Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The Saturation of the Gas Phase Acidity of the nHF/AlF_3 and nHF/GeF_4 (n=1-6) Superacids Caused by Increasing Number of Surrounding HF Molecules

Marcin Czapla[1], Iwona Anusiewicz[1,2], and Piotr Skurski[1,2,*]

[1] *Laboratory of Quantum Chemistry, Faculty of Chemistry, University of Gdańsk*
Wita Stwosza 63, 80-308 Gdańsk, Poland

[2] *Department of Technical Physics and Applied Mathematics*
Gdańsk University of Technology
Narutowicza 11/12, 80-233 Gdańsk, Poland

[*] corresponding author: piotr.skurski@ug.edu.pl

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) lowest energy structures of the *n*HF/AlF_3 superacids (*n*=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.

HF/AlF_3 (1)

13	-0.052742000	0.307135000	0.000000000
9	0.572194000	0.860846000	1.440159000
9	-1.618069000	-0.313995000	0.000000000
9	0.572194000	-1.613145000	0.000000000
9	0.572194000	0.860846000	-1.440159000
1	-0.200971000	-2.143723000	0.000000000

E_{B3LYP} = -642.809121

E_{QCISD} = -641.546427

2HF/AlF_3 (1)

13	0.687734134	-0.145096908	0.000000000
9	-0.620862594	-1.267970603	0.000000000
9	1.486980814	-0.010440205	-1.452528001
9	1.486980814	-0.010440205	1.452528001
9	-0.533096561	1.334873741	0.000000000
9	-2.608094832	0.139930189	0.000000000
1	-1.481963822	1.042715063	0.000000000
1	-2.073837349	-0.663553342	0.000000000

E_{B3LYP} = -743.321036

E_{QCISD} = -741.853556

3HF/AlF_3 (1)

13	1.085379360	0.261339009	0.000000000
9	0.195071829	-1.392017228	0.000000000
9	-0.355071944	1.211732319	0.000000000
9	1.896668126	0.289646855	1.453544992
9	1.896668126	0.289646855	-1.453544992
9	-2.746770685	0.811396148	0.000000000
1	-0.813696562	-1.507389933	0.000000000
1	-1.848369537	1.171276456	0.000000000
9	-2.152537293	-1.530655259	0.000000000
1	-2.531054079	-0.623460666	0.000000000

E_{B3LYP} = -843.826916

E_{QCISD} = -842.155583

4HF/AlF_3 (1)

13	0.000000000	0.000000000	0.381708742
9	0.000000000	0.000000000	2.051036742
9	-1.823871087	0.844406607	0.262447742
9	1.823871087	-0.844406607	0.262447742
9	0.657463214	1.308986008	-0.529745258
9	-0.657463214	-1.308986008	-0.529745258
1	2.485747874	-0.303026316	-0.198337258
1	-2.485747874	0.303026316	-0.198337258
9	3.030645354	0.897132425	-0.967911258
1	2.180359386	1.340919906	-0.958372258
9	-3.030645354	-0.897132425	-0.967911258
1	-2.180359386	-1.340919906	-0.958372258

E_{B3LYP} = -944.324434

E_{QCISD} = -942.454081

5HF/AlF_3 (1)

13	-0.436562000	-0.325796000	0.314542000
9	0.616351000	1.040167000	0.244830000
9	-0.580148000	-1.211922000	1.723373000
9	1.005860000	-1.440039000	-0.413696000
9	-1.934108000	0.936660000	0.860326000
9	-1.388162000	-0.649007000	-1.087676000
9	2.944659000	1.707102000	-0.029249000
9	-3.512739000	0.564283000	-0.984684000
1	-2.693160000	0.941741000	0.257479000
1	1.950737000	-1.171094000	-0.482359000
1	-2.824396000	-0.022439000	-1.303115000
1	1.996592000	1.629765000	0.123189000
9	3.285337000	-0.661770000	-0.569494000
1	3.312096000	0.288121000	-0.377811000

E_{B3LYP} = -1044.828397

E_{QCISD} = -1042.754639

6HF/AlF_3 (1)

13	0.000000000	0.000000000	0.506402425
9	-1.083919700	-1.004808453	-0.384871574
9	1.083919700	1.004808453	-0.384871574
9	0.000000000	0.000000000	2.178669423
9	1.342771905	-1.448887465	0.391494426
9	-1.342771905	1.448887465	0.391494426
9	3.637631346	-1.030594598	-0.256721073
9	3.393813525	1.254569467	-1.125770572
9	-3.637631346	1.030594598	-0.256721073
1	-2.287540636	1.321553670	0.155576926
1	2.287540636	-1.321553670	0.155576926
1	-3.703916883	0.140803379	-0.632754573
1	2.461005891	1.334204597	-0.900112074
1	3.703916883	-0.140803379	-0.632754573
1	-2.461005891	-1.334204597	-0.900112074
9	-3.393813525	-1.254569467	-1.125770572

E_{B3LYP} = -1145.332138

E_{QCISD} = -1143.055084

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) higher energy structures of the *n*HF/AlF_3 superacids (*n*=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.

