Coordinates of the lowest energy ion-radical and hemibonded isomers in Å evaluated at the MP2/6-31+G* level of theory and CCSD(T)/aug-cc-pVTZ energies at the MP2/6-31+G* structure.

Ion-radical Isomers

$(NH_3)_2^+$ -112.65271300 a.u.

H	1.685936	-0.950073	0.161938
N	1.335100	0.000339	0.000347
H	1.684634	0.615020	0.743638
H	0.269648	-0.000395	-0.000140
H	1.685270	0.336113	-0.903632
H	-2.127265	-0.820696	-0.001022
N	-1.510477	-0.000539	-0.001443
H	-2.125888	0.820666	-0.000945

$(H_2O)_2^+$ -152.29595821 a.u.

H	1.590109	-0.827179	0.029916
O	1.204667	0.040161	-0.240035
H	1.659406	0.771789	0.239827
H	0.168544	0.059712	-0.108640
H	-2.061942	0.490143	-0.257413
O	-1.358555	-0.093886	0.117055

$(HF)_2^+$ -200.18994685 a.u.

H	0.081872	-0.066630	0.004450
F	-1.370823	-0.133854	0.008754
H	1.546186	0.782029	0.006905
F	1.120173	-0.101221	0.015077

$(PH_3)_2^+$ -685.16995900 a.u.

H	2.412934	-1.290206	0.216426
P	1.934091	0.000234	-0.000121
H	2.418552	0.830639	1.008381
H	0.528416	0.003383	-0.000114
H	2.417941	0.455848	-1.224692
H	-2.987888	-1.052721	0.006478
P	-2.050164	0.000195	-0.000626
H	-2.993071	1.048486	0.005041

$(H_2S)_2^+$ -797.59314673 a.u.

H	1.917316	-1.230823	0.114184
S	1.746446	0.084039	-0.117877
H	1.971752	0.476167	1.149678
H	0.352704	0.073255	-0.036422
H	-2.310533	1.116385	-0.287118
S	-1.863808	-0.100959	0.071096

$(HCl)_2^+$ -920.30138486 a.u.

H	1.909375	-1.147891	0.067353
Cl	1.695880	0.140052	0.123919
H	0.237381	0.086038	0.109349
Cl	-1.549060	0.116570	0.098721

$(NH_3)_3^+$ -169.16661467 a.u.

H	3.16849917015	-0.03408674749	0.09105229508
N	2.32288772797	0.52874387072	-0.01567701495
H	2.44186743649	1.04696965129	-0.88764837464
H	2.35687158705	1.22590482452	0.72981100575
H	0.83170298918	-0.44229382824	0.01056754919
N	-0.05208182848	-1.04445209890	0.02485035999
H	-0.06231623547	-1.61836802709	0.87255926877
H	-0.05281991138	-1.66834676884	-0.78675873641
H	-0.91661868825	-0.45165223992	0.00195380560
N	-2.51210249915	0.54352368384	-0.01739884492
H	-2.67345761635	1.47261634711	0.38706029769
H	-3.41410886907	0.25544329074	-0.41322136768

$(H_2O)_3^+$ -228.68214812 a.u.

H	0.82413718253	0.33979222097	-0.02853018632
O	-2.22366966847	-0.58484454297	0.00708562292
H	-3.18719315875	-0.40011838364	-0.08378615259
O	2.05151660691	-0.43101466973	0.03800452549
H	2.17997340147	-1.23286970300	0.57873166845
H	2.65414889778	-0.49204422393	-0.72734358860
O	-0.02573380919	0.96821614837	-0.09911891970
H	-0.89613563601	0.46180070376	-0.03208954392
H	0.00909723410	1.68810306559	0.56650335600

$(HF)_3^+$ -300.58425826 a.u.

H	2.81584888775	0.02383783355	0.02160861973
F	1.96251778860	0.47374313023	0.00540492784
H	0.93839486379	-0.21510584587	0.00251572509
F	0.00922120855	-0.82542633027	-0.00039463430
H	-0.84508495366	-0.32482037375	-0.00552841497
F	-2.29875629875	0.40777475628	-0.00330911813

$(PH_3)_3^+$ -1027.93242618 a.u.

