

Supporting Information
Of
Unsupported Donor-acceptor complexes of noble gases with group 13
elements

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Cartesian coordinates of the optimized geometries calculated at BP86(D3BJ)/def2-TZVPP

B1-Ar

NImag=0

Sum of electronic and zero-point Energies = -934.742165
Sum of electronic and thermal Energies = -934.732967
Sum of electronic and thermal Enthalpies = -934.732023
Sum of electronic and thermal Free Energies= -934.778852

5	0.218729000	0.000061000	0.000084000
6	-0.184634000	1.518089000	0.146745000
1	-0.100728000	1.964236000	1.149080000
1	0.205250000	2.218135000	-0.603810000
6	-0.184585000	-0.886156000	1.241228000
1	-0.100808000	-1.977256000	1.126140000
1	0.205345000	-0.586412000	2.222809000
6	-0.184468000	-0.631916000	-1.387971000
1	0.205484000	-1.631927000	-1.618873000
1	-0.100510000	0.013058000	-2.275508000
6	-2.051005000	-0.000061000	-0.000023000
1	-3.147692000	-0.000115000	0.000026000
8	-1.629332000	-0.823990000	-1.074180000
8	-1.629466000	1.342186000	-0.176525000

8	-1.629374000	-0.518212000	1.250649000
18	3.137419000	0.000020000	0.000016000

B1-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-3161.200606
Sum of electronic and thermal Energies	=	-3161.191471
Sum of electronic and thermal Enthalpies	=	-3161.190527
Sum of electronic and thermal Free Energies	=	-3161.237551

5	-0.349529000	0.000004000	-0.000018000
6	-0.762810000	1.518554000	-0.130281000
1	-0.673102000	2.139167000	0.774311000
1	-0.375355000	2.071710000	-0.996181000
6	-0.762794000	-0.646630000	1.380106000
1	-0.673461000	-1.740399000	1.464927000
1	-0.375015000	-0.173661000	2.292138000
6	-0.762772000	-0.872110000	-1.249986000
1	-0.375216000	-1.898543000	-1.296007000
1	-0.673055000	-0.399053000	-2.239767000
6	-2.628385000	0.000007000	0.000052000
1	-3.725013000	0.000022000	0.000127000
8	-2.207835000	-0.999688000	-0.913188000
8	-2.207892000	1.290702000	-0.409116000

8	-2.207751000	-0.290886000	1.322404000
36	2.530729000	0.000022000	0.000011000

B1-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-736.664775
Sum of electronic and thermal Energies	=	-736.655735
Sum of electronic and thermal Enthalpies	=	-736.654791
Sum of electronic and thermal Free Energies	=	-736.701675

5	0.742506000	-0.000109000	0.000058000
6	1.173555000	-0.905038000	1.224569000
1	1.074193000	-0.460424000	2.227169000
1	0.790612000	-1.934519000	1.242447000
6	1.173328000	1.512912000	0.171354000
1	1.074114000	2.158724000	-0.715127000
1	0.790258000	2.043323000	1.053800000
6	1.173521000	-0.608200000	-1.395910000
1	0.790351000	-0.109282000	-2.296491000
1	1.074520000	-1.698848000	-1.511911000
6	3.037759000	0.000151000	-0.000006000
1	4.134298000	0.000267000	-0.000004000
8	2.618979000	-0.267967000	-1.327558000
8	2.619078000	-1.015586000	0.895897000

8	2.618843000	1.283826000	0.431643000
54	-2.141575000	0.000003000	-0.000001000

B2-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-1186.299591
Sum of electronic and thermal Energies	=	-1186.288941
Sum of electronic and thermal Enthalpies	=	-1186.287997
Sum of electronic and thermal Free Energies	=	-1186.337909

5	0.000000000	0.000000000	0.405267000
6	0.000000000	-1.563717000	0.085245000
1	0.932434000	-2.101204000	0.313961000
1	-0.848541000	-2.134072000	0.490432000
6	1.354218000	0.781858000	0.085245000
1	1.353479000	1.858114000	0.313961000
1	2.272432000	0.332178000	0.490432000
6	-1.354218000	0.781858000	0.085245000
1	-1.423890000	1.801894000	0.490432000
1	-2.285913000	0.243090000	0.313961000
14	0.000000000	0.000000000	-2.020088000
1	0.000000000	0.000000000	-3.491510000
8	-1.254054000	0.906454000	-1.395264000
8	-0.157985000	-1.539270000	-1.395264000