2HF/AlF_3 (2)

13	0.000000000	0.000000000	0.075590212
9	-2.036414827	0.500951207	-0.109263788
9	2.036414827	-0.500951207	-0.109263788
9	0.532255869	1.357597359	-0.787051788
9	-0.532255869	-1.357597359	-0.787051788
9	0.000000000	0.000000000	1.745763212
1	2.348762414	0.252372217	-0.570100788
1	-2.348762414	-0.252372217	-0.570100788

E_{B3LYP} = -743.307101

E_{QCISD} = -741.844198

2HF/AlF_3 (3)

13	-0.644757000	0.245744000	0.186463000
9	-1.095843000	-1.133573000	-1.195119000
9	-1.407318000	-0.710748000	1.332598000
9	1.030853000	0.174077000	0.130034000
9	-1.397072000	1.597232000	-0.416943000
1	-1.541927000	-1.860188000	-0.805920000
1	2.745462000	0.042054000	0.038199000
9	3.666970000	-0.079937000	-0.034603000

E_{B3LYP} = -743.303476

E_{QCISD} = -741.839513

3HF/AlF_3 (2)

13	0.437202000	-0.195353000	-0.045558000
9	1.094688000	-0.456793000	1.492711000
9	0.886200000	-1.061796000	-1.399815000
9	2.193561000	1.038134000	-0.150198000
9	-1.239018000	-1.196215000	0.307499000
9	-0.525318000	1.223671000	-0.258953000
9	-2.866563000	0.586777000	-0.008751000
1	-2.045285000	-0.652033000	0.226084000
1	2.558384000	0.857929000	0.692387000
1	-2.088675000	1.129691000	-0.168648000

E_{B3LYP} = -843.816389

E_{QCISD} = -842.149545

3HF/AlF_3 (3)

13	0.127625000	0.652708000	-0.115926000
9	0.994420000	-0.287580000	1.294686000
9	1.106999000	-0.113125000	-1.301004000
9	-1.440544000	0.061957000	-0.063303000
9	0.426234000	2.258747000	0.174075000
9	2.529881000	-1.604463000	0.027222000
1	1.692525000	-0.915649000	0.959567000
1	2.177590000	-1.185476000	-0.763441000
1	-3.044096000	-0.577407000	-0.015308000
9	-3.893116000	-0.960723000	0.015682000

E_{B3LYP} = -843.815076

E_{QCISD} = -842.146267

4HF/AlF_3 (2)

E_{B3LYP} = -944.327311

E_{QCISD} = -942.452334

13	-1.508666343	0.143698933	0.000000000
9	-2.313062605	0.266832029	-1.453339500
9	-0.326890641	1.586398529	0.000000000
9	-0.298229664	-1.081664761	0.000000000
9	-2.313062605	0.266832029	1.453339500
9	2.010431928	1.615317421	0.000000000
9	1.762832033	-2.368816957	0.000000000
1	0.691531767	1.586157213	0.000000000
1	0.876613936	-1.987174536	0.000000000
1	2.537876474	0.782883235	0.000000000
9	3.257385715	-0.442035356	0.000000000
1	2.740696436	-1.266805515	0.000000000

5HF/AlF_3 (2)

13	1.605508000	0.128828000	-0.071361000
9	1.520859000	-0.056032000	1.613467000
9	3.085971000	0.107995000	-0.824597000
9	0.680512000	-1.328347000	-0.676289000
9	0.522062000	1.375195000	-0.539436000
9	-1.551250000	-1.868757000	-0.698794000
9	-3.053122000	-0.067689000	-0.314281000
9	-1.830965000	2.054992000	-0.304126000
1	-0.355622000	-1.578341000	-0.654971000
1	-0.884232000	1.901438000	-0.385940000
1	-2.191840000	-1.130513000	-0.478822000
1	-2.624223000	0.802229000	-0.240496000
1	-0.109126000	-0.268782000	2.067843000
9	-1.008127000	-0.373000000	1.812954000