H	-4.22043303393	0.52528824517	0.61392853487
P	-2.96285114556	0.69299551945	-0.00245202281
H	-3.28092437324	1.89987863311	-0.65969262250
H	-0.05150987734	-0.58092301834	1.12413829360
H	3.96147859659	0.31665358382	-0.76169544849
P	2.84210009183	0.66567798475	0.01828402002
H	3.53915118967	0.87855954590	1.22329908639
H	2.77708614628	2.01547096544	-0.37771484751

H	1.08388873268	-2.18152362018	-0.02299256540
P	-0.04060578873	-1.36296183718	-0.02160407148
H	-1.17167687567	-2.17552467953	-0.03401835264
H	-0.04060993236	-0.56580572676	-1.15716956448

$(H_2S)_3^+$ -1196.59256017 a.u.

S	2.54629227899	-1.18252648868	0.14298033698
H	1.00275390103	0.55667435300	0.18015246029
H	3.49778742732	-0.83281583799	1.02714749662
S	0.02558203486	1.52817793387	0.19350180920
H	0.16230558447	1.89118908014	-1.09421149820
H	-1.04522013783	0.67227390432	-0.00196710838
S	-2.66876857534	-0.87900327053	-0.18027128032
H	-3.70853440378	-0.41062724266	0.52353637036
H	-3.26935074099	-0.73165327141	-1.36914861091

$(HCl)_3^+$ -1380.71803589 a.u.

H	1.19169059887	-0.65787251393	-0.08074314857
Cl	2.87362239104	0.63397957553	0.25933984163
H	-0.81947488792	-0.55476281689	-0.22078656515
Cl	0.16952173778	-1.48609185017	-0.28332982080
H	-2.95502645702	0.73147523657	-1.09176579357
Cl	-2.24439334838	0.80740751210	-0.01930179460

$(NH_3)_4^+$ -225.67390053 a.u.

H	0.04587712961	0.00845206697	1.69585278620
N	0.03795786762	0.00975986959	0.67337377924
H	-0.12143797823	-0.97459540179	0.33423800833
H	-0.73370018703	0.64600456875	0.34199735770
H	0.39817770814	-3.34089408850	-0.01672425797
N	-0.39513697269	-2.73441107085	-0.22836398328
H	-1.20705929983	-3.17450022402	0.20637492027
H	-0.54241491151	-2.80855312099	-1.23560895501
H	-1.94460675567	2.75752131698	0.10290199129
N	-2.09890443623	1.79555977559	-0.20177828057
H	-3.01533932996	1.53114718808	0.16172796558
H	-2.20171707703	1.83666941858	-1.21640412575
H	0.95832684305	0.35892878934	0.33714344195
N	2.70089053381	1.01981657138	-0.22637674044
H	2.94464389068	1.43677173469	-1.13193739993
H	3.57153466132	1.02596547373	0.31720189674

$(H_2O)_4^+$ -305.05841597 a.u.

H	0.97808445236	-0.09957796960	-0.25213147739
O	-1.16394409700	2.36759346028	0.22104614909
H	-1.01269461226	3.31126608545	-0.01470859085
O	0.01908810196	0.03005802560	-0.58274069388
H	-0.59720099231	-0.72188597408	-0.26283003843

H	-0.33868072061	0.92244504305	-0.30851315118
O	2.48847912440	-0.21137080541	0.16984950669
H	2.83433656557	-0.56755529790	1.00828497696
H	3.20346971614	-0.29372807541	-0.48756550426
O	-1.49804444731	-1.93308615598	0.16773051450
H	-1.86675469560	-2.55608376180	-0.48511438652
H	-2.07402744621	-1.97439045043	0.95272405752

$(HF)_4^+$ -400.96592290 a.u.

H	2.85565872305	0.26033608081	1.90772876541
F	2.20286648926	0.61270016173	1.30195447460
H	1.15649238423	-0.14588841822	0.83566411563
F	0.35800497216	-0.68042871180	0.45283455377
H	-0.31064421914	-0.10816126260	-0.16813473891
F	-1.07807483321	0.61105716782	-0.89453657696
H	-1.87334167120	0.23169750713	-1.30096231140
F	-3.31569423439	-0.31795484075	-2.10112924665

$(PH_3)_4^+$ -1370.69138375 a.u.

