Supporting Information

Unveiling distinct bonding patterns in noble gas hydrides via interference energy analysis

Lucas Araujo,[a,b] Marco A. C. Nascimento,[a] Thiago M. Cardozo[a] and Felipe Fantuzzi*[c]*

a. Instituto de Química, Universidade Federal do Rio de Janeiro, Av. Athos da Silveira Ramos, 149, CT, A-622, Cid. Univ., Rio de Janeiro, RJ 21941-909, Brazil.
E-mail: thiago@iq.ufrj.br

b. Center for Theoretical Chemistry, Faculty of Chemistry and Biochemistry, Ruhr University Bochum, Universitätsstraße 150, 44801 Bochum, Germany.

c. School of Chemistry and Forensic Science, University of Kent, Park Wood Rd, Canterbury CT2 7NH, UK.
E-mail: f.fantuzzi@kent.ac.uk

Table of Contents

1. Optimization and frequencies: CCSD(T)/aug-cc-pVTZ results

Table S1: Molecular parameters calculated at the CCSD(T)/aug-cc-pVTZ level. Bond lengths, absolute energies, zero-point energy (zpe) and fundamental vibrational frequencies.

Species	Bond length (Å)	Energy (a.u.)	ZPE (a.u.)	Frequencies (cm^{-1})
HeH^+	0.77615	-2.975393255079	0.00730227	3205.33
NeH^+	0.99234	-128.897819263410	0.00671000	2945.35
ArH^+	1.28211	-527.199804389098	0.00621645	2728.70

2. Orbital extents and orbital plots

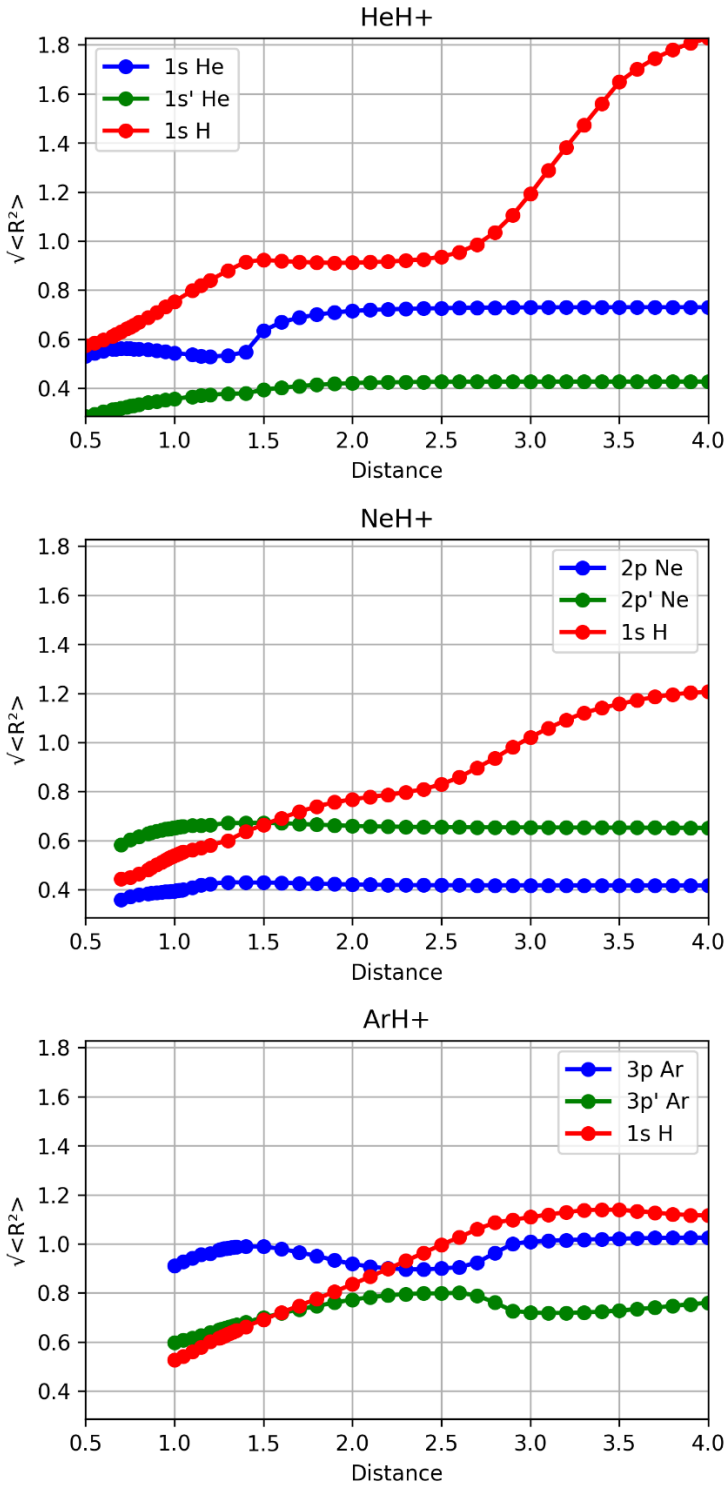

Figure S1: SCGVB orbital extents derived from the square root of ⟨R²⟩, calculated at the SCGVB(2,3)/aug-cc-pVTZ level across various interatomic distances (in Å) for the NgH^+ species discussed.

