2 level of theory. Some of these systems are potentially important in astrophysics. The calculated values are found in good agreement with the available data. Many data are reported to be first time in literature.

1. Introduction

The rare gas hydride ions (RgH^+) has been found of immense interest because of their significant role in a variety of physical and chemical processes occurring in astrophysics and in the laboratory. The HeH^+ is thought to be the first among the molecules formed in the evolution of early universe. Recent astrophysical detection in interstellar space of this ion by Gusten et al. [1] unambiguously proved to be a path to the formation of molecular hydrogen in the universe. Role of HeH^+ in the ion chemistry of early universe was presented by Bovino et al. [2]. The existence of this ion in low temperature and low density white dwarfs was demonstrated by Harris et al. [3]. Recent investigation by Mousis et al. [4] also suggested that the rare gases could be trapped by H_3^+ ions to form RgH_3^+, which following dissociation reaction (viz. $RgH_3^+ \rightarrow RgH^+ + H_2$; Rg = Ar, Kr, Xe) produce RgH^+, in the protoplanetary disks outside the solar system.

The existence and formation of HeH^+ was studied experimentally using mass-spectroscopic analysis by Hogness and Lunn [5]. Experimental investigation of a number of protonated rare gases was studied from the spectra of discharge emission by Johns [6]. Fourier transform emission spectroscopy of NeH^+ was observed by Ram et al. [7]. Structure and molecular properties of KrH^+ were investigated from infrared spectral analysis by Linnartz et al. [8], Hunter and Lias [9] and Molski [10]. Spectroscopic properties of XeH^+ were investigated using Fourier transform emission spectroscopy by Roger et al. [11] and submilimeter wave spectroscopy by Peterson et al. [12]. To date no experimental investigation is reported in literature for RnH^+.

Early quantum mechanical study for the structure and some properties of HeH^+ were reported by

Beach [13] using MO method, Toh [14] applying James-Coolidge method of expanding wave function and Evett [15] as an extension of this method with the use of more accurate wave function. Among the recent theoretical investigations, ab initio MO study for the various properties of HeH^+, NeH^+, ArH^+ and KrH^+ were studied by Schutte [16] at the MP4(SDQ)//6-311++G(3df,3dp) level along with some experimental values for comparison. Ground state molecular constants using correlated wave function at the self-consistent coupled electron pair approach (SCEP/CEPA) were investigated for NeH^+ and KrH^+ by Rosmus and Reinsch [17], for ArH^+ by Rosmus [18] and for XeH^+ by Klein and Rosmus [19]. All electron and effective core potential studies were done by Lundell et al. [20] for ArH^+, KrH^+ and XeH^+ using Gaussian and modified Gaussian ($+VP^s(2p)^s$) basis sets at the MP2 level. Multireference spin-orbit CI method study for the potential energy and constants have been performed for XeH^+ by Alekseyev et al. [21] using RECP basis set for Xe and aug-cc-pVQZ basis set for H. Another recent calculations have been reported by Ferrante et al. [22] for KrH^+, XeH^+ and RnH^+ at the relativistic CCSD(T) method using contracted triple-zeta basis sets. Most of the theoretical calculations were done so far used a variety of basis sets and methodologies, so a comparison is very critical for any system.

In this article, we shall report optimized geometries, vibrational frequencies, dissociation energies and various molecular properties using several basis sets for the ground $^1\Sigma^+$ state of the rare gas hydride ions HeH^+, NeH^+, ArH^+, KrH^+, XeH^+ and RnH^+. The reported data are found consistent with the available data and many of them are found to be new in literature.