E_{B3LYP} = -1044.824900

E_{QCISD} = -1042.746714

5HF/AlF_3 (3)

13	0.000000000	0.000000000	0.160995001
9	-0.854381244	1.207413566	1.039532393
9	0.000000000	0.000000000	-1.523202779
9	-1.663784653	-1.095752335	0.244818413
9	1.663784653	1.095752335	0.244818413
9	0.854381244	-1.207413566	1.039532393
9	-3.159911545	0.435715958	1.415253364
9	3.159911545	-0.435715958	1.415253364
1	2.415974526	0.655055992	0.680746559
1	-2.415974526	-0.655055992	0.680746559
1	2.401325047	-1.018783284	1.436428206
1	-2.401325047	1.018783284	1.436428206
1	0.000000000	0.000000000	-3.224562605
9	0.000000000	0.000000000	-4.158217746

E_{B3LYP} = -1044.823960

E_{QCISD} = -1042.748596

5HF/AlF_3 (4)

13	-1.907286000	-0.216426000	0.014475000
9	-2.466040000	0.002268000	1.570574000
9	-2.941594000	-0.538399000	-1.249982000
9	-1.160518000	1.431734000	-0.428369000
9	-0.451347000	-1.132142000	-0.025510000
9	0.840933000	2.381691000	0.308201000
9	2.932776000	1.419610000	-0.375405000
9	3.495885000	-0.893118000	0.145165000
1	-0.287989000	1.849468000	-0.108517000
1	2.790427000	-1.554908000	0.111617000
1	1.703995000	1.991265000	0.041366000
1	3.186712000	0.503693000	-0.168816000
1	0.747152000	-1.998699000	0.017028000
9	1.600395000	-2.446898000	0.046343000

E_{B3LYP} = -1044.819996

E_{QCISD} = -1042.748294

6HF/AlF_3 (2)

13	0.517843000	-0.031210000	-0.041316000
9	0.000308000	-1.125888000	1.168465000
9	1.809369000	-0.464132000	-1.093968000
9	-0.152968000	1.524923000	-0.189242000
9	1.925918000	0.676719000	1.201625000
9	-0.795772000	-0.830816000	-1.256276000
9	-1.786167000	-2.548608000	0.158688000
9	3.943149000	0.245042000	-0.109571000
9	-2.464964000	2.525055000	-0.123285000
1	-1.383097000	-1.496146000	-0.838603000
1	2.834876000	0.605359000	0.861294000
1	-1.245239000	-2.193458000	0.856370000
1	3.333072000	-0.130206000	-0.745461000
1	-1.542804000	2.313961000	-0.181669000
1	-3.083092000	0.966074000	0.160144000
9	-3.106170000	0.035500000	0.290788000

E_{B3LYP} = -1145.321814

E_{QCISD} = -1143.040372

6HF/AlF_3 (3)

13	-2.124143000	-0.312842000	0.176423000
9	-0.810639000	-1.358904000	-0.178885000
9	-2.058966000	0.237363000	1.752590000
9	-3.555830000	-0.750997000	-0.550983000
9	-1.573873000	1.191183000	-0.771496000
9	-0.023814000	2.834635000	-0.197348000
9	2.304205000	2.309227000	-0.479918000
9	3.387334000	0.509671000	0.753320000
9	1.103263000	-2.859714000	-0.391295000
1	-0.900375000	1.913895000	-0.509984000
1	3.379257000	-0.403982000	0.437899000
1	0.934378000	2.633011000	-0.285050000
1	2.761924000	1.603425000	0.006001000
1	0.316104000	-2.308124000	-0.321378000
9	3.302251000	-1.793156000	-0.093100000
1	2.457197000	-2.245061000	-0.206945000

E_{B3LYP} = -1145.318030

E_{QCISD} = -1143.045420

6HF/AlF_3 (4)

13	2.384684762	-0.221766222	0.000000000
9	0.763547619	-0.824324726	0.000000000
9	3.146770426	-0.430592145	-1.461646958
9	3.146770426	-0.430592145	1.461646958
9	1.872404156	1.584795224	0.000000000
9	-0.328945644	2.477402186	0.000000000
9	-1.556771232	-1.367556357	0.000000000
9	-2.325886423	0.969031383	0.000000000
9	-2.733249663	-3.905446770	0.000000000
1	0.944291436	1.953514443	0.000000000
1	-0.580714181	-1.274335277	0.000000000
1	-1.119539722	1.928614053	0.000000000
1	-2.130789639	0.019323497	0.000000000
1	-2.364982139	-3.055172660	0.000000000
1	-4.081827087	1.699599046	0.000000000
9	-4.876243536	2.174783089	0.000000000

