Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for Binding of the Atomic Cations Hydrogen through Argon to Water and Hydrogen Sulfide

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Complex	Term Symbol	Atom	X	Y	Z
H_2OH^+	$^1A'$	H	−1.764524250	−0.452504876	0.000000000
		O	0.000011932	0.085528815	0.000000000
		H	0.882167425	−0.452562634	1.528173652
		H	0.882167425	−0.452562634	−1.528173652
H_2OLi^+	$^1A_1$	Li	0.000000000	0.000000000	−2.606863119
		O	0.000000000	0.000000000	0.880925209
		H	0.000000000	1.445727505	1.984226304
		H	0.000000000	−1.445727505	1.984226304
H_2OBe^+	$^2A_1$	Be	0.000000000	0.000000000	−2.045592745
		O	0.000000000	0.000000000	0.905012644
		H	0.000000000	1.498922856	1.962215377
		H	0.000000000	−1.498922856	1.962215377
H_2OB^+	$^1A_1$	B	0.000000000	0.000000000	−1.843697338
		O	0.000000000	0.000000000	0.992212616
		H	0.000000000	1.544275082	2.011807100
		H	0.000000000	−1.544275082	2.011807100
H_2OC^+	$^2B_2$	C	0.000000000	0.000000000	−1.645040084
		O	0.000000000	0.000000000	0.987243811
		H	0.000000000	1.582491284	1.966023680
		H	0.000000000	−1.582491284	1.966023680
H_2ON^+	$^3A''$	N	−0.024521332	0.000000000	−1.585729932
		O	0.104609300	0.000000000	1.153740126
		H	−0.659872159	1.541985354	1.861069939
		H	−0.659872159	−1.541985354	1.861069939
H_2ON^+	$^1A_1$	N	0.000000000	0.000000000	−1.445060360
		O	0.000000000	0.000000000	1.016859642
		H	0.000000000	1.616068918	1.970049205
		H	0.000000000	−1.616068918	1.970049205
H_2OO^+	$^2A'$	O	−0.019100363	0.000000000	−1.405253495
		O	0.086129907	0.000000000	1.166020504
		H	−0.531992223	1.598828317	1.898716345
		H	−0.531992223	−1.598828317	1.898716345
H_2OO^+	$^2A''$	O	−0.020214907	0.000000000	−1.483784647
		O	0.128595605	0.000000000	1.260476109
		H	−0.860183218	1.508048033	1.772329022
		H	−0.860183218	−1.508048033	1.772329022
H_2OO^+	$^4A''$	O	−0.013700716	0.000000000	−1.996353229
		O	0.122592239	0.000000000	1.720633034
		H	−0.864237476	1.492925122	2.188303713
		H	−0.864237476	−1.492925122	2.188303713
H_2OF^+	$^1A'$	F	−0.015714364	0.000000000	−1.320817654
		O	0.123464419	0.000000000	1.339887668
		H	−0.831799914	1.542665483	1.813613565
		H	−0.831799914	−1.542665483	1.813613565
H_2ONe^+	$^2A'$	Ne	0.008158217	0.000000000	−2.317346334
		O	0.102429308	0.000000000	2.646372642
		H	−0.894612838	1.537267206	2.193264088
		H	−0.894612838	−1.537267206	2.193264088

H_2ONa^+	$^1A_1$	Na	0.000000000	0.000000000	−1.939000464
		O	0.000000000	0.000000000	2.349844791
		H	0.000000000	1.436189172	3.463140381
		H	0.000000000	−1.436189172	3.463140381
H_2OMg^+	$^2A_1$	Mg	0.000000000	0.000000000	−1.699525044
		O	0.000000000	0.000000000	2.170283364
		H	0.000000000	1.458904554	3.265930777
		H	0.000000000	−1.458904554	3.265930777
H_2OAl^+	$^1A_1$	Al	0.000000000	0.000000000	−1.593219091
		O	0.000000000	0.000000000	2.264625915
		H	0.000000000	1.472332434	3.350818879
		H	0.000000000	−1.472332434	3.350818879
H_2OAl^+	$^3B_2$	Al	0.000000000	0.000000000	−1.461128573
		O	0.000000000	0.000000000	2.070522378
		H	0.000000000	1.495143594	3.123391914
		H	0.000000000	−1.495143594	3.123391914
H_2OSi^+	$^2B_2$	Si	0.000000000	0.000000000	−1.427263115
		O	0.000000000	0.000000000	2.107898833
		H	0.000000000	1.505395678	3.155089407