2. Computational methods

We employed three sets of basis function- B1: 6-31++G(3df,3pd), B2: 6-311++G(3df,3pd) and B3: aug-cc-pvTZ for the atoms H, He, Ne, Ar and Kr [23]. For heavier atoms Xe and Rn, we employed the Stuttgart-REL-ECP basis set [23] in all the three sets B1 to B3. The rare gas ions RgH^+ (Rg=He, Ne, Ar, Kr, Xe and Rn) were optimized at the second-order Moller-Plesset perturbation theory (MP2). The vibrational frequencies were calculated at the MP2 level. Different molecular properties, like the dipole moment (μ), force constant (k), rotational constant (B) and Mulliken population charge (q) were obtained from MP2 calculations. Single point energy calculations were performed using quadratic configuration interaction single-double including triples terms QCISD(T) at the MP2 optimized geometries. Dissociation energies to $Rg(^1S) + H^+$ and $Rg^+(^2P) + H(^2S)$ were evaluated using QCISD(T) energy of the composite ions and isolated atom/ions and included the ZPE at the MP2 level. All the calculations described above are performed employing Gaussian 03 program system [24].

3. Results and Discussion

To get an idea, the MP2 potential energy curves only for the ArH^+ system using the three basis sets have been plotted in Figure 1. The curves have a relative deep and harmonic shape, in contrast to flat curve of RgH neutral van der Waals molecule. The other ions follow the similar nature in their potential energy curves, except the energy gap among different basis sets. It is to be worth mentioning at this point that, in case of Rg= He, Ne, Ar and Kr, the dissociation limit ($Rg + H^+$) is the lowest. This is clearly depicted in Figure 2, where the variation of MP2 Mulliken population charge of Rg and H in RgH^+ obtained using B3 basis set at the different internuclear distances are shown. Results of using other basis sets are omitted as they are very close and will overlap in the figure. The ground state of XeH^+ and RnH^+ would dissociate to ($Rg^+ + H$), because this lies well below the total energy value of ($Rg + H^+$). This happens since the ionization potential of Xe and Rn are less than the ionization potential of H. For XeH^+ and RnH^+, the MP2 population analysis at large R are not in accordance with the formation of ($Rg^+ + H$) and it is also checked using natural bond analysis. There may have an avoided crossing at large R with the excited $^1\Sigma^+$ state or intersection between ($Rg^+ + H$) and ($Rg + H^+$) potential energy curves. Such a possibility of intersection has been mentioned by

Ferrante et al. [22] for XeH^+ and RnH^+ ions in the range 2.70-2.80 Å and at the long range by Rogers et al. [11]. Because of this reason, charges are plotted up to 3 Å for XeH^+ and RnH^+ in Figure 2. Methods including spin-orbit effect may reveal the true shape of potential curves at large internuclear distances.

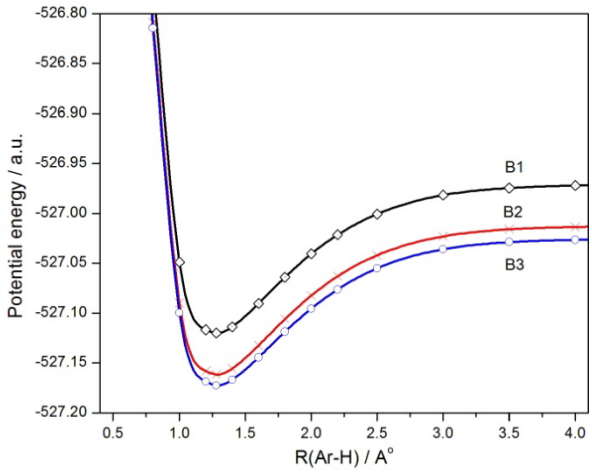

Figure 1: Variation of potential energy with internuclear distance R of ArH^+ ion for different basis sets B1: 6-31++G(3df,3pd); B2: 6-311++G(3df,3pd); B3: Aug-cc-pvTZ.