E_{B3LYP} = -1145.300623

E_{QCISD} = -1143.024505

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) lowest energy structures of the $((n\text{-}1)HF/AlF_4)^-$ anions (n=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.:

AlF_4^-

13	0.000000000	0.000000000	-0.000000001
9	-0.991466818	0.991466818	-0.991466814
9	0.991466818	-0.991466818	-0.991466814
9	-0.991466810	-0.991466810	0.991466814
9	0.991466810	0.991466810	0.991466814

E_{B3LYP} = -642.372316

E_{QCISD} = -641.101412

$(HF/AlF_4)^-$

13	0.000000000	0.000000000	-0.705592152
9	1.624687894	0.000000000	-1.233222580
9	0.000000000	0.000000000	1.033330503
9	-0.812343947	-1.407020989	-1.233222580
9	-0.812343947	1.407020989	-1.233222580
9	0.000000000	0.000000000	3.531653332
1	0.000000000	0.000000000	2.578160375

E_{B3LYP} = -742.884405

E_{QCISD} = -741.410792

$(2HF/AlF_4)^-$

13	0.000000000	0.000000000	0.689342582
9	1.387206378	0.000000000	-0.342057776
9	-1.387206378	0.000000000	-0.342057776
9	0.000000000	1.412519776	1.635745501
9	0.000000000	-1.412519776	1.635745501
9	-3.495889889	0.000000000	-1.719334503
9	3.495889889	0.000000000	-1.719334503
1	-2.698613370	0.000000000	-1.203731834
1	2.698613370	0.000000000	-1.203731834

E_{B3LYP} = -843.393642

E_{QCISD} = -841.717947

$(3HF/AlF_4)^-$

13	0.000000000	0.000000000	-0.514444190
9	-0.803569497	1.391823196	0.097186761
9	0.000000000	0.000000000	-2.207479108
9	-0.803569497	-1.391823196	0.097186761
9	1.607138993	0.000000000	0.097186761
9	-2.015210589	-3.490447128	0.851733018
9	-2.015210589	3.490447128	0.851733018
9	4.030421177	0.000000000	0.851733018
1	3.125904307	0.000000000	0.573905803
1	-1.562952154	-2.707112540	0.573905803
1	-1.562952154	2.707112540	0.573905803

E_{B3LYP} = -943.900378

E_{QCISD} = -942.023011

$(4HF/AlF_4)^-$

13	0.000000000	0.000000000	0.000000000
9	-0.988148743	-0.988148745	0.988148744
9	0.988148743	0.988148745	0.988148744
9	0.988148745	-0.988148743	-0.988148744
9	-0.988148745	0.988148743	-0.988148744
9	2.464621712	-2.464621705	-2.464621709
9	-2.464621705	-2.464621712	2.464621709
9	2.464621705	2.464621712	2.464621709
1	-1.919978328	-1.919978333	1.919978330
1	1.919978333	-1.919978328	-1.919978330
1	1.919978328	1.919978333	1.919978330
1	-1.919978333	1.919978328	-1.919978330
9	-2.464621712	2.464621705	-2.464621709

E_{B3LYP} = -1044.404891

E_{QCISD} = -1042.326175

$(5HF/AlF_4)^-$

13	0.500004389	-0.336020429	0.000000000
9	0.644475297	-1.302886840	-1.400654201
9	0.644475297	-1.302886840	1.400654201
9	-1.051163492	0.409710909	0.000000000
9	1.699341326	0.879740418	0.000000000
9	0.918047805	-2.728135915	3.516797830
9	-3.415048996	1.109176979	0.000000000
9	0.918047805	-2.728135915	-3.516797830
9	3.581815276	2.624691893	0.000000000
1	0.818798636	-2.206536084	2.738607022
1	2.889008412	1.986423872	0.000000000
1	-2.491397550	0.852392632	0.000000000
1	0.818798636	-2.206536084	-2.738607022
1	-4.102717363	2.629345291	0.000000000
9	-4.540419614	3.459971289	0.000000000

E_{B3LYP} = -1144.905254

E_{QCISD} = -1142.624000

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) lowest energy structures of the *n*HF/GeF_4 superacids (*n*=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.