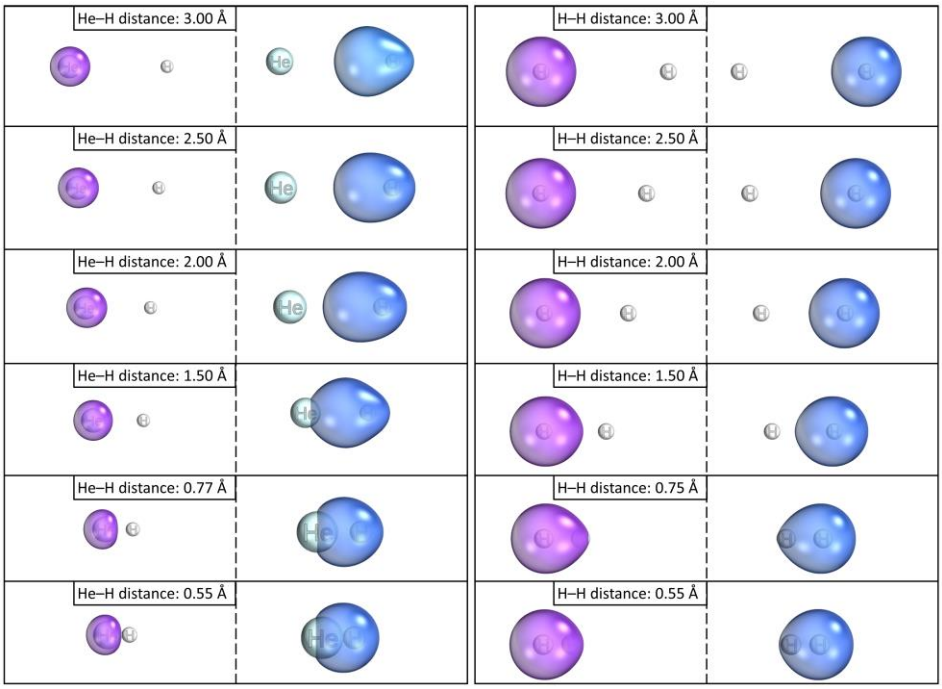

Figure S2: SCGVB/aug-cc-pVTZ orbitals for HeH^+ and H_2 at various interatomic distances along their potential energy curves. For helium, only the orbital with the largest overlap with the hydrogen 1s orbital at the energy minimum is shown for simplicity.

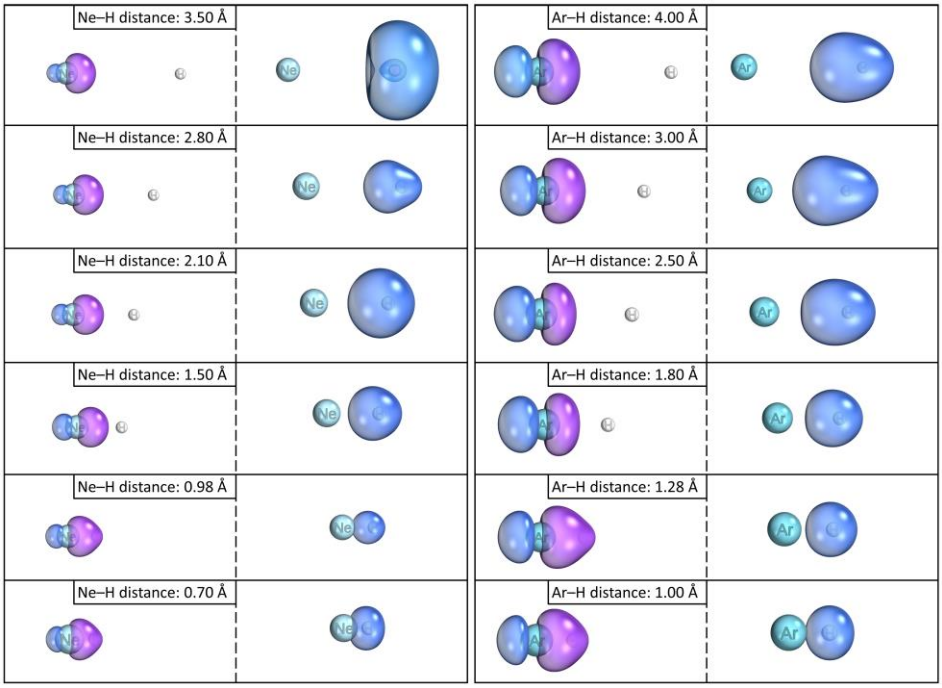

Figure S3: SCGVB/aug-cc-pVTZ orbitals for NeH^+ and ArH^+ at various interatomic distances along their potential energy curves. For the noble gases, only the orbital with the largest overlap with the hydrogen 1s orbital at the energy minimum is shown for simplicity.

3. CCSD(T) potential energy curves

Table S2: CCSD(T)/aug-cc-pVTZ potential energy curves for HeH^+, NeH^+ and ArH^+. Distances are given in angstroms (Å) and the absolute energies in atomic units (a.u.).

Distance He–H (Å)	Energy (a.u.)	Distance Ne–H (Å)	Energy (a.u.)	Distance Ar–H (Å)	Energy (a.u.)
0.500	-2.87130819	0.700	-128.78169613	1.000	-527.12668563
0.596	-2.94384602	0.794	-128.85849052	1.091	-527.17263314
0.692	-2.97031901	0.888	-128.88960251	1.182	-527.19368149
0.788	-2.97531871	0.982	-128.89775531	1.273	-527.19976012
0.884	-2.97054994	1.076	-128.89467103	1.364	-527.19700318
0.980	-2.96180211	1.170	-128.88654098	1.455	-527.18923940
1.076	-2.95199760	1.264	-128.87662010	1.545	-527.17885075
1.172	-2.94258548	1.358	-128.86657701	1.636	-527.16729878
1.268	-2.93422728	1.452	-128.85724291	1.727	-527.15546603
1.364	-2.92715529	1.545	-128.84900354	1.818	-527.14387788
1.460	-2.92136937	1.639	-128.84198605	1.909	-527.13284022
1.556	-2.91675096	1.733	-128.83616231	2.000	-527.12252478
1.652	-2.91313090	1.827	-128.83141837	2.091	-527.11302021
1.747	-2.91033018	1.921	-128.82760528	2.182	-527.10436349
1.843	-2.90818230	2.015	-128.82457060	2.273	-527.09655930
1.939	-2.90654354	2.109	-128.82217472	2.364	-527.08959168
2.035	-2.90529564	2.203	-128.82029390	2.455	-527.08343073
2.131	-2.90434442	2.297	-128.81882213	2.545	-527.07803745
2.227	-2.90361659	2.391	-128.81767055	2.636	-527.07336201
2.323	-2.90305623	2.485	-128.81676691	2.727	-527.06935026
2.419	-2.90262128	2.579	-128.81605424	2.818	-527.06594236
2.515	-2.90228047	2.673	-128.81548864	2.909	-527.06307512
2.611	-2.90201066	2.767	-128.81503664	3.000	-527.06068393
2.707	-2.90179481	2.861	-128.81467269	3.091	-527.05870516
2.803	-2.90162028	2.955	-128.81437718	3.182	-527.05707740
2.899	-2.90147777	3.048	-128.81413500	3.273	-527.05574421
2.995	-2.90136029	3.142	-128.81393455	3.364	-527.05465496
3.091	-2.90126258	3.236	-128.81376698	3.455	-527.05376551
3.187	-2.90118064	3.330	-128.81362562	3.545	-527.05303836
3.283	-2.90111140	3.424	-128.81350549	3.636	-527.05244224
3.379	-2.90105246	3.518	-128.81340287	3.727	-527.05195148
3.475	-2.90100193	3.612	-128.81331488	3.818	-527.05154531
3.571	-2.90095833	3.706	-128.81323929	3.909	-527.05120702
3.667	-2.90092049	3.800	-128.81317425	4.000	-527.05092330
3.763	-2.90088747	3.894	-128.81311819	4.091	-527.05068356
3.859	-2.90085848	3.988	-128.81306976	4.182	-527.05047945
3.955	-2.90083303	4.082	-128.81302778	4.273	-527.05030437
4.051	-2.90081058	4.176	-128.81299126	4.364	-527.05015313
4.146	-2.90079072	4.270	-128.81295934	4.455	-527.05002162
4.242	-2.90077313	4.364	-128.81293131	4.545	-527.04990658
4.338	-2.90075751	4.458	-128.81290657	4.636	-527.04980541