8	1.412040000	0.632816000	-1.395264000
18	0.000000000	0.000000000	3.293619000

B2-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-3412.758161
Sum of electronic and thermal Energies	=	-3412.747579
Sum of electronic and thermal Enthalpies	=	-3412.746635
Sum of electronic and thermal Free Energies	=	-3412.797896

5	-0.158350000	-0.000157000	0.000077000
6	-0.487599000	0.063954000	-1.562399000
1	-0.235327000	1.009820000	-2.065250000
1	-0.100565000	-0.771577000	-2.164272000
6	-0.487649000	1.321123000	0.836665000
1	-0.235595000	1.283863000	1.907289000
1	-0.100595000	2.260066000	0.413875000
6	-0.487809000	-1.385232000	0.725865000
1	-0.100774000	-1.488617000	1.750409000
1	-0.235753000	-2.293743000	0.158216000
14	-2.592927000	0.000076000	-0.000030000
1	-4.064413000	0.000140000	-0.000071000
8	-1.970646000	-1.310764000	0.823301000
8	-1.970474000	-0.057672000	-1.546858000

8	-1.970486000	1.368517000	0.723423000
36	2.728804000	0.000001000	0.000004000

B2-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-988.222519
Sum of electronic and thermal Energies	=	-988.212030
Sum of electronic and thermal Enthalpies	=	-988.211086
Sum of electronic and thermal Free Energies	=	-988.262815

5	-0.542548000	-0.000907000	0.000043000
6	-0.889681000	-1.304431000	-0.862919000
1	-0.575076000	-1.269457000	-1.917330000
1	-0.556715000	-2.259683000	-0.428839000
6	-0.890553000	1.398716000	-0.696944000
1	-0.575714000	2.293942000	-0.138843000
1	-0.556565000	1.500582000	-1.740906000
6	-0.888939000	-0.096731000	1.560809000
1	-0.554040000	0.755859000	2.171366000
1	-0.576086000	-1.028261000	2.057152000
14	-2.990834000	0.000240000	0.000071000
1	-4.462596000	-0.000248000	0.000905000
8	-2.373961000	-0.077035000	1.547367000
8	-2.374688000	-1.301087000	-0.841035000

8	-2.375549000	1.379409000	-0.706593000
54	2.323145000	0.000237000	-0.000154000

B3-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-1225.625110
Sum of electronic and thermal Energies	=	-1225.612418
Sum of electronic and thermal Enthalpies	=	-1225.611474
Sum of electronic and thermal Free Energies	=	-1225.665818

5	0.000000000	0.000000000	0.744812000
6	-0.579807000	1.451218000	0.427037000
1	-1.571580000	1.672385000	0.848569000
1	0.093230000	2.295476000	0.641403000
6	-0.966888000	-1.227736000	0.427037000
1	-0.662537000	-2.197221000	0.848569000
1	-2.034555000	-1.066998000	0.641403000
6	1.546695000	-0.223482000	0.427037000
1	1.941325000	-1.228478000	0.641403000
1	2.234118000	0.524836000	0.848569000
14	0.000000000	0.000000000	-1.692113000
8	1.544768000	-0.036422000	-1.046433000
8	-0.740841000	1.356020000	-1.046433000
8	-0.803927000	-1.319597000	-1.046433000

6	0.000000000	0.000000000	-3.535046000
1	0.384381000	-0.954618000	-3.917511000
1	-1.018914000	0.144426000	-3.917511000
1	0.634533000	0.810193000	-3.917511000
18	0.000000000	0.000000000	3.660341000

B3-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-3452.083603
Sum of electronic and thermal Energies	=	-3452.070979
Sum of electronic and thermal Enthalpies	=	-3452.070035
Sum of electronic and thermal Free Energies	=	-3452.124573

5	0.000000000	0.000000000	0.163483000
6	-0.582069000	1.450170000	-0.163487000
1	-1.579194000	1.666412000	0.248512000
1	0.085164000	2.295926000	0.063925000
6	-0.964850000	-1.229172000	-0.163487000
1	-0.653558000	-2.200829000	0.248512000
1	-2.030913000	-1.074209000	0.063925000
6	1.546919000	-0.220998000	-0.163487000
1	1.945748000	-1.221717000	0.063925000
1	2.232753000	0.534416000	0.248512000
14	0.000000000	0.000000000	-2.282365000