HF/GeF_4 (1)

32	-0.168038000	0.300088000	0.000000000
9	1.554728000	0.406403000	0.000000000
9	-0.750992000	-0.452078000	1.425909000
9	-0.750992000	-0.452078000	-1.425909000
9	-0.750992000	1.920699000	0.000000000
9	1.075528000	-2.259767000	0.000000000
1	1.981690000	-2.071416000	0.000000000

E_{B3LYP} = -2577.126797

E_{QCISD} = -2574.535547

2HF/GeF_4 (1)

32	0.277517000	0.611286000	0.000000000
9	0.911564000	-1.015422000	0.000000000
9	-1.821195000	-0.964245000	0.000000000
9	1.705105000	1.576414000	0.000000000
9	-0.542850000	0.986860000	1.454110000
9	-0.542850000	0.986860000	-1.454110000
9	-0.542850000	-3.231584000	0.000000000
1	0.244000000	-2.726317000	0.000000000
1	-1.626860000	-1.884765000	0.000000000

E_{B3LYP} = -2677.623700

E_{QCISD} = -2674.830455

3HF/GeF_4 (1)

32	0.980586000	0.036801000	0.032549000
9	1.580812000	-1.019428000	-1.171808000
9	-0.300668000	1.101629000	-0.512067000
9	0.650466000	-0.586246000	1.596122000
9	-0.857556000	-1.519134000	-0.402602000
9	2.262180000	1.165475000	0.281943000
1	-1.749570000	-1.402675000	-0.091864000
1	-1.913457000	1.604374000	-0.352902000
9	-2.840856000	1.587714000	-0.194490000
1	-3.270758000	0.045360000	0.165530000
9	-3.210484000	-0.888307000	0.318198000

E_{B3LYP} = -2778.122574

E_{QCISD} = -2775.126631

4HF/GeF_4 (1)

32	-1.335337000	0.002049000	-0.067381000
9	-2.690792000	0.773500000	-0.804437000
9	-1.938271000	-0.551098000	1.436801000
9	-0.227059000	1.353317000	0.072586000
9	-0.823053000	-1.139602000	-1.242576000
9	0.590799000	-0.989984000	0.976022000
9	2.631073000	-1.856428000	-0.176416000
9	2.249029000	2.072477000	0.315870000
1	1.316753000	-1.421286000	0.522353000
1	1.331532000	1.853579000	0.273377000
1	3.225983000	-1.119779000	-0.293252000
9	3.928670000	0.293306000	-0.379936000
1	3.372952000	1.022522000	-0.127510000

E_{B3LYP} = -2878.620767

E_{QCISD} = -2875.421609

5HF/GeF_4 (1)

32	1.765108000	-0.079810000	-0.011967000
9	1.582922000	-0.988006000	1.430153000
9	3.428341000	0.369518000	-0.058152000
9	1.485734000	-0.932478000	-1.472154000
9	0.979564000	1.479746000	0.039249000
9	-0.679612000	-0.451238000	0.068001000
9	-2.269009000	-2.350984000	0.051080000
9	-4.339485000	-0.949644000	-0.041171000
9	-3.724455000	1.491397000	-0.067869000
1	-1.193486000	-1.262773000	0.066143000
1	-2.844891000	1.850863000	-0.011097000
1	-3.124214000	-1.923883000	0.014982000
1	-4.141044000	-0.016349000	-0.051118000
9	-1.418248000	2.534440000	0.083385000
1	-0.591596000	2.081289000	0.071331000

E_{B3LYP} = -2979.118753

E_{QCISD} = -2975.716926

6HF/GeF_4 (1)

32	-1.362991000	-0.286459000	-0.012828000
9	-0.991887000	-2.032435000	-0.031001000
9	-2.166562000	-0.185927000	-1.525325000
9	3.472813000	0.489750000	-0.606872000
9	0.298697000	0.219680000	0.053109000
9	-2.292903000	-0.250072000	1.428889000
9	-1.672413000	1.829947000	0.029353000
9	3.248580000	-1.817119000	0.321551000
9	1.214520000	-3.254491000	0.014004000
9	0.213554000	3.319582000	-0.043241000
9	2.490096000	2.530212000	0.395402000
1	3.371485000	-0.395262000	-0.254780000
1	0.353214000	-2.849838000	-0.005039000
1	2.482762000	-2.376654000	0.204690000
1	1.111380000	2.990204000	0.114341000
1	-0.893193000	2.432538000	0.003541000
1	2.859595000	1.723558000	0.024911000

E_{B3LYP} = -3079.620174

E_{QCISD} = -3076.015532

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) higher energy structures of the *n*HF/GeF_4 superacids (*n*=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.