4.434	-2.90074361	4.552	-128.81288463	4.727	-527.04971600
4.530	-2.90073121	4.645	-128.81286474	4.818	-527.04963665
4.626	-2.90072013	4.739	-128.81284726	4.909	-527.04956595
4.722	-2.90071021	4.833	-128.81283156	5.000	-527.04950272
4.818	-2.90070129	4.927	-128.81281741	5.091	-527.04944600
4.914	-2.90069326	5.021	-128.81280463	5.182	-527.04939495
5.010	-2.90068601	5.115	-128.81279305	5.273	-527.04934889
5.106	-2.90067945	5.209	-128.81278253	5.364	-527.04930716
5.202	-2.90067350	5.303	-128.81277295	5.455	-527.04926925
5.298	-2.90066809	5.397	-128.81276421	5.545	-527.04923476
5.394	-2.90066315	5.491	-128.81275623	5.636	-527.04920325
5.490	-2.90065865	5.585	-128.81274892	5.727	-527.04917444
5.586	-2.90065453	5.679	-128.81274222	5.818	-527.04914801
5.682	-2.90065076	5.773	-128.81273606	5.909	-527.04912372
5.778	-2.90064729	5.867	-128.81273039	6.000	-527.04910134
5.874	-2.90064411	5.961	-128.81272518	6.091	-527.04908069
5.970	-2.90064117	6.055	-128.81272036	6.182	-527.04906161
6.066	-2.90063847	6.148	-128.81271592	6.273	-527.04904393
6.162	-2.90063597	6.242	-128.81271181	6.364	-527.04902754
6.258	-2.90063367	6.336	-128.81270800	6.455	-527.04901233
6.354	-2.90063153	6.430	-128.81270447	6.545	-527.04899818
6.449	-2.90062955	6.524	-128.81270120	6.636	-527.04898501
6.545	-2.90062772	6.618	-128.81269815	6.727	-527.04897273
6.641	-2.90062601	6.712	-128.81269532	6.818	-527.04896129
6.737	-2.90062443	6.806	-128.81269269	6.909	-527.04895059
6.833	-2.90062296	6.900	-128.81269024	7.000	-527.04894060
6.929	-2.90062159	6.994	-128.81268795	7.091	-527.04893126
7.025	-2.90062031	7.088	-128.81268581	7.182	-527.04892250
7.121	-2.90061911	7.182	-128.81268381	7.273	-527.04891430
7.217	-2.90061800	7.276	-128.81268195	7.364	-527.04890660
7.313	-2.90061695	7.370	-128.81268020	7.455	-527.04889938
7.409	-2.90061598	7.464	-128.81267856	7.545	-527.04889259
7.505	-2.90061506	7.558	-128.81267703	7.636	-527.04888621
7.601	-2.90061421	7.652	-128.81267559	7.727	-527.04888021
7.697	-2.90061340	7.745	-128.81267423	7.818	-527.04887455
7.793	-2.90061265	7.839	-128.81267296	7.909	-527.04886923
7.889	-2.90061194	7.933	-128.81267176	8.000	-527.04886420
7.985	-2.90061127	8.027	-128.81267064	8.091	-527.04885946
8.081	-2.90061064	8.121	-128.81266958	8.182	-527.04885499
8.177	-2.90061005	8.215	-128.81266858	8.273	-527.04885076
8.273	-2.90060950	8.309	-128.81266763	8.364	-527.04884676
8.369	-2.90060897	8.403	-128.81266674	8.455	-527.04884297
8.465	-2.90060847	8.497	-128.81266590	8.545	-527.04883939
8.561	-2.90060801	8.591	-128.81266511	8.636	-527.04883600
8.657	-2.90060756	8.685	-128.81266435	8.727	-527.04883278
8.753	-2.90060714	8.779	-128.81266364	8.818	-527.04882973
8.848	-2.90060675	8.873	-128.81266296	8.909	-527.04882683
8.944	-2.90060637	8.967	-128.81266232	9.000	-527.04882409
9.040	-2.90060602	9.061	-128.81266172	9.091	-527.04882147