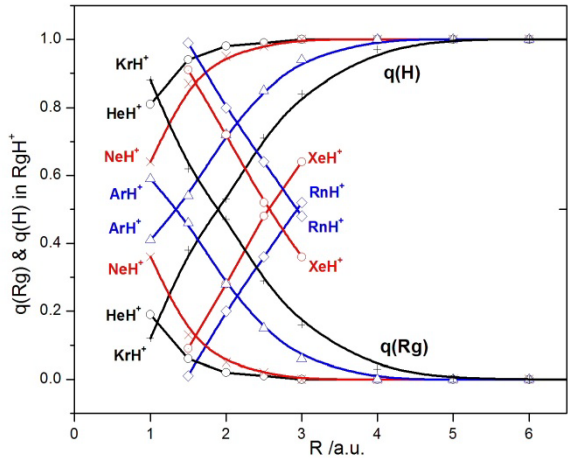

Figure 2: Variation q(Rg) & q(H) with internuclear distance R in RgH^+ ions.

The optimized geometries, vibrational frequencies, dissociation energies and various molecular properties of all the ions are listed in the following tables along with the available data for comparison. From Table 1, for HeH^+, we see that our calculated R_e using B1 and B3 basis sets and $D_e(He + H^+)$ using all the sets are almost same and are in very good agreement with the experimental values quoted in Schutte [16]. No data is available in literature for the dissociation limit $D_e(He^+ + H)$. Other molecular properties reported here are found consistent with the only available data by Schutte [16]. The data obtained by Schutte [16] for most of the systems are found over estimated compared to the available experimental values.

Table 1: Spectroscopic constants and molecular properties of HeH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	0.7742	0.7733	0.7743	0.7743[a]	0.7751[c]
ω_e (cm^{-1})	3220.7	3225.3	3208.7	2911[b]	3218.8[c]
q(Rg) at R_e	0.21	0.29	0.32		0.31[c]
D_e (Rg + H^+) (eV)	1.83	1.84	1.84	1.85[a]	1.90[d]
D_e (Rg^+ + H) (eV)	12.76	12.75	12.77		
Dipole moment (D)	1.2885	1.2909	1.2962		1.2487[c]
Force cons. (mdyne/Å)	7.2504	7.2711	7.1964		7.2420[c]
Rotational cons. (GHz)	1047.37	1049.71	1047.00	1006.42[b]	1044.80[c]
IR intensity (km/mol)	813.09	807.36	808.09		788.24[c]
E(Thermal) (kcal/mol)	6.085	6.092	6.068		6.083[c]
C_V (cal/mol-K)	4.968	4.968	4.968		4.968[c]
S (cal/mol-K)	36.320	36.315	36.320		36.325[c]

[a]Values quoted in Reference [16]; [b]reference [6]; [c]reference [16]; [d]reference [15].

For NeH^+, in Table 2, we see that R_e and ω_e using B2 basis sets are in good agreement with the experimental values. Results obtained using basis set B3 for other quantities are almost close to those obtained using basis set B2. Our calculated $D_e(Ne + H^+)$ is found to be better than the available theoretical value. The other's calculated value for the force constant is too much overestimated.

Table 2: Spectroscopic constants and molecular properties of NeH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	0.9864	0.9890	0.9951	0.9912[a]	0.996[d]
ω_e (cm^{-1})	2935.2	2908.5	2916.2	2903.8[a]	2896[d]
q(Rg) at R_e	0.29	0.37	0.37		0.40[e]
D_e (Rg + H^+) (eV)	2.18	2.16	2.14	2.08[b]	2.45[e]
D_e (Rg^+ + H) (eV)	10.04	10.03	10.00		
Dipole moment (D)	2.7799	2.7972	2.8151		2.6197[e]
Force cons. (mdyne/Å)	5.3604	5.2630	5.2907		12.6998[e]
Rotational cons. (GHz)	541.36	531.52	531.93	536.03[c]	531.23[d]
IR intensity (km/mol)	837.25	841.29	852.14		1001.06[e]
E(Thermal) (kcal/mol)	5.677	5.639	5.650		7.940[e]
C_V (cal/mol-K)	4.968	4.968	4.968		4.968[e]
S (cal/mol-K)	41.903	41.913	41.937		42.334[e]

[a]References [7]; [b]Values quoted in reference [16]; [c]reference [6]; [d]reference [17]; [e]reference [16].

