

Supplementary data for “Relativistic density  
functional theory modeling of plutonium and  
americium higher oxide molecules”

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Calculated equilibrium geometries of plutonium and americium oxide molecules (standard .xyz files separated by empty lines. Units: angströms). See comment (second) lines for identification.

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8
Pu206 pbe0.xyz
Pu      0.000      -1.644      0.000
O       0.000      -1.761     -1.733
O       0.000      -1.761      1.733
O      -1.266      0.000      0.000
Pu      0.000      1.644      0.000
O       1.266      0.000      0.000
O       0.000      1.761     -1.733
O       0.000      1.761      1.733
```

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8
Pu206 b3lyp.xyz
Pu      0.000      -1.661      0.000
O       1.283      0.000      0.000
O       0.000      -1.806      1.755
O       0.000      -1.806     -1.755
Pu      0.000      1.661      0.000
O      -1.283      0.000      0.000
O       0.000      1.806      1.755
O       0.000      1.806     -1.755
```

```
8
Am206 pbe0.xyz
Am      0.000      -1.649      0.000
O       0.000      -1.741      1.725
O       0.000      -1.741     -1.725
O       1.265      0.000      0.000
Am      0.000      1.649      0.000
O      -1.265      0.000      0.000
O       0.000      1.741      1.725
O       0.000      1.741     -1.725
```

8  
Am206 b3lyp.xyz  
Am 0.000 -1.676 0.000  
O 0.000 -1.783 -1.751  
O 0.000 -1.783 1.751  
O -1.276 0.000 0.000  
Am 0.000 1.676 0.000  
O 1.276 0.000 0.000  
O 0.000 1.783 -1.751  
O 0.000 1.783 1.751

8  
PuAm06 pbe0.xyz  
Pu 0.000 1.632 0.000  
O 0.000 1.765 -1.735  
O 0.000 1.765 1.735  
O 1.273 0.000 0.000  
Am 0.000 -1.644 0.000  
O -1.273 -0.000 0.000  
O 0.000 -1.720 -1.722  
O 0.000 -1.720 1.722

8  
PuAm06 b3lyp.xyz  
Pu 0.000 0.000 -1.656  
O 0.000 -1.756 -1.810  
O 0.000 1.756 -1.810  
O -1.278 0.000 0.000  
Am 0.000 0.000 1.669  
O 1.278 0.000 0.000  
O 0.000 -1.746 1.762  
O 0.000 1.746 1.762

9  
 Pu207 pbe0.xyz  
 Pu 0.068 -1.669 0.000  
 0 0.128 -1.575 1.735  
 0 0.139 -1.600 -1.735  
 0 -0.931 -3.158 0.000  
 0 1.213 0.212 0.000  
 Pu -0.023 1.672 0.000  
 0 -1.260 2.923 0.000  
 0 -1.253 0.318 0.000  
 0 1.280 2.835 0.000

9  
 Pu207 b3lyp.xyz  
 Pu 0.069 -1.689 0.000  
 0 0.166 -1.610 1.757  
 0 0.119 -1.605 -1.757  
 0 -0.947 -3.198 0.000  
 0 1.229 0.218 0.000  
 Pu -0.024 1.693 0.000  
 0 -1.288 2.948 0.000  
 0 -1.263 0.313 0.000  
 0 1.297 2.872 0.000

9  
 Am207 pbe0.xyz  
 Am 0.083 -1.656 0.000  
 0 0.093 -1.661 1.723  
 0 0.085 -1.678 -1.723  
 0 -0.962 -3.410 0.000  
 0 1.259 0.301 0.000  
 Am -0.026 1.683 0.000  
 0 -1.348 2.862 0.000  
 0 -1.230 0.274 0.000  
 0 1.238 2.907 0.000