8	1.544639000	-0.053900000	-1.638268000
8	-0.725641000	1.364647000	-1.638268000
8	-0.818999000	-1.310747000	-1.638268000
6	0.000000000	0.000000000	-4.125427000
1	0.368655000	-0.960788000	-4.507932000
1	-1.016394000	0.161129000	-4.507932000
1	0.647739000	0.799659000	-4.507932000
36	0.000000000	0.000000000	3.075998000

B3-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-1027.547812
Sum of electronic and thermal Energies	=	-1027.535272
Sum of electronic and thermal Enthalpies	=	-1027.534328
Sum of electronic and thermal Free Energies	=	-1027.589936

5	0.259102000	-0.000035000	0.000017000
6	0.601794000	-1.558098000	0.115567000
1	0.205457000	-2.063616000	1.009507000
1	0.353389000	-2.165124000	-0.769283000
6	0.601699000	0.879203000	1.291508000
1	0.205367000	1.906135000	1.282191000
1	0.353191000	0.416606000	2.259714000
6	0.601765000	0.678939000	-1.407114000

1	0.353528000	1.748794000	-1.490399000
1	0.205487000	0.157516000	-2.291898000
14	2.718169000	-0.000009000	0.000057000
8	2.077922000	0.549819000	-1.445325000
8	2.077913000	-1.526586000	0.246599000
8	2.077867000	0.976878000	1.198727000
6	4.561664000	-0.000053000	-0.000011000
1	4.944427000	1.028633000	-0.025828000
1	4.944444000	-0.492110000	0.903718000
1	4.944266000	-0.536742000	-0.878048000
54	-2.665381000	-0.000012000	-0.000005000

B4-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-1646.023405
Sum of electronic and thermal Energies	=	-1646.011556
Sum of electronic and thermal Enthalpies	=	-1646.010612
Sum of electronic and thermal Free Energies	=	-1646.063458

5	0.000000000	0.000000000	1.049551000
6	0.975478000	-1.221047000	0.722416000
1	2.043273000	-1.051766000	0.924922000
1	0.680364000	-2.193006000	1.142709000
6	0.569719000	1.455313000	0.722416000

1	-0.110780000	2.295409000	0.924922000
1	1.559017000	1.685715000	1.142709000
6	-1.545197000	-0.234265000	0.722416000
1	-2.239381000	0.507291000	1.142709000
1	-1.932493000	-1.243643000	0.924922000
14	0.000000000	0.000000000	-1.363060000
8	-1.547797000	-0.036293000	-0.755052000
8	0.805330000	-1.322285000	-0.755052000
8	0.742467000	1.358578000	-0.755052000
17	0.000000000	0.000000000	-3.382394000
18	0.000000000	0.000000000	3.902814000

B4-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-3872.482105
Sum of electronic and thermal Energies	=	-3872.470313
Sum of electronic and thermal Enthalpies	=	-3872.469369
Sum of electronic and thermal Free Energies	=	-3872.522470

5	0.000000000	0.000000000	0.469092000
6	-0.974680000	1.221553000	0.131648000
1	-2.040557000	1.057588000	0.349445000
1	-0.672710000	2.196483000	0.540736000
6	-0.570556000	-1.454874000	0.131648000

1	0.104381000	-2.295968000	0.349445000
1	-1.565855000	-1.680825000	0.540736000
6	1.545236000	0.233321000	0.131648000
1	2.238565000	-0.515658000	0.540736000
1	1.936176000	1.238381000	0.349445000
14	0.000000000	0.000000000	-1.953474000
8	1.547492000	0.059055000	-1.347629000
8	-0.824889000	1.310640000	-1.347629000
8	-0.722603000	-1.369695000	-1.347629000
17	0.000000000	0.000000000	-3.973171000
36	0.000000000	0.000000000	3.329166000

B4-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-1447.946736
Sum of electronic and thermal Energies	=	-1447.935034
Sum of electronic and thermal Enthalpies	=	-1447.934089
Sum of electronic and thermal Free Energies	=	-1447.988388

5	-0.064292000	-0.000509000	-0.001109000
6	0.292518000	1.130550000	-1.078655000
1	0.025278000	0.892884000	-2.119713000
1	-0.078374000	2.138898000	-0.841097000
6	0.292649000	-1.499475000	-0.440554000