2HF/GeF_4 (2)

32	-0.240683000	0.103150000	0.000000000
9	0.443761000	-1.495460000	0.000000000
9	-1.169253000	0.199894000	1.434482000
9	1.114064000	1.162619000	0.000000000
9	2.654165000	-3.151381000	0.000000000
9	-1.169253000	2.642594000	0.000000000
9	-1.169253000	0.199894000	-1.434482000
1	1.886704000	-2.630119000	0.000000000
1	-0.522914000	3.305877000	0.000000000

E_{B3LYP} = -2677.615445

E_{QCISD} = -2674.823695

3HF/GeF_4 (2)

32	-0.492316000	-0.093241000	0.000000000
9	-1.094910000	-0.735774000	1.466175000
9	1.220430000	0.224699000	0.000000000
9	-1.094910000	-0.735774000	-1.466175000
9	0.486307000	-2.317078000	0.000000000
9	-1.108117000	1.538899000	0.000000000
1	1.432721000	-2.345353000	0.000000000
1	2.823981000	-0.842834000	0.000000000
9	2.998124000	-1.760651000	0.000000000
1	-0.532443000	3.265187000	0.000000000
9	-0.110267000	4.092239000	0.000000000

E_{B3LYP} = -2778.112658

E_{QCISD} = -2775.118792

3HF/GeF_4 (3)

32	-0.260784000	0.197759000	0.000000000
9	-0.212827000	0.180244000	1.748102000
9	-0.287833000	-1.853533000	0.000000000
9	-1.995506000	0.532594000	0.000000000
9	-0.212827000	2.390251000	0.000000000
9	1.561234000	0.180374000	0.000000000
9	-0.212827000	0.180244000	-1.748102000
1	0.635542000	-2.203861000	0.000000000
1	-1.121248000	2.617708000	0.000000000
9	2.096036000	-2.218866000	0.000000000
1	2.211717000	-1.263902000	0.000000000

E_{B3LYP} = -2778.090862

E_{QCISD} = -2775.097448

4HF/GeF_4 (2)

32	0.000000000	0.000000000	0.000000000
9	0.000000000	0.000000000	-1.744263078
9	-1.601931342	-1.301888281	0.000000000
9	1.601931342	1.301888281	0.000000000
9	1.186150736	-1.372781640	0.000000000
9	-1.186150736	1.372781640	0.000000000
9	0.000000000	0.000000000	1.744263078
1	-2.456465881	-0.813621282	0.000000000
1	2.456465881	0.813621282	0.000000000
9	-3.408241558	0.307397315	0.000000000
1	-2.741283393	0.996834830	0.000000000
9	3.408241558	-0.307397315	0.000000000
1	2.741283393	-0.996834830	0.000000000

E_{B3LYP} = -2878.599339

E_{QCISD} = -2875.402882

5HF/GeF_4 (2)

32	-0.304888000	0.184144000	0.200982000
9	0.184465000	-0.251770000	-1.403059000
9	-1.613600000	1.311212000	-0.218376000
9	-0.802548000	-0.199681000	1.804176000
9	1.012225000	1.330819000	0.535794000
9	1.092295000	-1.433072000	0.661256000
9	3.248365000	-1.255455000	-0.512468000
9	3.356418000	1.250388000	-0.422795000
9	-3.778350000	0.084707000	-0.735340000
9	-1.834867000	-1.429671000	-0.253233000
1	1.922323000	-1.465474000	0.157674000
1	2.498762000	1.464163000	-0.073478000
1	3.439981000	-0.318840000	-0.561424000
1	-3.192724000	0.814426000	-0.598639000
1	-2.691555000	-1.054177000	-0.459137000

E_{B3LYP} = -2979.110667

E_{QCISD} = -2975.713852

5HF/GeF_4 (3)

32	-0.821795000	-0.303916000	0.165224000
9	0.254874000	1.064329000	0.374818000
9	-0.582919000	-1.130214000	-1.318597000
9	-2.280041000	0.596174000	-0.173889000
9	-1.262467000	-1.130366000	1.596885000
9	1.095203000	-1.387426000	0.653243000
9	3.077461000	-1.393288000	-0.802036000
9	4.249221000	0.798196000	-0.538294000
9	2.519039000	2.322848000	0.523285000
9	-4.901938000	1.086981000	-0.804998000
1	1.853117000	-1.447452000	0.053619000
1	1.652146000	1.954142000	0.542751000
1	3.608084000	-0.597171000	-0.748303000
1	3.683879000	1.453156000	-0.142475000
1	-4.015689000	0.917543000	-0.586508000