For ArH^+, in Table 3, it is clear that our results obtained using B3 for R_e and ω_e are in good agreement with the available experimental values. Very good agreement is obtained for $D_e(Ar + H^+)$ of 4.00 eV in comparison to the experimental value of 4.02 eV. The values for the $D_e(Ar^+ + H)$ limit truncated to second place are found same using three basis sets. It is to be mentioned that the tabulated values in this article of Lundell et al. [20] are those obtained using MP2/LANL1DZ.

Table 3: Spectroscopic constants and molecular properties of ArH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	1.2849	1.2781	1.2810	1.2804 [a]	1.2829[d]
ω_e (cm^{-1})	2784.8	2758.9	2737.8	2710.9 [a]	2723.0[e]
q(Rg) at R_e	0.61	0.55	0.58		0.57[c]
D_e (Rg + H^+) (eV)	3.99	4.00	3.94	4.02[b]	4.15[c]
D_e (Rg^+ + H) (eV)	5.95	5.95	5.95		
Dipole moment (D)	2.0299	2.0382	2.0699		1.9283[c]
Force cons. (mdyne/Å)	4.7181	4.6306	4.5601		4.6855[c]
Rotational cons. (GHz)	316.30	314.72	313.29	313.61[a]	310.58[e]
IR intensity (km/mol)	562.98	566.00	564.29		529.89[c]
E(Therm) (kcal/mol)	5.462	5.425	5.395		5.449[c]
C_V (cal/mol-K)	4.969	4.969	4.969		4.969[c]
S (cal/mol-K)	44.963	44.973	44.982		44.967[c]

[a]Reference [6]; [b]Values quoted in reference [16]; [c]reference [16]; [d]reference [20]; [e]refeference [18].

The results of KrH^+ are listed in Table 4, where we see that our calculated values using basis sets B2 and B3 are underestimated for R_e and overestimated for ω_e in comparison to the experimental values, but consistent with the theoretical values. Ferrante et al. [22] suggested reconfirmation of the

experimental values of Johns [6] from the point of systematic agreement of their calculated values with other theoretical values. Very good agreement is found for the dissociation limit D_e (Kr + H^+).

Table 4: Spectroscopic constants and molecular properties of KrH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	1.3742	1.4177	1.4126	1.4212[a,b]	1.4184[e]
ω_e (cm^{-1})	3010.5	2573.9	2576.1	2494.7[a]	2570.9[e]
q(Rg) at R_e	0.65	0.66	0.73		0.76[h]
D_e (Rg + H^+) (eV)	4.88	4.53	4.54	4.51[c]	4.58[f]
D_e (Rg^+ + H) (eV)	5.27	4.87	4.94		4.79[f]
Dipole moment (D)	1.7914	1.8985	1.8864	1.967[d]	1.94[g]
Force cons. (mdyne/Å)	5.4453	3.9807	3.9873		3.9713[e]
Rotational cons. (GHz)	268.73	252.49	224.31	240.98[a]	252.13[g]
IR intensity (km/mol)	373.78	408.14	409.58		369.01[e]
E(Therm) (kcal/mol)	5.785	5.161	5.164		5.157[e]
C_V (cal/mol-K)	4.968	4.969	4.969		5.748[e]
S (cal/mol-K)	47.459	47.583	47.569		47.584[e]

[a]Reference [6]; [b]reference [8]; [c]reference [9]; [d]reference [10]; [e]reference [16]; [f]reference [22]; [g]reference [17]; [h]reference [20].