1	0.023714000	-2.281330000	0.286038000
1	-0.076560000	-1.798554000	-1.433044000
6	0.292339000	0.368061000	1.517314000
1	-0.077782000	-0.342142000	2.271849000
1	0.022774000	1.388035000	1.831357000
14	2.372953000	0.000277000	0.000141000
8	1.775977000	0.275706000	1.526088000
8	1.775923000	1.184339000	-1.000136000
8	1.775985000	-1.458664000	-0.523987000
17	4.394202000	-0.000294000	-0.000088000
54	-2.876454000	0.000000000	0.000099000

B5-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-934.859210
Sum of electronic and thermal Energies	=	-934.850311
Sum of electronic and thermal Enthalpies	=	-934.849367
Sum of electronic and thermal Free Energies	=	-934.895631

6	2.084051000	0.000177000	0.000046000
6	1.518245000	-1.176331000	0.843604000
1	1.688275000	-2.143982000	0.343224000
1	1.962730000	-1.198570000	1.848780000
6	1.518113000	-0.142358000	-1.440580000

1	1.688047000	0.774777000	-2.028466000
1	1.962615000	-1.001758000	-1.962431000
6	1.517938000	1.318986000	0.596870000
1	1.962093000	2.200571000	0.113161000
1	1.688200000	1.369900000	1.685016000
5	-0.127676000	-0.000146000	0.000039000
8	0.077968000	1.349728000	0.311053000
8	0.078369000	-0.944370000	1.013612000
8	0.078292000	-0.405751000	-1.324508000
1	3.184298000	0.000300000	0.000026000
18	-3.066944000	-0.000011000	-0.000022000

B5-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-3161.317010
Sum of electronic and thermal Energies	=	-3161.308133
Sum of electronic and thermal Enthalpies	=	-3161.307189
Sum of electronic and thermal Free Energies	=	-3161.354014

6	2.674955000	-0.000219000	-0.000160000
6	2.109298000	0.306511000	1.414251000
1	2.279676000	-0.537267000	2.103354000
1	2.554721000	1.219682000	1.834222000
6	2.108822000	-1.378263000	-0.441638000

1	2.279217000	-1.553298000	-1.516901000
1	2.553969000	-2.198669000	0.139258000
6	2.109154000	1.071493000	-0.972663000
1	2.554329000	0.978763000	-1.973602000
1	2.279762000	2.090081000	-0.586352000
5	0.458896000	0.000165000	0.000042000
8	0.670288000	0.822150000	-1.115323000
8	0.670439000	0.555003000	1.269638000
8	0.669977000	-1.376828000	-0.154224000
1	3.775232000	-0.000408000	-0.000285000
36	-2.518622000	0.000015000	0.000017000

B5-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-736.779881
Sum of electronic and thermal Energies	=	-736.771047
Sum of electronic and thermal Enthalpies	=	-736.770103
Sum of electronic and thermal Free Energies	=	-736.817088

6	3.106456000	0.000000000	0.000073000
6	2.541170000	-1.367371000	-0.471515000
1	2.711933000	-1.518407000	-1.550484000
1	2.987522000	-2.200371000	0.090463000
6	2.541158000	1.092183000	-0.948171000

1	2.711609000	2.102076000	-0.539237000
1	2.987768000	1.022302000	-1.950468000
6	2.540955000	0.275229000	1.420020000
1	2.987280000	1.178347000	1.860601000
1	2.711544000	-0.583735000	2.090277000
5	0.881207000	0.000005000	-0.000162000
8	1.103289000	0.527232000	1.281866000
8	1.103478000	-1.373872000	-0.184509000
8	1.103577000	0.846579000	-1.097740000
1	4.206820000	0.000039000	0.000165000
54	-2.158735000	-0.000001000	0.000002000

B6-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-1903.826149
Sum of electronic and thermal Energies	=	-1903.815640
Sum of electronic and thermal Enthalpies	=	-1903.814696
Sum of electronic and thermal Free Energies	=	-1903.865462

6	2.238875000	0.000051000	-0.000230000
6	1.787859000	-0.659077000	1.323723000
1	1.851438000	-1.752479000	1.261842000
1	2.396924000	-0.298982000	2.163743000
6	1.787386000	-0.816958000	-1.233037000

1	1.850766000	-0.216797000	-2.149130000
1	2.396342000	-1.724538000	-1.341300000
6	1.787559000	1.476174000	-0.091328000
1	2.396371000	2.023597000	-0.823401000
1	1.851360000	1.969467000	0.886444000
5	-0.288566000	-0.000062000	0.000129000
16	0.038807000	1.641991000	-0.760592000
16	0.039303000	-0.162252000	1.802442000
16	0.038814000	-1.479836000	-1.041521000
1	3.344827000	0.000107000	-0.000406000
18	-3.451447000	0.000019000	0.000085000

