Supporting Information

Neutral and Multicharged Ions of Small Aluminum Oxides: Structures, Spectroscopy and Energetics

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Table of Contents

Examples of input files for the computations of AlO_2, Al_2O and Al_2O_2 species.

```
   ***,OAlO RCCSD(T)/AVTZ computations
        memory,500,M;
basis=avtz;
 {symmetry,nosym;}
  angstrom
        geometry={
  al
  o    1 1.76
  o    2 1.33        1 145.0
   }
    {rhf;wf,29,1,1;}
    {rccsd(t); }
  optg;
  frequencies;
```

```
***,AlAlO+ RCCSD(T)/AVTZ computations
       memory,500,M;
       basis=avtz;
       geomtyp=xyz;
geometry={
  Al        -4.2364844317        0.2977281855       -1.4521386536
  Al        -1.4761094606        0.3008230192        0.1415662631
  O          0.0377138923        0.3025187954        1.0155723905
 }
 {rhf,maxdis=10,iptyp='KAIN',nitord=20; shift,-1.0,-0.5;wf,33,1,1;
  maxit,300;}
   {rccsd(t);wf,33,1,1;}
 optg;
 frequencies;
 put,molden,alalo+doubccsdt1.molden;
```

```
***,Al2O2 CCSD(T/AVTZ Computations
   MEMORY,400.0,M;
  basis=avtz;

  geometry={
 o
 al   1 1.763083
  o    2 1.763083        1 92.953
 al    3 1.763083        2 87.047        1 0.000
  }

 {hf;wf,42,1,0;}
   {ccsd(t); }
 optg;
 frequencies;
put,molden,al2o2sngrectcass.molden;
```