E_{B3LYP} = -2979.110055

E_{QCISD} = -2975.710226

5HF/GeF_4 (4)

32	-0.310582000	0.318977000	0.160966000
9	0.505174000	-1.243117000	-0.300465000
9	-1.791060000	-0.802427000	1.097791000
9	1.129133000	1.294382000	-0.849160000
9	0.644333000	0.327576000	1.626504000
9	-1.276554000	0.110190000	-1.354130000
9	-1.158668000	1.798587000	0.512002000
1	-2.550958000	-0.977471000	0.504580000
1	2.083028000	1.003140000	-0.723266000
9	-3.384704000	-1.016282000	-0.727248000
1	-2.741563000	-0.562875000	-1.270881000
9	3.345978000	0.491658000	-0.554197000
1	3.304754000	-0.431247000	-0.243781000
1	1.910750000	-1.752960000	0.078656000
9	2.867771000	-1.792330000	0.160434000

E_{B3LYP} = -2979.102095

E_{QCISD} = -2975.703747

6HF/GeF_4 (2)

32	2.066409000	-0.143282000	-0.012962000
9	1.794530000	-0.897991000	1.502018000
9	1.737601000	-1.088924000	-1.405897000
9	3.767119000	0.135249000	-0.062580000
9	1.459631000	1.495331000	-0.112156000
9	-0.358486000	-0.293261000	0.049325000
9	-1.685524000	-2.376378000	0.198245000
9	-4.128290000	-1.955106000	-0.052021000
9	-4.597374000	0.468567000	-0.451349000
9	-3.008235000	2.067042000	0.635215000
1	-0.838521000	-1.125070000	0.112645000
1	-4.009619000	1.114757000	-0.064143000
1	-2.635222000	-2.280256000	0.106331000
1	-4.373047000	-1.042700000	-0.204264000
1	-2.156073000	2.331618000	0.298960000
9	-0.772783000	2.811552000	-0.259857000
1	0.013715000	2.291958000	-0.203248000

E_{B3LYP} = -3079.616070

E_{QCISD} = -3076.011103

6HF/GeF_4 (3)

32	0.000000000	0.000000000	0.000000000
9	0.376687000	-0.560724000	1.684631000
9	1.909328000	0.629154000	-0.229522000
9	-1.909328000	-0.629154000	0.229522000
9	0.418682000	-1.587415000	-0.597152000
9	-0.418682000	1.587415000	0.597152000
9	-0.376687000	0.560724000	-1.684631000
1	2.060775000	1.535367000	-0.632295000
1	-2.060775000	-1.535367000	0.632295000
9	2.171153000	2.749058000	-1.278759000
1	1.382132000	2.917319000	-1.824803000
9	-2.171153000	-2.749058000	1.278759000
1	-1.382132000	-2.917319000	1.824803000
1	0.265862000	-1.966188000	2.293973000
9	-0.092077000	-2.819422000	2.557964000
1	-0.265862000	1.966188000	-2.293973000
9	0.092077000	2.819422000	-2.557964000

E_{B3LYP} = -3079.606432

E_{QCISD} = -3076.005231

6HF/GeF_4 (4)

32	-0.545624000	0.374283000	-0.122934000
9	-1.487485000	1.545186000	-0.996274000
9	0.393943000	-0.894494000	0.755545000
9	-2.039467000	0.167042000	1.305218000
9	0.900310000	0.459895000	-1.475754000
9	0.210707000	1.596893000	0.913417000
9	-1.367739000	-0.982306000	-0.994589000
9	2.932401000	-0.705235000	-1.315474000
9	-3.449246000	-1.500541000	0.239722000
9	2.721572000	-1.852463000	0.833012000
1	-2.730201000	-0.473064000	1.032360000
1	1.798124000	-0.026248000	-1.399713000
1	-2.796472000	-1.536812000	-0.457196000
1	3.008626000	-1.152245000	-0.452146000
1	1.849442000	-1.534503000	1.041692000
9	2.785984000	1.190211000	1.066640000
1	1.921612000	1.528133000	1.185739000

E_{B3LYP} = -3079.595273

E_{QCISD} = -3075.997437

The Cartesian coordinates (in Å) of the B3LYP/6-311++G(d,p) lowest energy structures of the $((n\text{-}1)HF/GeF_5)^-$ anions (n=1-6). The corresponding B3LYP/6-311++G(d,p) and QCISD/6-311++G(d,p) energies are given in a.u.