9.136	-2.90060568	9.155	-128.81266114	9.182	-527.04881899
9.232	-2.90060536	9.248	-128.81266059	9.273	-527.04881663
9.328	-2.90060505	9.342	-128.81266007	9.364	-527.04881438
9.424	-2.90060477	9.436	-128.81265958	9.455	-527.04881224
9.520	-2.90060449	9.530	-128.81265911	9.545	-527.04881021
9.616	-2.90060423	9.624	-128.81265866	9.636	-527.04880827
9.712	-2.90060398	9.718	-128.81265824	9.727	-527.04880642
9.808	-2.90060375	9.812	-128.81265783	9.818	-527.04880465
9.904	-2.90060352	9.906	-128.81265745	9.909	-527.04880296
10.000	-2.90060331	10.000	-128.81265708	10.000	-527.04880136

4. SCGVB potential energy curves and the GPF-EP results

```
 $CONTRL ICHARG=1 MULT=1 SCFTYP=RHF VBTYP=VB2000 ISPHER=1 MAXIT=199 $END
 $SYSTEM MEMORY=100000000 $END
 $BASIS GBASIS=ACCT $END
 $DATA
HeH+ SC
C1
HELIUM          2.0      0.000000000          0.000000000          0.000000000
HYDROGEN        1.0      0.77           0.000000000          0.000000000
$END
 $VB2000
#! SC(2,3)/aug-cc-pVTZ

HeH+ 1 GROUPS (1 Spin-Coupled(2,3) Group)


 $01LENHANCE
 3
 1,1,1
 2,1,1
 3,1,2

 $GPFEP
 partition_0.77.txt dmatrix_0.77.txt

 $READGUESS
 heh_0.75.guess

 $WRITEGUESS
 heh_0.77.guess

 $MACROITER
 250

 $MOLDEN

 $END
```

Figure S4: Example of an input file for VB2000, as distributed with GAMESS, used for the SCGVB calculations.

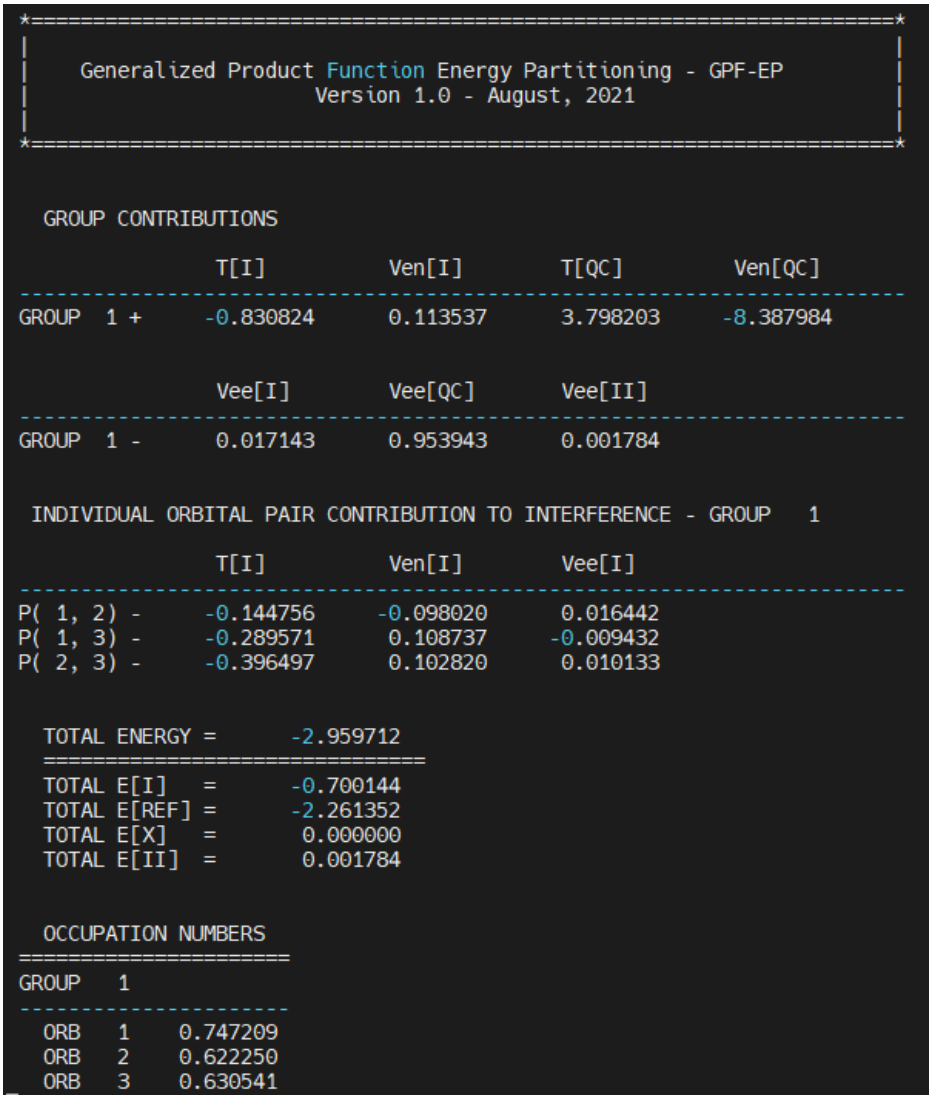

Figure S5: Example of a partition file generated by the GPF-EP module of VB2000.

Table S3: IEA data for HeH^+ at the SCGVB(2,3)/aug-cc-pVTZ level.