B6-Kr

NImag=0

Sum of electronic and zero-point Energies = -4130.284468

Sum of electronic and thermal Energies = -4130.273974

Sum of electronic and thermal Enthalpies = -4130.273030

Sum of electronic and thermal Free Energies= -4130.324135

6	2.755256000	0.000135000	-0.000053000
6	2.303782000	0.998012000	-1.091522000
1	2.368155000	2.032024000	-0.730542000
1	2.913569000	0.883578000	-1.997782000
6	2.303878000	0.446392000	1.409996000

1	2.368355000	-0.383231000	2.124977000
1	2.913664000	1.288486000	1.763956000
6	2.304013000	-1.444207000	-0.318569000
1	2.913889000	-2.171763000	0.233659000
1	2.368377000	-1.648594000	-1.394537000
5	0.223291000	-0.000094000	0.000094000
16	0.556222000	-1.788923000	0.277303000
16	0.555922000	0.654301000	-1.687772000
16	0.555969000	1.134564000	1.410507000
1	3.861133000	0.000237000	-0.000061000
36	-2.930972000	-0.000037000	0.000004000

B6-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-1705.748328
Sum of electronic and thermal Energies	=	-1705.737884
Sum of electronic and thermal Enthalpies	=	-1705.736940
Sum of electronic and thermal Free Energies	=	-1705.787899

6	3.133343000	0.000153000	-0.000251000
6	2.682494000	-0.119062000	1.473729000
1	2.748250000	-1.157786000	1.821149000
1	3.294240000	0.525308000	2.119327000
6	2.682311000	-1.216882000	-0.840233000

1	2.747916000	-0.998629000	-1.913568000
1	3.294011000	-2.098180000	-0.604914000
6	2.682097000	1.336083000	-0.634050000
1	3.293543000	1.572983000	-1.515101000
1	2.747911000	2.156446000	0.091665000
5	0.586770000	-0.000083000	0.000177000
16	0.935967000	1.247318000	-1.313268000
16	0.936549000	0.513805000	1.736968000
16	0.936372000	-1.761145000	-0.423412000
1	4.239140000	0.000239000	-0.000387000
54	-2.543010000	-0.000025000	0.000021000

B7-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-1576.581953
Sum of electronic and thermal Energies	=	-1576.575682
Sum of electronic and thermal Enthalpies	=	-1576.574738
Sum of electronic and thermal Free Energies	=	-1576.613090

5	0.000000000	0.000000000	0.282427000
15	0.000000000	1.330559000	-1.015670000
15	-1.152298000	-0.665279000	-1.015670000
15	1.152298000	-0.665279000	-1.015670000
18	0.000000000	0.000000000	2.460724000

B7-Kr**NImag=0**

Sum of electronic and zero-point Energies = -3803.045049
Sum of electronic and thermal Energies = -3803.038827
Sum of electronic and thermal Enthalpies = -3803.037883
Sum of electronic and thermal Free Energies= -3803.076836

5	0.000000000	0.000000000	-0.234527000
15	0.000000000	1.322149000	-1.554042000
15	-1.145015000	-0.661075000	-1.554042000
15	1.145015000	-0.661075000	-1.554042000
36	0.000000000	0.000000000	1.975126000

B7-Xe**NImag=0**

Sum of electronic and zero-point Energies = -1378.516183
Sum of electronic and thermal Energies = -1378.509994
Sum of electronic and thermal Enthalpies = -1378.509050
Sum of electronic and thermal Free Energies= -1378.548460

5	0.000000000	0.000000000	-0.616580000
15	0.000000000	1.314724000	-1.957110000
15	-1.138585000	-0.657362000	-1.957110000
15	1.138585000	-0.657362000	-1.957110000