H	1.97183681221	3.30929043487	-1.25052587416
P	2.36076828287	2.31346798191	-0.33308584803
H	3.49272510028	1.87089977009	-1.04563278419
H	3.05080873183	3.16805482034	0.54908695340
H	0.56571882768	-3.65168109021	-1.54050892690
P	0.82918113569	-3.25423463857	-0.21481892043
H	0.27700237860	-4.39071693025	0.40821216013
H	2.16962409847	-3.68671792239	-0.17997621252
H	-0.36296278315	1.27795321043	1.35149604760
P	-0.03167882246	0.00187954358	0.91155814436
H	1.21696578486	-0.33794949924	1.41342205644
H	-0.97637889600	-0.89473777558	1.39658579952
H	-3.76832457753	0.97493438159	-1.70809277465
P	-3.27228046134	0.88083418737	-0.39011309614
H	-0.01907525288	-0.03092551334	-0.47248901442
H	-4.48045434245	1.25130827131	0.23787287067

$(H_2S)_4^+$ -1595.59156935 a.u.

H	-3.20864541452	-2.75953691295	0.11372530928
S	-2.49275704358	-1.92605440899	0.88064904776
H	-3.51337193080	-1.08757021857	1.10608818317
H	0.67060737291	3.55196500973	0.66337959013
S	-0.37059034389	3.20930342213	-0.11652312808
H	-0.05542880831	0.93686080018	-0.79220130530
H	2.55255061373	-2.15102570859	1.82111988150
S	2.84010448631	-1.08114878277	1.06720943045
H	3.81955409839	-1.68993490896	0.38467247201
H	1.09146076156	-0.70517416691	-0.41154066154
S	0.07257637593	-0.34351441205	-1.25755235312
H	-0.94065308001	-0.88538526746	-0.50731330449

$(HCl)_4^+$ -1841.10538335 a.u.

H	-0.35341660378	-0.95565181448	-0.06976900447
Cl	-1.36705729923	-1.25889348088	-0.99517295988
H	-2.30124059075	-0.47215579074	-0.48845065595
Cl	-3.88635264941	0.83657228576	0.30771249770
H	1.79731225716	0.09689767861	0.56023559745
Cl	0.93410075051	-0.64274909249	1.19783163039
H	4.41245030361	1.30174536648	-0.15624460024
Cl	3.22932448550	1.42116165744	-0.64279058519

Hemibonded

$(NH_3)_2^+$ -112.64440839 a.u.

H	-1.363590	-0.716402	0.667551
N	-1.081358	-0.000027	-0.000008
H	-1.363667	0.936250	0.286648
H	-1.363719	-0.219946	-0.954155
H	1.363551	0.716840	-0.667058
N	1.081199	0.000040	-0.000003
H	1.363485	0.219370	0.954300
H	1.363648	-0.936031	-0.287197

$(H_2O)_2^+$ -152.28467104 a.u.

H	1.344319	-0.793212	0.281152
O	1.106868	0.014638	-0.239330
H	1.319208	0.779740	0.352116
H	-1.117457	-0.814235	-0.378435
O	-0.888707	0.003164	0.131173
H	-1.109137	0.757906	-0.470505

$(HF)_2^+$ -200.17225903 a.u.

H	1.183530	-0.921482	-0.128953
F	0.997126	0.034486	-0.156903
H	-1.099516	0.882753	-0.214369
F	-0.913024	-0.072980	-0.179961

$(PH_3)_2^+$ -685.17828973 a.u.

H	-1.62258742798	-1.08812100390	0.84564886412
P	-1.35160134797	-0.00586344441	0.00133220822
H	-2.41419929095	-0.02493928736	-0.92286747952
H	-1.62832503706	1.10420896360	0.80676883984
H	1.63094953247	-1.10633626820	-0.80097574834
P	1.34847460348	0.00359152958	0.00266649309
H	2.40525659798	0.02406660357	0.93331240924
H	1.62316548016	1.08612791676	-0.84014601561

$(H_2S)_2^+$ -797.62982887 a.u.

H	1.544205	-1.013981	0.743184
S	1.412276	0.001441	-0.128596
H	1.539570	0.955532	0.810411
H	-1.545244	-1.006538	-0.745602
S	-1.407175	0.006521	0.128008
H	-1.534258	0.963204	-0.808440

$(HCl)_2^+$ -920.34270874 a.u.