Dist He-H	E[TOT]	T[TOT]	V[TOT]	E[I]	T[I]	V[I]	E[QC]	T[QC]	V[QC]
0.50	-2.855123	3.424664	-6.279787	-0.91049	-0.818277	-0.092213	-1.946452	4.242941	-6.189393
0.55	-2.901199	3.297388	-6.198587	-0.846194	-0.849164	0.00297	-2.056611	4.146552	-6.203163
0.60	-2.929822	3.193851	-6.123673	-0.801251	-0.851634	0.050383	-2.130184	4.045485	-6.175669
0.65	-2.946719	3.109768	-6.056487	-0.765925	-0.845692	0.079768	-2.182468	3.95546	-6.137928
0.67	-2.951093	3.080777	-6.03187	-0.756029	-0.839995	0.083965	-2.19677	3.920772	-6.117541
0.70	-2.955696	3.041583	-5.997279	-0.738719	-0.835577	0.096857	-2.218716	3.87716	-6.095875
0.73	-2.958393	3.007071	-5.965464	-0.721781	-0.832756	0.110975	-2.238376	3.839827	-6.078203
0.75	-2.959335	2.986386	-5.945721	-0.710859	-0.83146	0.120601	-2.25025	3.817846	-6.068097
0.77	-2.959712	2.967379	-5.927091	-0.700144	-0.830824	0.13068	-2.261352	3.798203	-6.059555
0.80	-2.959403	2.941784	-5.901187	-0.685236	-0.830475	0.14524	-2.275971	3.772259	-6.048231
0.85	-2.957124	2.905908	-5.863032	-0.663539	-0.830682	0.167143	-2.295442	3.73659	-6.032032
0.90	-2.953349	2.877297	-5.830646	-0.645248	-0.830829	0.185582	-2.310004	3.708126	-6.018131
0.95	-2.948673	2.854783	-5.803456	-0.6293	-0.831225	0.201925	-2.321304	3.686008	-6.007312
1.00	-2.943511	2.837323	-5.780834	-0.614671	-0.831871	0.2172	-2.330795	3.669194	-5.999989
1.10	-2.932784	2.814496	-5.74728	-0.590651	-0.830494	0.239844	-2.344126	3.64499	-5.989116
1.15	-2.927557	2.807852	-5.735409	-0.579286	-0.829231	0.249945	-2.350264	3.637083	-5.987347
1.20	-2.922549	2.803633	-5.726182	-0.568649	-0.825533	0.256884	-2.355899	3.629166	-5.985065
1.30	-2.913376	2.801033	-5.714409	-0.546994	-0.807103	0.260108	-2.368392	3.608136	-5.976528
1.40	-2.905393	2.80419	-5.709583	-0.517134	-0.76362	0.246486	-2.390259	3.56781	-5.958069
1.50	-2.897556	2.820207	-5.717763	-0.349012	-0.483171	0.134159	-2.549782	3.303378	-5.85316
1.60	-2.892806	2.829043	-5.721849	-0.300206	-0.414643	0.114436	-2.593579	3.243686	-5.837265
1.70	-2.889164	2.837551	-5.726715	-0.271552	-0.378749	0.107197	-2.618423	3.2163	-5.834724
1.80	-2.886399	2.845366	-5.731765	-0.252368	-0.353902	0.101533	-2.634724	3.199268	-5.833991
1.90	-2.884318	2.851951	-5.736269	-0.239783	-0.335836	0.096052	-2.645152	3.187787	-5.832939
2.00	-2.882757	2.857458	-5.740215	-0.232222	-0.323661	0.09144	-2.651108	3.181119	-5.832227
2.10	-2.881586	2.861815	-5.743401	-0.227664	-0.315246	0.087581	-2.654468	3.177061	-5.831529
2.20	-2.880702	2.865364	-5.746066	-0.224926	-0.309418	0.084492	-2.656308	3.174782	-5.831091
2.30	-2.88003	2.868049	-5.748079	-0.223219	-0.30525	0.082031	-2.657336	3.173299	-5.830635
2.40	-2.879517	2.870143	-5.74966	-0.222131	-0.302238	0.080106	-2.657907	3.172381	-5.830287
2.50	-2.87912	2.871784	-5.750904	-0.221416	-0.300039	0.078623	-2.658224	3.171823	-5.830046
2.60	-2.87881	2.873055	-5.751865	-0.220937	-0.298431	0.077494	-2.658391	3.171486	-5.829878
2.70	-2.878565	2.874049	-5.752614	-0.220609	-0.297258	0.076648	-2.658474	3.171307	-5.82978
2.80	-2.878369	2.874829	-5.753198	-0.220382	-0.296411	0.076029	-2.658505	3.17124	-5.829745
2.90	-2.878211	2.875452	-5.753663	-0.22022	-0.295803	0.075583	-2.658509	3.171255	-5.829764
3.00	-2.878082	2.875949	-5.754031	-0.220104	-0.295375	0.075271	-2.658497	3.171324	-5.82982
3.10	-2.877976	2.876351	-5.754327	-0.220021	-0.295081	0.075061	-2.658474	3.171432	-5.829907
3.20	-2.877888	2.87668	-5.754568	-0.219961	-0.294885	0.074924	-2.658445	3.171565	-5.830011
3.30	-2.877814	2.87695	-5.754764	-0.219921	-0.29476	0.074839	-2.658411	3.17171	-5.830122
3.40	-2.877751	2.877176	-5.754927	-0.219896	-0.294685	0.074789	-2.658373	3.171861	-5.830235
3.50	-2.877697	2.877364	-5.755061	-0.219881	-0.294645	0.074764	-2.658334	3.172009	-5.830344

3.60	-2.877652	2.87752	-5.755172	-0.219875	-0.294627	0.074751	-2.658295	3.172147	-5.830442
3.70	-2.877612	2.877653	-5.755265	-0.219877	-0.294626	0.074749	-2.658254	3.172279	-5.830532
3.80	-2.877578	2.877769	-5.755347	-0.219884	-0.294639	0.074755	-2.658213	3.172408	-5.83062
3.90	-2.877549	2.877866	-5.755415	-0.219895	-0.294661	0.074766	-2.658173	3.172527	-5.830699
4.00	-2.877523	2.877953	-5.755476	-0.219907	-0.294688	0.07478	-2.658134	3.172641	-5.830774

Table S4: IEA data for NeH^+ at the SCGVB(2,3)/aug-cc-pVTZ level.