GeF_5^-

32	0.000000000	0.000000000	0.000208000
9	0.000000000	0.000000000	1.777983000
9	0.000000000	1.538744000	-0.890055000
9	0.000000000	-1.538744000	-0.890055000
9	1.805531000	0.000000000	0.000693000
9	-1.805531000	0.000000000	0.000693000

E_{B3LYP} = -2576.664238

E_{QCISD} = -2574.065767

$(HF/GeF_5)^-$

32	0.334907000	0.360825000	0.000000000
9	1.114634000	-0.069922000	1.524150000
9	-1.274831000	1.086803000	0.000000000
9	1.114634000	1.976683000	0.000000000
9	1.114634000	-0.069922000	-1.524150000
9	-0.469425000	-1.303437000	0.000000000
9	-2.588655000	-2.668330000	0.000000000
1	-1.815949000	-2.113260000	0.000000000

E_{B3LYP} = -2677.173467

E_{QCISD} = -2674.373237

$(2HF/GeF_5)^-$

32	-0.000778723	-0.000011421	0.000000000
9	0.001055279	-0.000005912	-1.829413500
9	1.755495272	0.008368632	0.000000000
9	-0.875360326	-1.522644037	0.000000000
9	-0.889815127	1.514220052	0.000000000
9	0.001055279	-0.000005912	1.829413500
9	0.005112482	0.000054051	-4.368084000
9	0.005112482	0.000054051	4.368084000
1	0.003531083	0.000033127	-3.421528500
1	0.003531083	0.000033127	3.421528500

E_{B3LYP} = -2777.680213

E_{QCISD} = -2774.678262

$(3HF/GeF_5)^-$

32	-0.158058000	0.115673000	0.000000000
9	-0.186120000	-1.704946000	0.000000000
9	-0.009761000	1.928270000	0.000000000
9	-1.028800000	0.157403000	1.518668000
9	1.622527000	0.032198000	0.000000000
9	-1.028800000	0.157403000	-1.518668000
9	-1.028800000	4.280589000	0.000000000
9	-1.694319000	-3.784753000	0.000000000
9	3.790426000	-1.416091000	0.000000000
1	-0.681098000	3.402851000	0.000000000
1	2.974533000	-0.950484000	0.000000000
1	-1.162769000	-3.004574000	0.000000000

E_{B3LYP} = -2878.181301

E_{QCISD} = -2874.978405

$(4HF/GeF_5)^-$

32	0.045100000	0.270171000	0.000000000
9	-1.281364000	1.496319000	0.000000000
9	1.300004000	-1.033655000	0.000000000
9	1.266536000	1.516680000	0.000000000
9	-0.584135000	-0.365851000	1.534354000
9	-0.584135000	-0.365851000	-1.534354000
9	3.847515000	-1.533872000	0.000000000
9	-2.905890000	3.505241000	0.000000000
9	-0.584135000	-2.009188000	3.584075000
9	-0.584135000	-2.009188000	-3.584075000
1	2.930800000	-1.322545000	0.000000000
1	-0.537710000	-1.452627000	2.831565000
1	-2.310953000	2.776618000	0.000000000
1	-0.537710000	-1.452627000	-2.831565000

E_{B3LYP} = -2978.680067

E_{QCISD} = -2975.276950

$(5HF/GeF_5)^-$

32	0.201444000	0.081377000	0.000000000
9	1.263227000	-1.371337000	0.000000000
9	1.562435000	1.167913000	0.000000000
9	-0.549715000	-0.438044000	1.513674000
9	-0.549715000	-0.438044000	-1.513674000
9	-0.938285000	1.532496000	0.000000000
9	3.722419000	-2.253277000	0.000000000
9	-3.579595000	1.562588000	0.000000000
9	-0.397586000	4.128895000	0.000000000
9	-0.549715000	-2.076308000	-3.603780000
9	-0.549715000	-2.076308000	3.603780000
1	2.848302000	-1.911279000	0.000000000
1	-0.516665000	-1.535052000	2.842061000
1	-2.643066000	1.529456000	0.000000000
1	-0.516665000	-1.535052000	-2.842061000
1	-0.521915000	3.200706000	0.000000000

E_{B3LYP} = -3079.176735

E_{QCISD} = -3075.573072