In Table 5, our calculated values of R_e, ω_e, D_e (Xe^+ + H) and rotational constant for XeH^+ are found in good agreement with the available data. Some data are reported as first time. Finally, in Table 6, our results for RnH^+ are listed along with the only available theoretical values of Ferrante et al. [22]. Their relativistic and non-relativistic values are found almost same for R_e and D_e (Rn + H^+). The spin-orbit effect has a strong influence on the ground state dissociation [21-22] and so the difference of 0.05-0.07 eV in our D_e values for both the RnH^+ and XeH^+ compared to the available values may be due to this SO effect. Because of radioactive instability of Rn, experimental investigation on RnH^+ is probably difficult. In this sense, our reported values for RnH^+ may be a benchmark to the future investigations.

Table 5: Spectroscopic constants and molecular properties of XeH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	1.5931	1.5931	1.5963	1.6028[a]	1.598[d]
ω_e (cm^{-1})	2349.7	2353.2	2329.6	2270.0[a]	2322.0[c]
q(Rg) at R_e	0.85	0.86	0.97		0.98[f]
D_e (Rg + H^+) (eV)	5.19	5.23	5.26		5.28[d]
D_e (Rg^+ + H) (eV)	3.81	3.83	3.86	3.81[b]	3.64[d]
Dipole moment (D)	1.5047	1.5031	1.5104		1.55[e]
Force cons. (mdyne/Å)	3.3032	3.1330	3.2469		
Rotational cons. (GHz)	199.09	199.09	198.29	196.69[a]	194.57[e]
IR intensity (km/mol)	237.78	239.70	242.53		
E(Therm) (kcal/mol)	4.840	4.845	4.812		
C_V (cal/mol-K)	4.840	4.971	4.971		
S (cal/mol-K)	49.391	49.391	49.391		

[a]Reference [11]; [b]reference [12]; [c]reference [21]; [d]reference [22]; [e]reference [19]; [f]reference [20].

Table 6: Spectroscopic constants and molecular properties of RnH^+ in its ground $^1\Sigma^+$ state

Spectroscopic data	Basis set			Other values	
	B1: 6-31++G (3df,3pd)	B2: 6-311++G (3df,3pd)	B3: Aug-cc-pVTZ	Expt	Theo
R_e (Å)	1.6861	1.6749	1.6771		1.700[a]
ω_e (cm^{-1})	2203.6	2242.3	2238.4		
q(Rg) at R_e	0.96	0.89	0.90		
D_e (Rg + H^+) (eV)	5.61	5.70	5.61		5.64[a]
D_e (Rg^+ + H) (eV)	3.36	3.42	3.34		3.68[a]
Dipole moment (D)	1.1649	1.1472	1.1709		1.025[b]
Force cons. (mdyne/Å)	2.8963	2.9991	2.9885		
Rotational cons. (GHz)	177.19	179.56	179.08		
IR intensity (km/mol)	171.91	171.74	154.88		
E(Therm) (kcal/mol)	4.632	4.687	4.681		
C_V (cal/mol-K)	4.973	4.973	4.973		
S (cal/mol-K)	51.165	51.139	51.144		

[a]Reference [22, non-relativistic value]; [b]reference [22, relativistic value].

To get a comparative idea, we have plotted our various spectroscopic constants using only basis set B3 along with available experimental and/or other's theoretical values. Results of using other basis sets are omitted as they are very close and will overlap in the figures. In Figure 3, the variation of R_e for different RgH^+ are plotted. Except KrH^+, our calculated R_e values are underestimated by only 0.001-0.006 Å in comparison to experimental values, which is already mentioned. Note that R_e increases with increasing Z, ie. rare gas members (Rg) in RgH^+, which is obvious and consequently ω_e decreases, as shown in Figure 4. Our calculated vales of ω_e for KrH^+ and XeH^+ are slightly overestimated, but the experimental value for HeH^+ is underestimated by about 300 cm^{-1} in contrast to our calculated and other theoretical values. Consistency has also been achieved for charge q(Rg) at the equilibrium geometry, as shown in Figure 5. From this figure, it is clear that the charge of Rg at the equilibrium geometry is more for the higher members of rare gases and this is obvious due to their higher proton affinity. Consistent dissociation values are obtained as clear from Figures 6 and 7 for D_e(Rg + H^+) and D_e(Rg^+ + H), respectively. Limited results are available in literature for the dissociation energy D_e (Rg^+ + H).