Distance Ne-H	E[TOT]	T[TOT]	V[TOT]	E[I]	T[I]	V[I]	E[QC]	T[QC]	V[QC]
0.70	-128.528523	129.333642	-257.862165	-0.851093	-1.340546	0.489453	-127.679037	130.674188	-258.353225
0.75	-128.575662	129.129926	-257.705588	-0.799015	-1.294266	0.49525	-127.778361	130.424192	-258.202553
0.80	-128.605614	128.970506	-257.57612	-0.751815	-1.249573	0.497758	-127.855611	130.220079	-258.075689
0.85	-128.623675	128.845758	-257.469433	-0.707638	-1.202792	0.495155	-127.917925	130.04855	-257.966476
0.87	-128.628439	128.803842	-257.432281	-0.69225	-1.190437	0.498187	-127.938103	129.994279	-257.932382
0.90	-128.633508	128.748176	-257.381684	-0.668085	-1.16368	0.495596	-127.967366	129.911856	-257.879222
0.93	-128.636541	128.700149	-257.33669	-0.644385	-1.135589	0.491204	-127.994115	129.835738	-257.829853
0.95	-128.63764	128.671859	-257.309499	-0.62897	-1.117515	0.488545	-128.010632	129.789374	-257.800006
0.96	-128.637956	128.65873	-257.296686	-0.622046	-1.110649	0.488603	-128.017874	129.769379	-257.787252
0.97	-128.638127	128.646238	-257.284365	-0.614693	-1.102343	0.48765	-128.025395	129.748581	-257.773976
0.98	-128.638164	128.634354	-257.272518	-0.606967	-1.092758	0.485791	-128.033153	129.727112	-257.760266
0.99	-128.638077	128.622983	-257.26106	-0.598807	-1.081562	0.482754	-128.041218	129.704545	-257.745762
1.00	-128.637875	128.612367	-257.250242	-0.590174	-1.068664	0.47849	-128.049638	129.681031	-257.730668
1.01	-128.637567	128.602156	-257.239723	-0.58121	-1.055238	0.474029	-128.058279	129.657394	-257.715673
1.02	-128.637162	128.592459	-257.229621	-0.571749	-1.040338	0.468589	-128.067313	129.632797	-257.700111
1.03	-128.636668	128.583312	-257.21998	-0.562245	-1.025412	0.463167	-128.076303	129.608724	-257.685026
1.04	-128.636091	128.57453	-257.210621	-0.551951	-1.008595	0.456644	-128.085988	129.583125	-257.669114
1.05	-128.635436	128.566304	-257.20174	-0.54091	-0.990124	0.449214	-128.096337	129.556428	-257.652767
1.10	-128.631234	128.531421	-257.162655	-0.476135	-0.878529	0.402393	-128.156594	129.40995	-257.566543
1.15	-128.626126	128.504974	-257.1311	-0.422186	-0.782529	0.360344	-128.205085	129.287503	-257.492588
1.20	-128.62056	128.484195	-257.104755	-0.384843	-0.71055	0.325706	-128.236632	129.194745	-257.431376
1.30	-128.608938	128.4578	-257.066738	-0.337905	-0.607466	0.269561	-128.27169	129.065266	-257.336956
1.40	-128.597788	128.447993	-257.045781	-0.315329	-0.562407	0.247078	-128.28307	129.0104	-257.293469
1.50	-128.587764	128.447976	-257.03574	-0.292253	-0.509423	0.21717	-128.296046	128.957399	-257.253444
1.60	-128.579249	128.454292	-257.033541	-0.274146	-0.466755	0.192609	-128.305588	128.921047	-257.226635
1.70	-128.572311	128.463911	-257.036222	-0.260342	-0.433482	0.173141	-128.312423	128.897393	-257.209817
1.80	-128.566823	128.47475	-257.041573	-0.249397	-0.405867	0.156469	-128.317859	128.880617	-257.198475
1.90	-128.562558	128.485542	-257.0481	-0.2409	-0.383254	0.142354	-128.322078	128.868796	-257.190874
2.00	-128.559275	128.495483	-257.054758	-0.234583	-0.365389	0.130806	-128.325106	128.860872	-257.185978
2.10	-128.55676	128.50409	-257.06085	-0.230006	-0.351479	0.121473	-128.327167	128.855569	-257.182735
2.20	-128.554839	128.511226	-257.066065	-0.226786	-0.341056	0.11427	-128.328463	128.852282	-257.180746
2.30	-128.55337	128.517041	-257.070411	-0.224441	-0.332897	0.108456	-128.32934	128.849938	-257.179277

2.40	-128.552243	128.521538	-257.073781	-0.222832	-0.326896	0.104064	-128.32982	128.848434	-257.178255
2.50	-128.551372	128.525126	-257.076498	-0.221713	-0.322477	0.100764	-128.330068	128.847603	-257.177671
2.60	-128.550692	128.527943	-257.078635	-0.220927	-0.319231	0.098304	-128.330173	128.847174	-257.177346
2.70	-128.550157	128.530139	-257.080296	-0.220372	-0.316855	0.096484	-128.33019	128.846994	-257.177185
2.80	-128.549731	128.532014	-257.081745	-0.219965	-0.315033	0.095069	-128.330169	128.847047	-257.177217
2.90	-128.549388	128.53337	-257.082758	-0.219693	-0.31378	0.094087	-128.330097	128.84715	-257.177246
3.00	-128.549108	128.534447	-257.083555	-0.219521	-0.31292	0.093399	-128.329986	128.847367	-257.177353
3.10	-128.548878	128.535316	-257.084194	-0.219426	-0.312356	0.09293	-128.32985	128.847672	-257.177522
3.20	-128.548687	128.53602	-257.084707	-0.219386	-0.312014	0.092628	-128.329697	128.848034	-257.177731
3.30	-128.548526	128.536603	-257.085129	-0.219388	-0.311837	0.09245	-128.329533	128.84844	-257.177974
3.40	-128.548391	128.537084	-257.085475	-0.219416	-0.311798	0.092383	-128.329369	128.848882	-257.178251
3.50	-128.548275	128.537466	-257.085741	-0.21947	-0.311827	0.092357	-128.329196	128.849293	-257.17849
3.60	-128.548177	128.537794	-257.085971	-0.219536	-0.311918	0.092381	-128.32903	128.849712	-257.178742
3.70	-128.548092	128.538062	-257.086154	-0.219611	-0.312037	0.092427	-128.32887	128.850099	-257.17897
3.80	-128.54802	128.538277	-257.086297	-0.21969	-0.31217	0.09248	-128.328717	128.850447	-257.179164
3.90	-128.547957	128.538444	-257.086401	-0.219768	-0.312307	0.092538	-128.328575	128.850751	-257.179325
4.00	-128.547902	128.538583	-257.086485	-0.219845	-0.312439	0.092595	-128.328442	128.851022	-257.179465

Table S5: IEA data for ArH^+ at the SCGVB(2,3)/aug-cc-pVTZ level.