H	1.47599937523	-1.20622996260	0.00444142585
Cl	1.32314887928	0.08205471404	-0.00472478062
H	-1.47600886155	1.20622889244	0.00444142682
Cl	-1.32315412798	-0.08205531414	-0.00472480623

$(NH_3)_3^+$ -169.14920589 a.u.

H	-1.69935561035	-1.16533291252	0.80895316713
N	-1.90278738799	-0.58736481473	-0.00382321824
H	-2.81804409121	-0.14460783509	0.05330268686
H	-1.76811653442	-1.08951785977	-0.87893130135
H	0.50895435061	0.47675396097	0.00258517594
N	-0.41755408396	0.96272421216	0.00758408561
H	-0.60420329864	1.50948911362	-0.83075820041
H	-0.60322027099	1.49353469862	0.85632589091
H	2.26168563794	-1.32573349360	0.14422034531
N	2.21639507456	-0.31727241904	-0.00600200058
H	2.80421870269	0.09777192707	0.71828446606
H	2.70172723575	-0.14548013758	-0.88762389248

$(H_2O)_3^+$ -228.66721292 a.u.

O	0.93777295795	0.98172501537	-0.11561701190
H	1.44123351139	1.14559825539	0.71722517851
H	-0.03626650523	1.05523673238	0.09472770019
O	0.88400881719	-1.02803418756	0.11328079484
H	1.37781950251	-1.21681338691	-0.72024726834
H	-0.09285280126	-1.04830173855	-0.09661172555
O	-1.61237442688	0.04412506725	0.00162484595
H	-2.20960261981	-0.07399553295	0.76702918323
H	-2.20490699347	0.19458487716	-0.76175569385

$(HF)_3^+$ -300.56247861 a.u.

H	0.50643698504	0.46702902490	0.03057640940
F	-0.40652057199	0.82205854974	0.08393068699
H	-2.25730743615	0.13719103937	-0.03486771277
F	-1.53487520867	-0.57989597984	-0.03205494611
H	2.71309878261	0.06709394085	-0.00316616383
F	1.84058141209	-0.30953204837	-0.04758830082

$(PH_3)_3^+$ -1027.93646724 a.u.

H	-0.62205384038	-1.78759547181	0.01766743572
P	-1.79563646566	-1.02817238033	-0.01274362986
H	-2.69361512918	-1.83447889949	-0.74262451673
H	-2.27151533959	-1.13179516712	1.29954579151
H	2.93234254685	-1.29647140691	-0.87571345507
P	2.42171389633	-0.33463343192	0.01941557897
H	2.96277101934	-0.90762505996	1.18809699481
H	3.44521648453	0.61478515970	-0.17470945917
H	-0.26378678875	1.49085322485	-1.29478585016
P	-0.74448314248	1.40388752996	0.01386255085
H	0.15710446835	2.18151897913	0.76354306925
H	-1.90581844186	2.18755144206	-0.01900913428

$(H_2S)_3^+$ -1196.62432893 a.u.

S	-1.31845999551	-1.33166275583	0.12332121149
H	-2.60193806857	-1.34030084020	-0.27794975756
H	-0.82080716032	-1.52662943460	-1.10982859826
S	2.29036813320	-0.14618144892	-0.03471055623
H	3.04272103864	-0.05374670434	1.06897843024
H	3.22113370988	0.35946731413	-0.85372314427
S	-1.11456601637	1.46702958537	-0.09728956223
H	-1.32696525818	1.62249161617	1.22136896507
H	0.22057445181	1.27097718577	0.02548658138

$(HCl)_3^+$ -1380.74045828 a.u.

H	0.63300230021	-0.67462606198	0.01029790377
Cl	-0.52860995679	-1.31560966410	0.01881033490
H	-2.42215537763	0.74568520000	1.12467645705
Cl	-1.95238496170	0.87268561637	-0.07690032258
H	3.23188354705	-0.03253806188	-0.82022512077
Cl	2.43984590860	0.45408050142	0.06917216150

$(NH_3)_4^+$ -225.65738091 a.u.