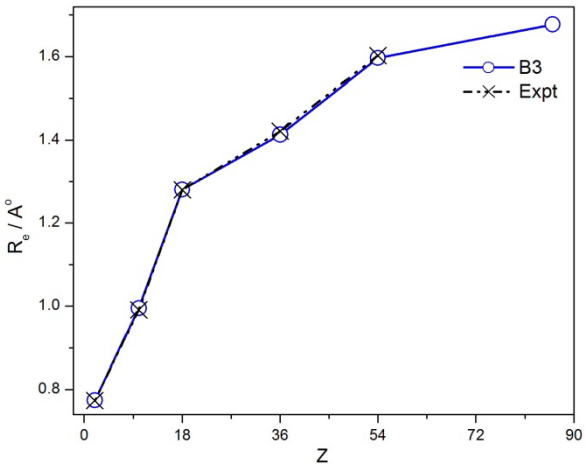

Figure 3: Variation of R_e with Z of Rg for different RgH^+ ions.

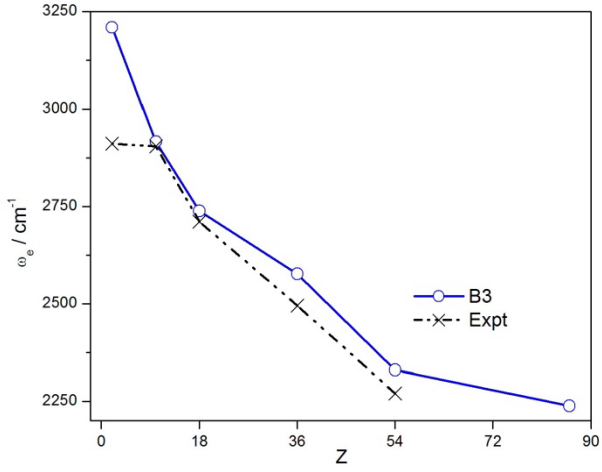

Figure 4: Variation of ω_e with Z of Rg for different RgH^+ ions.

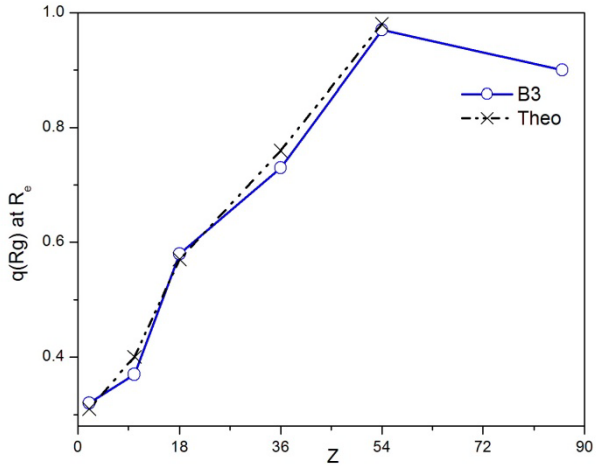

Figure 5: Variation of q(Rg) at R_e with Z of Rg for different RgH^+ ions.