Distances Ar-H	E[TOT]	T[TOT]	V[TOT]	E[I]	T[I]	V[I]	E[QC]	T[QC]	V[QC]
1.00	-526.905306	527.542213	-1054.447519	-0.557998	-0.915894	0.357896	-526.348667	528.458107	-1054.806774
1.05	-526.934359	527.381726	-1054.316085	-0.540141	-0.905537	0.365396	-526.395686	528.287263	-1054.682949
1.10	-526.954146	527.247392	-1054.201538	-0.517235	-0.887868	0.370633	-526.438456	528.13526	-1054.573716
1.15	-526.966914	527.134776	-1054.10169	-0.493914	-0.870622	0.376708	-526.474612	528.005398	-1054.48001
1.20	-526.974358	527.040195	-1054.014553	-0.463558	-0.862979	0.399421	-526.512413	527.903174	-1054.415587
1.25	-526.977824	526.960785	-1053.938609	-0.4482	-0.849276	0.401076	-526.531334	527.810061	-1054.341395
1.26	-526.978125	526.946589	-1053.924714	-0.445079	-0.845584	0.400505	-526.534772	527.792173	-1054.326945
1.27	-526.978314	526.932834	-1053.911148	-0.441623	-0.84248	0.400857	-526.53843	527.775314	-1054.313744
1.28	-526.978396	526.919435	-1053.897831	-0.438002	-0.840017	0.402015	-526.542144	527.759452	-1054.301596
1.29	-526.978379	526.906586	-1053.884965	-0.434325	-0.838012	0.403687	-526.545814	527.744598	-1054.290412
1.30	-526.978266	526.894228	-1053.872494	-0.430698	-0.836262	0.405564	-526.549339	527.73049	-1054.279829
1.31	-526.978066	526.882261	-1053.860327	-0.427092	-0.834595	0.407503	-526.552754	527.716856	-1054.26961
1.32	-526.977781	526.870719	-1053.8485	-0.423541	-0.833043	0.409502	-526.55603	527.703762	-1054.259792
1.33	-526.977418	526.859584	-1053.837002	-0.420049	-0.831581	0.411532	-526.559169	527.691165	-1054.250334
1.34	-526.976981	526.848843	-1053.825824	-0.416615	-0.8302	0.413585	-526.562175	527.679043	-1054.241218
1.35	-526.976474	526.838484	-1053.814958	-0.413238	-0.82889	0.415652	-526.565053	527.667374	-1054.232427
1.40	-526.973039	526.791986	-1053.765025	-0.397562	-0.822022	0.42446	-526.577343	527.614008	-1054.191351
1.50	-526.962971	526.721417	-1053.684388	-0.369094	-0.81177	0.442676	-526.595819	527.533187	-1054.129006
1.60	-526.950619	526.673771	-1053.62439	-0.34359	-0.802886	0.459296	-526.609001	527.476657	-1054.085658
1.70	-526.937486	526.642543	-1053.580029	-0.320414	-0.790583	0.470169	-526.619009	527.433126	-1054.052135
1.80	-526.924429	526.623303	-1053.547732	-0.299218	-0.771634	0.472416	-526.627074	527.394937	-1054.022011
1.90	-526.911921	526.612013	-1053.523934	-0.279443	-0.746468	0.467025	-526.634206	527.358481	-1053.992687
2.00	-526.900203	526.606491	-1053.506694	-0.261685	-0.716885	0.4552	-526.64011	527.323376	-1053.963486

2.10	-526.889397	526.605263	-1053.49466	-0.246036	-0.686059	0.440023	-526.64483	527.291322	-1053.936152
2.20	-526.879548	526.607394	-1053.486942	-0.23262	-0.657133	0.424513	-526.648302	527.264527	-1053.912829
2.30	-526.870664	526.612314	-1053.482978	-0.22124	-0.63131	0.41007	-526.65072	527.243624	-1053.894344
2.40	-526.862723	526.619673	-1053.482396	-0.211454	-0.607509	0.396055	-526.652499	527.227182	-1053.879681
2.50	-526.855685	526.629183	-1053.484868	-0.203082	-0.582815	0.379733	-526.653775	527.211998	-1053.865773
2.60	-526.849525	526.641183	-1053.490708	-0.193589	-0.54993	0.356341	-526.657016	527.191113	-1053.848129
2.70	-526.844105	526.655224	-1053.499329	-0.186024	-0.501262	0.315238	-526.659108	527.156486	-1053.815594
2.80	-526.839322	526.673672	-1053.512994	-0.176719	-0.411451	0.234732	-526.663545	527.085123	-1053.748668
2.90	-526.835543	526.692665	-1053.528208	-0.162029	-0.302656	0.140627	-526.67421	526.995321	-1053.669531
3.00	-526.832892	526.706013	-1053.538905	-0.150007	-0.245156	0.095149	-526.683408	526.951169	-1053.634577
3.10	-526.830859	526.716905	-1053.547764	-0.14096	-0.205	0.06404	-526.690321	526.921905	-1053.612226
3.20	-526.829272	526.725662	-1053.554934	-0.133861	-0.173649	0.039788	-526.695766	526.899311	-1053.595077
3.30	-526.828028	526.732754	-1053.560782	-0.128242	-0.148171	0.019929	-526.700096	526.880925	-1053.581021
3.40	-526.827049	526.738566	-1053.565615	-0.123805	-0.127286	0.003481	-526.703525	526.865852	-1053.569377
3.50	-526.826276	526.743183	-1053.569459	-0.120265	-0.109914	-0.010351	-526.706272	526.853097	-1053.559369
3.60	-526.825664	526.746892	-1053.572556	-0.11741	-0.095323	-0.022087	-526.708501	526.842215	-1053.550716
3.70	-526.825174	526.749857	-1053.575031	-0.115081	-0.082983	-0.032098	-526.71033	526.83284	-1053.54317
3.80	-526.824781	526.752213	-1053.576994	-0.113157	-0.072502	-0.040655	-526.711854	526.824715	-1053.536569
3.90	-526.824462	526.7541	-1053.578562	-0.11155	-0.063587	-0.047963	-526.713135	526.817687	-1053.530822
4.00	-526.8242	526.755637	-1053.579837	-0.110319	-0.056672	-0.053647	-526.7141	526.812309	-1053.526409