		H	0.000000000	−1.505395678	3.155089407
H_2OSi^+	$^4A_2$	Si	0.000000000	0.000000000	−1.367305420
		O	0.000000000	0.000000000	2.017914886
		H	0.000000000	1.523659182	3.033925103
		H	0.000000000	−1.523659182	3.033925103
H_2OP^+	$^3A''$	P	−0.007619735	0.000000000	−1.312153002
		O	0.070895962	0.000000000	2.154084263
		H	−0.445602424	1.509866296	3.064793745
		H	−0.445602424	−1.509866296	3.064793745
H_2OP^+	$^1A_1$	P	0.000000000	0.000000000	−1.260246701
		O	0.000000000	0.000000000	2.053808939
		H	0.000000000	1.537748776	3.063112938
		H	0.000000000	−1.537748776	3.063112938
H_2OS^+	$^2A'$	S	−0.006638902	0.000000000	−1.209995801
		O	0.062092291	0.000000000	2.053729406
		H	−0.387223555	1.548669216	2.943641048
		H	−0.387223555	−1.548669216	2.943641048
H_2OS^+	$^2A''$	S	−0.009420158	0.000000000	−1.252198434
		O	0.112005909	0.000000000	2.151221341
		H	−0.739139764	1.490477788	2.841057543
		H	−0.739139764	−1.490477788	2.841057543
H_2OS^+	$^4A''$	S	−0.005603490	0.000000000	−1.648454260
		O	0.062117359	0.000000000	2.823185741
		H	−0.403889409	1.461731875	3.809832741
		H	−0.403889409	−1.461731875	3.809832741
H_2OCl^+	$^1A'$	Cl	−0.008195732	0.000000000	−1.127239783
		O	0.111131595	0.000000000	2.146776737
		H	−0.737879009	1.519147643	2.786322745
		H	−0.737879009	−1.519147643	2.786322745
H_2OCl^+	$^3A'$	Cl	−0.006246835	0.000000000	−1.419486877
		O	0.115549369	0.000000000	2.730267632
		H	−0.807216475	1.491221964	3.295049457
		H	−0.807216475	−1.491221964	3.295049457
H_2OAr^+	$^2A'$	Ar	−0.001138085	0.000000000	−1.391867136
		O	0.124822818	0.000000000	3.074753832
		H	−0.968126073	1.515335178	3.178806227
		H	−0.968126073	−1.515335178	3.178806227

Complex	Term Symbol	Atom	X	Y	Z
H_2SH^+	$^1A'$	H	−2.162843888	−1.243602880	0.000000000
		S	0.000005577	0.117300571	0.000000000
		H	1.081333243	−1.243714513	1.873056993
		H	1.081333243	−1.243714513	−1.873056993
H_2SLi^+	$^1A'$	Li	−0.050911154	0.000000000	−3.843310826
		S	0.108631599	0.000000000	0.752154242
		H	−1.552351698	1.846334943	1.271085298
		H	−1.552351698	−1.846334943	1.271085298
H_2SBe^+	$^2A'$	Be	−0.027635995	0.000000000	−3.185068348
		S	0.108638495	0.000000000	0.824101016
		H	−1.604207381	1.866174652	1.132870361
		H	−1.604207381	−1.866174652	1.132870361
H_2SB^+	$^1A'$	B	−0.013236403	0.000000000	−3.120356572
		S	0.106762010	0.000000000	0.979299676
		H	−1.626934397	1.866288894	1.158157690
		H	−1.626934397	−1.866288894	1.158157690
H_2SC^+	$^2A''$	C	−0.044522264	0.000000000	−2.546920756
		S	0.106703326	0.000000000	0.860385793
		H	−1.431708094	1.947048250	1.491704203
		H	−1.431708094	−1.947048250	1.491704203
H_2SN^+	$^3A''$	N	−0.028677342	0.000000000	−2.327664910
		S	0.111654981	0.000000000	0.932397419
		H	−1.576474666	1.891531121	1.344446509
		H	−1.576474666	−1.891531121	1.344446509
	$^1A_1$	N	0.000000000	0.000000000	−2.038802018
		S	0.000000000	0.000000000	0.747200061
		H	0.000000000	2.082616699	2.282702479
		H	0.000000000	−2.082616699	2.282702479
H_2SO^+	$^2A'$	O	−0.051210411	0.000000000	−1.940063511
		S	0.100511511	0.000000000	0.854535739
		H	−1.192066588	2.009760883	1.807367682
		H	−1.192066588	−2.009760883	1.807367682
	$^2A''$	O	−0.026251734	0.000000000	−2.097933767
		S	0.118374629	0.000000000	0.962496710
		H	−1.674245799	1.823161102	1.343352283