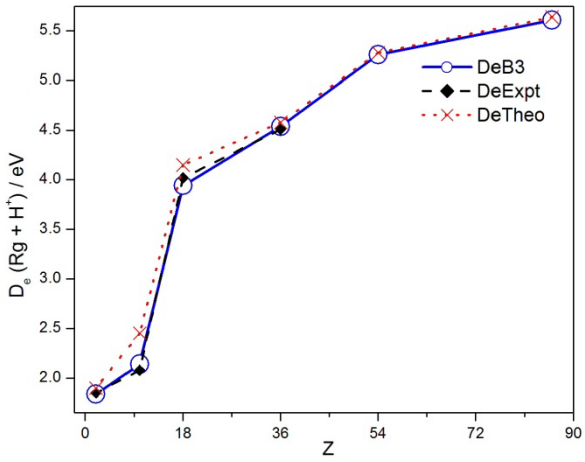

Figure 6: Variation of $D_e(Rg + H^+)$ with Z of Rg for different RgH^+ ions.

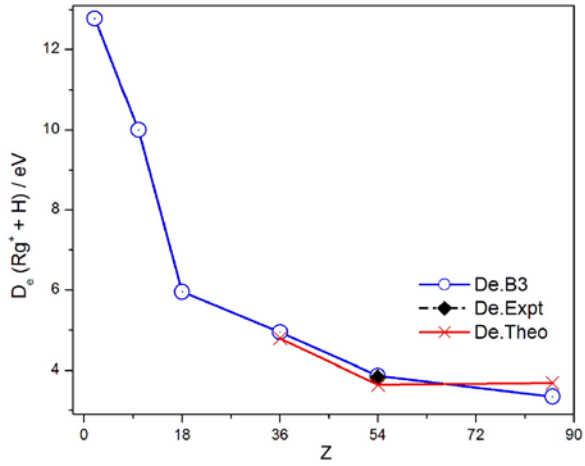

Figure 7: Variation of $D_e(Rg^+ + H)$ with Z of Rg for different RgH^+ ions.

4. Conclusions

In summary, we presented spectroscopic constants and various molecular properties of some rare gas hydride ions. Some of the systems have a significant importance in astrophysics. The calculated values are found in good agreement with the available data. Limited result is available for RnH^+. Many new data are reported for the first time in literature, which may serve as future references.

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References

[1] *Gusten, R., Wiesemeyer, H.D., Neufeld, D., Menten, K.M., Graf, U.U., Jacobs, K., Klein, B., Ricken, O., Risacher, C. and Stutzki, J. (2019) Astrophysical detection of the helium hydride ion HeH^+. Nature, 568, 357-363.* DOI:10.1038/s41586-019-1090-x

[2] *Bovino, S., Tacconi, M., Gianturco, F.A. and Gajlli, D. (2011) Ion chemistry in the early universe: Revisiting the*

role of HeH+ with new quantum calculations. Astron. Astrophys., A 529, 140-144.
DOI:10.1051/0004-6361/201116740

[3] Harris, G.J., Lynas-Gray, A.E., Miller, S. and Tennyson, J. (2004) The role of HeH+ in cool helium-rich white dwarfs. Astrophys. J., 617, L143-146.

[4] Mousis, O., Pauzat, F., Ellinger, Y., Ceccarelli, C. (2008) Sequestration of noble gases by H^+_3 in protoplanetary disks and outer solar system composition. Astrophys. J., 673, 637-646.

[5] Hogness, T.R. and Lunn, E.C. (1925) The ionization of hydrogen by electron impact as interpreted by positive ray analysis. Phys. Rev., 26, 44-55.
DOI:10.1103/PhysRev.26.44

[6] Johns, J.W.C. (1984) Spectra of the protonated rare gases. J. Mol. Spectrosc., 106, 124-133.
DOI:10.1016/0022-2852(84)90087-0

[7] Ram, R.S., Bernath, P.F. and Brault, J.W. (1985) Fourier transform emission spectroscopy of NeH^+. J. Mol. Spectrosc,. 113, 451-457.
DOI:10.1016/0022-2852(85)90281-4

[8] Linnartz, H., Zink, L.R. and Evenson, K.M. (1977) The pure rotational spectra of $^{84}KrH^+$ and $^{86}KrH^+$. J. Mol. Spectrosc., 184, 56-59.