Table S6: Chirgwin–Coulson coefficients along the potential energy curves of HeH^+, NeH^+ and ArH^+.

Distance He–H	closed-shell	bonding	Distance Ne–H	closed-shell	bonding	Distance Ar–H	closed-shell	bonding
0.50	0.2484	0.7516	0.70	0.5804	0.4196	1.00	0.4934	0.5067
0.55	0.2883	0.7117	0.75	0.6090	0.3910	1.05	0.4904	0.5096
0.60	0.3144	0.6856	0.80	0.6223	0.3777	1.10	0.4857	0.5143
0.65	0.3338	0.6663	0.85	0.6337	0.3663	1.15	0.4820	0.5180
0.67	0.3360	0.6640	0.87	0.6347	0.3653	1.20	0.4833	0.5167
0.70	0.3450	0.6551	0.90	0.6405	0.3596	1.25	0.4816	0.5184
0.73	0.3553	0.6448	0.93	0.6466	0.3534	1.26	0.4808	0.5193
0.75	0.3621	0.6380	0.95	0.6505	0.3495	1.27	0.4802	0.5198
0.77	0.3695	0.6306	0.96	0.6515	0.3485	1.28	0.4798	0.5202
0.80	0.3811	0.6189	0.97	0.6532	0.3468	1.29	0.4797	0.5203
0.85	0.4016	0.5985	0.98	0.6553	0.3447	1.30	0.4797	0.5203
0.90	0.4191	0.5809	0.99	0.6580	0.3420	1.31	0.4798	0.5202
0.95	0.4344	0.5657	1.00	0.6611	0.3388	1.32	0.4799	0.5202
1.00	0.4501	0.5498	1.01	0.6647	0.3353	1.33	0.4800	0.5200
1.10	0.4801	0.5199	1.02	0.6686	0.3314	1.34	0.4802	0.5198
1.15	0.4952	0.5048	1.03	0.6726	0.3275	1.35	0.4804	0.5197
1.20	0.5109	0.4890	1.04	0.6772	0.3229	1.40	0.4816	0.5185
1.30	0.5443	0.4557	1.05	0.6824	0.3176	1.50	0.4863	0.5137
1.40	0.5841	0.4159	1.10	0.7175	0.2825	1.60	0.4934	0.5066

1.50	0.7464	0.2537	1.15	0.7502	0.2498	1.70	0.5014	0.4986
1.60	0.8310	0.1689	1.20	0.7762	0.2238	1.80	0.5097	0.4903
1.70	0.8825	0.1174	1.30	0.8142	0.1859	1.90	0.5185	0.4815
1.80	0.9189	0.0810	1.40	0.8282	0.1719	2.00	0.5279	0.4721
1.90	0.9448	0.0552	1.50	0.8545	0.1455	2.10	0.5388	0.4612
2.00	0.9620	0.0380	1.60	0.8807	0.1194	2.20	0.5522	0.4478
2.10	0.9736	0.0264	1.70	0.9048	0.0952	2.30	0.5695	0.4306
2.20	0.9815	0.0185	1.80	0.9266	0.0734	2.40	0.5919	0.4081
2.30	0.9869	0.0131	1.90	0.9448	0.0552	2.50	0.6204	0.3796
2.40	0.9907	0.0093	2.00	0.9592	0.0408	2.60	0.6559	0.3441
2.50	0.9934	0.0066	2.10	0.9701	0.0299	2.70	0.7018	0.2981
2.60	0.9954	0.0046	2.20	0.9781	0.0218	2.80	0.7652	0.2348
2.70	0.9967	0.0032	2.30	0.9841	0.0159	2.90	0.8360	0.1640
2.80	0.9977	0.0022	2.40	0.9885	0.0115	3.00	0.8787	0.1213
2.90	0.9985	0.0016	2.50	0.9917	0.0083	3.10	0.9089	0.0911
3.00	0.9990	0.0010	2.60	0.9941	0.0060	3.20	0.9320	0.0680
3.10	0.9993	0.0006	2.70	0.9958	0.0042	3.30	0.9496	0.0504
3.20	0.9996	0.0004	2.80	0.9971	0.0029	3.40	0.9628	0.0373
3.30	0.9998	0.0002	2.90	0.9980	0.0020	3.50	0.9726	0.0275
3.40	0.9999	0.0001	3.00	0.9987	0.0013	3.60	0.9799	0.0202
3.50	1.0000	0.0000	3.10	0.9991	0.0009	3.70	0.9852	0.0148
3.60	1.0000	0.0000	3.20	0.9994	0.0006	3.80	0.9892	0.0108
3.70	1.0000	0.0000	3.30	0.9996	0.0003	3.90	0.9922	0.0078
3.80	1.0000	0.0000	3.40	0.9998	0.0002	4.00	0.9943	0.0057
3.90	1.0000	0.0000	3.50	0.9999	0.0002	-	-	-
4.00	1.0000	0.0000	3.60	0.9999	0.0000	-	-	-
-	-	-	3.70	0.9999	0.0000	-	-	-
-	-	-	3.80	1.0000	0.0000	-	-	-
-	-	-	3.90	1.0000	0.0000	-	-	-
-	-	-	4.00	1.0000	0.0000	-	-	-