9  
Am207 b3lyp.xyz  
Am 0.083 -1.677 0.000  
0 0.111 -1.688 1.747  
0 0.077 -1.696 -1.747  
0 -0.970 -3.439 0.000  
0 1.271 0.296 0.000  
Am -0.026 1.704 0.000  
0 -1.363 2.906 0.000  
0 -1.245 0.274 0.000  
0 1.257 2.946 0.000

9  
PuAm07 pbe0.xyz  
Am -0.082 -1.661 0.000  
0 -0.116 -1.670 -1.723  
0 -0.061 -1.677 1.723  
0 0.942 -3.426 0.000  
0 -1.252 0.306 0.000  
Pu 0.027 1.682 0.000  
0 1.322 2.868 0.000  
0 1.220 0.264 0.000  
0 -1.220 2.914 0.000

9  
PuAm07 b3lyp.xyz  
Am 0.082 -1.681 0.000  
0 0.122 -1.695 1.747  
0 0.065 -1.695 -1.747  
0 -0.954 -3.453 0.000  
0 1.264 0.303 0.000  
Pu -0.027 1.702 0.000  
0 -1.340 2.904 0.000  
0 -1.233 0.266 0.000  
0 1.242 2.945 0.000

10  
Pu208 pbe0.xyz  
Pu -1.707 0.091 0.000  
0 -1.745 0.157 1.743  
0 -1.745 0.157 -1.743  
0 -2.994 -1.099 0.000  
0 -0.301 1.258 0.000  
Pu 1.707 -0.091 0.000  
0 0.301 -1.258 0.000  
0 1.745 -0.157 1.743  
0 1.745 -0.157 -1.743  
0 2.994 1.099 0.000

10  
Pu208 b3lyp.xyz  
Pu -1.730 0.092 0.000  
0 -0.295 1.266 0.000  
0 -1.794 0.184 1.764  
0 -1.794 0.184 -1.764  
Pu 1.730 -0.092 0.000  
0 0.295 -1.266 0.000  
0 1.794 -0.184 1.764  
0 1.794 -0.184 -1.764  
0 -3.000 -1.151 0.000  
0 3.000 1.151 0.000

10  
Am208 pbe0.xyz  
Am -1.694 0.093 0.000  
0 -0.306 1.268 0.000  
0 -1.704 0.120 1.735  
0 -1.704 0.120 -1.735  
Am 1.694 -0.093 0.000  
0 0.306 -1.268 0.000  
0 1.704 -0.120 1.735  
0 1.704 -0.120 -1.735  
0 -3.013 -1.056 0.000  
0 3.013 1.056 0.000

10  
 PuAm08 pbe0.xyz  
 Pu 0.091 -1.698 0.000  
 0 1.258 -0.295 0.000  
 0 0.156 -1.738 1.743  
 0 0.156 -1.738 -1.743  
 Am -0.092 1.705 0.000  
 0 -1.266 0.313 0.000  
 0 -0.121 1.713 1.735  
 0 -0.121 1.713 -1.735  
 0 -1.096 -2.988 0.000  
 0 1.056 3.025 0.000

10  
 Am208 b3lyp.xyz  
 Am 1.715 -0.094 0.000  
 0 0.298 -1.280 0.000  
 0 1.729 -0.126 1.759  
 0 1.729 -0.126 -1.759  
 Am -1.715 0.094 0.000  
 0 -0.298 1.280 0.000  
 0 -1.729 0.126 1.759  
 0 -1.729 0.126 -1.759  
 0 3.059 1.068 0.000  
 0 -3.059 -1.068 0.000

10  
 PuAm08 b3lyp.xyz  
 Pu 0.092 1.720 0.000  
 0 1.267 0.287 0.000  
 0 0.184 1.784 1.764  
 0 0.184 1.784 -1.764  
 Am -0.094 -1.726 0.000  
 0 -1.279 -0.306 0.000  
 0 -0.126 -1.738 1.759  
 0 -0.126 -1.738 -1.759  
 0 -1.149 2.991 0.000  
 0 1.071 -3.069 0.000