[9] Hunter, E.P. and Lias, S.G. (1988) Evaluated gas phase basicities and proton affinities of molecules: an update. J. Phys. Chem. Ref. Data, 27, 413-656.
DOI:10.1063/1.556018

[10] Molski, M. (2002) Reduction of wave numbers of pure rotational and vibration-rotational transitions of KrH^+ $X\,^1\Sigma^+$ to parameters of radial functions. Mol. Phys., 100, 3545-3552.
DOI:10.1080/00268970210150531

[11] Rogers S.A., Brazier, C.R. Bernath, P.F. (1987) The infrared spectrum of XeH^+. J. Chem. Phys., 87, 159-162.
DOI:10.1063/1.453611

[12] Peterson, K.A., Petrmichl, R.H., McClain, R.L. and Wood, R.C. (1991) Submillimeter wave spectroscopy of XeH^+ and XeD^+. J. Chem. Phys., 95, 2352-2360.
DOI:10.1063/1.460941

[13] Beach, J.Y. (1936) Quantum mechanical treatment of helium hydride molecule ion HeH^+. J. Chem. Phys., 4, 353-357.
DOI:10.1063/1.1749857

[14] Toh, S. (1940) Evaluated quantum-mechanical treatment of helium hydride molecule ion HeH^+. Proc. Phys. Math. Soc. Japan, 22, 119-126.
DOI:10.11429/ppmsj1919.22.2_119

[15] Evett, A.A. (1956) Ground state of the helium hydride ion. J. Chem. Phys., 24, 150-152.
DOI:10.1063/1.1700818

[16] Schutte, C. J. H. (2002) An ab initio molecular orbital study of the argon hydride molecule– ions, ArH^+ and ArD^+, at the MP4(SDQ)/6-311++G(3df,3dp) level. III: a study of some physical properties of ArH^+, compared with those of HeH^+, NeH^+ and KrH^+ and the diatomic Van der Waals molecules He_2, Ne_2, Ar_2 and Kr_2. Chem. Phys. Lett., 353, 389-395.
DOI:10.1016/S0009-2614(02)00050-7

[17] Rosmus, P. and Reinsch, E.-A. (1980) Calculation of molecular vonstants for the ground states of the NeH^+ and KrH^+ Ions. Z. Naturforsch, 35A, 1066-1070.
DOI:10.1515/zna-1980-1011

[18] Rosmus, P. (1979) Molecular constants for the $^1\Sigma^+$ ground state of the ArH^+ ion. Theor. Chim. Acta. 51, 359-362.
DOI:10.1007/BF00548944

[19] Klein, R. and Rosmus, P. (1984) Calculation of infrared transition probabilities for the $^1\Sigma^+$ ground state of XeH^+. Z. Naturforsch, 39A, 349-353.
DOI:10.1515/zna-1984-0405

[20] Lundell, J. Nieminen, J. and H. Kunttu, H. (1993) All-electron and effective core potential studies on ground state ArH^+, KrH^+ and XeH^+ ions. Chem. Phys. Lett., 208, 247-255.
DOI:10.1016/0009-2614(93)89070-X

[21] Alekseyev, A.B., Liebermann, H.P. and Buenker, R. (2008) Spin–orbit configuration interaction study of the ultraviolet photofragmentation of XeH^+. Phys. Chem. Chem. Phys., 10, 5706-5713.
DOI:10.1039/b807078d

[22] Ferrante, F., Barone, G. and Duca, D. (2012) Relativistic coupled cluster calculations of the electronic structure of KrH^+, XeH^+ and RnH^+. Theor. Cem. Acc., 131, 1165-1171.
DOI:10.1007/s00214-012-1165-3

[23] Basis sets are taken from: http://www.basissetexchange.org/

[24] Frisch M. J., et al. (2003) Gaussian 03, Gaussian Inc., Wallingbond, CT.