54 0.000000000 0.000000000 1.688016000

B8-Ar

NImag=0

Sum of electronic and zero-point Energies = -7260.873382

Sum of electronic and thermal Energies = -7260.866012

Sum of electronic and thermal Enthalpies = -7260.865068

Sum of electronic and thermal Free Energies= -7260.908848

5 0.000000000 0.000000000 0.681727000

33 0.000000000 1.494082000 -0.603986000

33 -1.293913000 -0.747041000 -0.603986000

33 1.293913000 -0.747041000 -0.603986000

18 0.000000000 0.000000000 3.132555000

B8-Kr

NImag=0

Sum of electronic and zero-point Energies = -9487.335063

Sum of electronic and thermal Energies = -9487.327759

Sum of electronic and thermal Enthalpies = -9487.326815

Sum of electronic and thermal Free Energies= -9487.370737

5 0.000000000 0.000000000 0.322086000

33 0.000000000 1.480071000 -0.997746000

33 -1.281779000 -0.740036000 -0.997746000

33	1.281779000	-0.740036000	-0.997746000
36	0.000000000	0.000000000	2.699068000

B8-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-7062.805024
Sum of electronic and thermal Energies	=	-7062.797831
Sum of electronic and thermal Enthalpies	=	-7062.796887
Sum of electronic and thermal Free Energies	=	-7062.840658

5	0.000000000	0.000000000	0.036329000
33	0.000000000	1.465803000	-1.320839000
33	-1.269423000	-0.732902000	-1.320839000
33	1.269423000	-0.732902000	-1.320839000
54	0.000000000	0.000000000	2.418174000

Cartesian coordinates of the optimized geometries calculated at BP86/def2-TZVPP.

B7-Ar

NImag=0

Sum of electronic and zero-point Energies = -1576.565372
Sum of electronic and thermal Energies = -1576.559063
Sum of electronic and thermal Enthalpies = -1576.558119
Sum of electronic and thermal Free Energies= -1576.596630

5	0.000000000	0.000000000	0.277117000
15	0.000000000	1.331231000	-1.022098000
15	-1.152879000	-0.665615000	-1.022098000
15	1.152879000	-0.665615000	-1.022098000
18	0.000000000	0.000000000	2.478268000

B7-Kr

NImag=0

Sum of electronic and zero-point Energies = -3803.027129
Sum of electronic and thermal Energies = -3803.020872
Sum of electronic and thermal Enthalpies = -3803.019928
Sum of electronic and thermal Free Energies= -3803.059018

5	0.000000000	0.000000000	-0.246381000
15	0.000000000	1.323095000	-1.566203000

15	-1.145834000	-0.661547000	-1.566203000
15	1.145834000	-0.661547000	-1.566203000
36	0.000000000	0.000000000	1.991974000

B7-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-1378.496184
Sum of electronic and thermal Energies	=	-1378.489970
Sum of electronic and thermal Enthalpies	=	-1378.489026
Sum of electronic and thermal Free Energies	=	-1378.528525

5	0.000000000	0.000000000	-0.629141000
15	0.000000000	1.315455000	-1.970635000
15	-1.139217000	-0.657727000	-1.970635000
15	1.139217000	-0.657727000	-1.970635000
54	0.000000000	0.000000000	1.700449000

B8-Ar

NImag=0

Sum of electronic and zero-point Energies	=	-7260.855681
Sum of electronic and thermal Energies	=	-7260.848150
Sum of electronic and thermal Enthalpies	=	-7260.847206
Sum of electronic and thermal Free Energies	=	-7260.892456

5	0.000000000	0.000000000	0.623236000
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33	0.000000000	1.504268000	-0.643126000
33	-1.302734000	-0.752134000	-0.643126000
33	1.302734000	-0.752134000	-0.643126000
18	0.000000000	0.000000000	3.364074000

B8-Kr

NImag=0

Sum of electronic and zero-point Energies	=	-9487.315310
Sum of electronic and thermal Energies	=	-9487.307974
Sum of electronic and thermal Enthalpies	=	-9487.307029
Sum of electronic and thermal Free Energies	=	-9487.351176

5	0.000000000	0.000000000	0.305665000
33	0.000000000	1.482738000	-1.011130000
33	-1.284089000	-0.741369000	-1.011130000
33	1.284089000	-0.741369000	-1.011130000
36	0.000000000	0.000000000	2.738153000

B8-Xe

NImag=0

Sum of electronic and zero-point Energies	=	-7062.782955
Sum of electronic and thermal Energies	=	-7062.775732
Sum of electronic and thermal Enthalpies	=	-7062.774787
Sum of electronic and thermal Free Energies	=	-7062.818703

5	0.000000000	0.000000000	0.024300000
33	0.000000000	1.467385000	-1.332975000
33	-1.270792000	-0.733692000	-1.332975000
33	1.270792000	-0.733692000	-1.332975000
54	0.000000000	0.000000000	2.441537000