		H	−1.674245799	−1.823161102	1.343352283
	$^4A_2$	O	−0.000120106	0.000000000	−1.982682717
		S	−0.000538665	0.000000000	0.948276331
		H	0.009520024	2.815316336	0.654798256
		H	0.009520024	−2.815316336	0.654798256
H_2SF^+	$^1A'$	F	−0.028006568	0.000000000	−1.887015610
		S	0.115665466	0.000000000	1.023230295
		H	−1.575567381	1.865288975	1.510764418
		H	−1.575567381	−1.865288975	1.510764418
	$^3B_1$	F	0.000000000	0.000000000	−1.870867229
		S	0.000000000	0.000000000	1.051836202
		H	0.000000000	2.723328334	0.903635599
		H	0.000000000	−2.723328334	0.903635599
H_2SNe^+	$^2A'$	Ne	0.020883105	0.000000000	−3.664218375
		S	0.079743436	0.000000000	2.219121989
		H	−1.477257933	1.860524545	1.386596240
		H	−1.477257933	−1.860524545	1.386596240

H_2SNa^+	$^1A'$	Na	−0.014367061	0.000000000	−3.227816099
		S	0.107027704	0.000000000	2.143853880
		H	−1.538291579	1.840732429	2.716004773
		H	−1.538291579	−1.840732429	2.716004773
H_2SMg^+	$^2A'$	Mg	−0.010370293	0.000000000	−2.956563969
		S	0.107795740	0.000000000	2.085337014
		H	−1.589321505	1.849552819	2.481984355
		H	−1.589321505	−1.849552819	2.481984355
H_2SAl^+	$^1A'$	Al	−0.008297755	0.000000000	−2.925397194
		S	0.107438102	0.000000000	2.294883016
		H	−1.597604690	1.849131342	2.657783154
		H	−1.597604690	−1.849131342	2.657783154
	$^3A''$	Al	−0.01858625	7 0.000000000	−2.452200490
		S	0.106177573	0.000000000	1.897215487
		H	−1.439851150	1.883070187	2.648678045
		H	−1.439851150	−1.883070187	2.648678045
H_2SSi^+	$^2A''$	Si	−0.014692200	0.000000000	−2.452986662
		S	0.106377864	0.000000000	1.985620013
		H	−1.487110616	1.889797249	2.596572855
		H	−1.487110616	−1.889797249	2.596572855
H_2SP^+	$^3A''$	P	−0.010858010	0.000000000	−2.207656741
		S	0.109497396	0.000000000	1.980430208
		H	−1.574584361	1.868387825	2.424170872
		H	−1.574584361	−1.868387825	2.424170872
	$^1A_1$	P	0.000000000	0.000000000	−1.955210786
		S	0.000000000	0.000000000	1.683158025
		H	0.000000000	2.010028037	3.273103232
		H	0.000000000	−2.010028037	3.273103232
H_2SS^+	$^2A'$	S	−0.016467160	0.000000000	−1.976341240
		S	0.107317315	0.000000000	1.818729724
		H	−1.444855832	1.911857696	2.506610121
		H	−1.444855832	−1.911857696	2.506610121
	$^2A''$	S	−0.010255664	0.000000000	−2.050523678
		S	0.112727568	0.000000000	1.905793293
		H	−1.629684917	1.839191458	2.301752165
		H	−1.629684917	−1.839191458	2.301752165
	$^4A''$	S	−0.001398414	0.000000000	−2.681242435
		S	0.104853753	0.000000000	2.518466042
		H	−1.645325211	1.847442514	2.588750893
		H	−1.645325211	−1.847442514	2.588750893
H_2SCl^+	$^1A'$	Cl	−0.011729691	0.000000000	−1.845157562
		S	0.111902285	0.000000000	1.890749339
		H	−1.573374673	1.864091411	2.380571885
		H	−1.573374673	−1.864091411	2.380571885
	$^3A'$	Cl	0.001239572	0.000000000	−2.512589478
		S	0.102020971	0.000000000	2.618155745
		H	−1.644313593	1.860569277	2.550132737
		H	−1.644313593	−1.860569277	2.550132737
	$^3B_1$	Cl	0.000000000	0.000000000	−3.295126488
		S	0.000000000	0.000000000	3.323962406
		H	0.000000000	1.863975227	5.087547203
		H	0.000000000	−1.863975227	5.087547203
H_2SAr^+	$^2A'$	Ar	0.004970907	0.000000000	−2.623490712
		S	0.096459682	0.000000000	3.095999149
		H	−1.632574951	1.858530359	2.750895014
		H	−1.632574951	−1.858530359	2.750895014