H	1.66995003085	-0.08914706599	-0.40953972375
N	0.71201085588	-0.12644550257	-0.81835787764
H	0.48149819220	0.66981136185	-1.40797860349
H	0.48650718562	-1.01026502561	-1.26867413729
H	4.11635962599	-0.12966606964	-0.48351620377
N	3.45082122950	-0.01426891310	0.28167159084
H	3.67633051471	-0.74333620837	0.95915035688
H	3.69307350364	0.86970908749	0.73033256953
H	-4.10858853391	-0.04352612487	0.51692120448
N	-3.45555778969	-0.06388515358	-0.26722729737
H	-3.69201001025	-0.89829581943	-0.80503151430
H	-3.70492024621	0.72999724533	-0.85796023206
H	-0.47916431685	-0.79748639034	1.39150712349

N	-0.70534669314	0.00323563699	0.80635265707
H	-1.66381334913	-0.02532955334	0.39802772164
H	-0.47437998893	0.88340521194	1.26099845738

$(H_2O)_4^+$ -305.04183904 a.u.

O	0.33965609974	-0.58032978915	0.69166645451
H	1.21715237622	-0.36825761309	0.22974773260
H	-0.20261918406	-1.10234916472	0.05640404819
O	-0.51007059035	1.22143997046	0.36653946202
H	-0.49349145954	1.40176096325	1.33617708217
H	-1.38767134196	0.75928701559	0.15219482100
O	2.65654309760	-0.09266699822	-0.49290339126
H	3.46981476622	-0.57880139789	-0.26624226085
H	2.93502043576	0.70838278092	-0.97143721565
O	-2.42923566901	-0.41196138434	-0.41314909826
H	-2.81671666051	-0.30650353711	-1.30339594060
H	-3.14021438580	-0.79112630657	0.13858520351

$(HF)_4^+$ -400.94386949 a.u.

H	3.49062872383	0.04548621823	0.06383780234
F	2.64530775336	0.20889970259	-0.34457170427
H	1.45440473160	0.03524691069	0.33466860354
F	0.53484075928	-0.06850300064	0.79960907422
H	-3.49069665103	0.02705744214	-0.05543177919
F	-2.64852715106	0.20033903449	0.35461268046
H	-1.45542487440	0.04939631597	-0.32588225958
F	-0.53526568083	-0.03456493934	-0.79342338203

$(PH_3)_4^+$ -1370.69477760 a.u.

H	-0.39093335625	0.03353433740	-1.64785677510
P	0.02498929259	-1.25969124374	-1.30647745642
H	-1.06118543592	-2.03455139042	-1.75414309252
H	1.00927195625	-1.54724883795	-2.28231520775
H	2.95793434634	1.79901778975	0.50772668321
P	2.83154373227	0.58217014396	-0.20627255849
H	3.52228229700	1.02357428482	-1.36139504119
H	3.94541267654	-0.05462260457	0.39237000338
H	0.34461700352	-0.05344788929	1.57800549798
P	-0.52868734104	-1.10623791571	1.27497559403
H	0.18873950387	-2.21778005999	1.75448911152
H	-1.54414587674	-0.97218109758	2.25075947778
H	-3.39537984572	1.85533617303	1.17104028322
P	-2.39441668278	1.68843781509	0.18271815717
H	-3.25990523000	1.87031002327	-0.92369284194
H	-1.92977683261	3.02553802316	0.22414480781

$(H_2S)_4^+$ -1595.62050214 a.u.

H	-2.19878312874	-2.59531258706	-1.17102911124
S	-1.92537485578	-1.45013645266	-0.53185460899
H	-2.85765399305	-1.62179864567	0.41439131699
H	-1.21709307716	3.18150386558	0.99272553856
S	-1.27249751305	1.95738797529	0.45139710044
H	-2.13838420720	2.29645677776	-0.51250928357
H	0.22777859185	-1.41475023592	0.63054061362
S	1.44006219821	-1.07047542006	1.13721144337
H	2.09028215828	-2.11437565871	0.59425116754
H	0.78651471238	1.26331825401	-0.69400144497
S	1.82168493868	0.50907139917	-1.14390010988
H	2.76998458466	1.24476427680	-0.53813721593

$(HCl)_4^+$ -1841.13496852 a.u.

H	4.24179329429	0.54149683728	-0.10660296001
Cl	3.07051443919	1.04478253907	-0.27694620626
H	1.62925846933	-0.28486291231	0.62188636590
Cl	0.66272728019	-1.04433832816	1.10882387231
H	-4.24216815752	0.52429452238	0.16760078820
Cl	-3.06921329020	1.03483972716	0.30034433476
H	-1.63404766356	-0.27786261341	-0.63876589145
Cl	-0.66429399808	-1.02351154770	-1.13918215541