**Supplementary material to:**

G.A. Boyle, T. Govender, H.G. Kruger, T. Naicker and G.E.M. Maguire, *S. Afr. J. Chem.*, 2009, **62**, 129–133.

**Cartesian Coordinates**

The LANL2DZ basis was used for copper; for medium and low levels, the information is provided below.

Optimized coordinates for compound **18a**.

HF=0.0000879

```
%chk=CU_onium_alt.chk
%mem=1000mb
%nproclinda=1
%nprocshared=8
#p opt=gdiis oniom(rpbepbe/geneadmp/auto:b3lyp/6 31+g(d):uff) guess=read

Cu Onium alternate

1 2 1 2 1 2 1 1 1 1 1 1
 C C_3            0    3.000437    2.919753    1.793455 L
 C C_3            0    1.516224    3.298370    1.622555 L
 C C_3            0    0.813077    1.914794    1.570235 L H H_      5
0.0000
 C C_3            0    2.949870    1.366115    1.849651 L
 C C_3            0    1.156069    1.236826    0.202447 M
 C C_3            0    2.671674    0.895098    0.381006 L H H_      5
0.0000
 C C_3            0    1.624925    1.099682    2.602828 L
 C C_3            0    1.551967    1.672377    4.058080 L
 C C_3            0    1.201774    0.397037    2.743873 L
 O O_3            0    0.402080    0.060109    0.044754 M H H_     27
0.0000
 C C_R            0    0.819539    2.120276    1.031922 M
 O O_3            0    2.935094    0.491890    0.235043 L
 C C_3            0    3.140823    0.824062    1.123218 L
 C C_R            0    3.078604    2.317336    1.272228 L
 C C_R            0    1.882268    2.999079    0.992240 L
 C C_R            0    1.815642    4.389404    1.121792 L
 C C_R            0    2.940750    5.108675    1.533578 L
 C C_R            0    4.134065    4.438233    1.816699 L
 C C_R            0    4.205357    3.047362    1.687506 L
 C C_R            0    1.639716    3.030841    1.706647 M
 C C_R            0    1.150294    3.716049    2.816870 M
 C C_R            0    0.152020    3.490798    3.247258 M
 C C_R            0    0.948664    2.578871    2.554558 M
 N N_R            0    0.458760    1.926085    1.474587 M H H_     27
 C C_3            0    4.208415    0.753181    2.481353 L
 C C_3            0    2.360965    2.290902    2.987904 M
```

| | | | | |
|---|---|---|---|---|
| Cu | 0 | 1.359467 | 0.423437 | 0.549331 H |
| O O_R | 0 | 3.400808 | 0.782657 | 0.431380 M |
| O O_R | 0 | 1.908778 | 1.439706 | 0.009915 M |
| H H_ | 0 | 3.615852 | 3.300681 | 0.949737 L |
| H H_ | 0 | 3.421122 | 3.358195 | 2.723653 L |
| H H_ | 0 | 1.147848 | 3.897086 | 2.481842 L |
| H H_ | 0 | 1.345862 | 3.926701 | 0.728290 L |
| H H_ | 0 | 0.277163 | 1.968134 | 1.781468 L |
| H H_ | 0 | 3.334455 | 1.470958 | 0.301766 L |
| H H_ | 0 | 0.505198 | 1.619504 | 4.426951 L |
| H H_ | 0 | 2.188207 | 1.071206 | 4.742075 L |
| H H_ | 0 | 1.885260 | 2.717470 | 4.182669 L |
| H H_ | 0 | 1.766513 | 0.883682 | 3.567650 L |
| H H_ | 0 | 1.376034 | 1.039684 | 1.869616 L |
| H H_ | 0 | 0.120037 | 0.456040 | 2.990445 L |
| H H_ | 0 | 4.133730 | 0.442998 | 1.451961 L |
| H H_ | 0 | 2.360438 | 0.379739 | 1.782945 L |
| H H_ | 0 | 1.002742 | 2.454520 | 0.674655 L |
| H H_ | 0 | 0.891501 | 4.908949 | 0.903295 L |
| H H_ | 0 | 2.887907 | 6.185043 | 1.633668 L |
| H H_ | 0 | 5.004629 | 4.996671 | 2.135715 L |
| H H_ | 0 | 5.138101 | 2.543541 | 1.908428 L |
| H H_ | 0 | 2.651543 | 3.238977 | 1.379703 M |
| H H_ | 0 | 1.789540 | 4.419115 | 3.343282 M |
| H H_ | 0 | 0.555496 | 4.007972 | 4.111328 M |
| H H_ | 0 | 4.106560 | 0.348596 | 2.569406 L |
| H H_ | 0 | 5.094578 | 0.979528 | 1.851399 L |
| H H_ | 0 | 4.379548 | 1.172123 | 3.495102 L |
| H H_ | 0 | 2.502615 | 1.222260 | 3.190168 M |
| H H_ | 0 | 3.080501 | 2.580714 | 2.215665 M |
| H H_ | 0 | 2.599440 | 2.838092 | 3.903234 M |
| C C_R | 0 | 1.721502 | 3.927062 | 1.250013 M |
| H H_ | 0 | 0.795619 | 3.493912 | 0.882408 M |
| H H_ | 0 | 1.677317 | 4.911849 | 1.704727 M |
| C C_R | 0 | 2.914139 | 1.927447 | 0.540552 M |
| N N_R | 0 | 4.118741 | 1.220565 | 0.577583 M |
| C C_R | 0 | 4.258370 | 0.080185 | 0.090889 M |
| O O_R | 0 | 5.500401 | 0.509448 | 0.272003 M |
| C C_3 | 0 | 6.347806 | 0.550152 | 0.794926 M |
| C C_3 | 0 | 5.370243 | 1.658959 | 1.229962 M |
| H H_ | 0 | 6.926229 | 0.129886 | 1.617018 M |
| H H_ | 0 | 7.014589 | 0.860651 | 0.012231 M |
| H H_ | 0 | 5.682576 | 2.638533 | 0.864012 M |
| H H_ | 0 | 5.236895 | 1.698420 | 2.315056 M |
| C C_R | 0 | 2.885208 | 3.263518 | 1.153472 M |
| H H_ | 0 | 3.804655 | 3.694010 | 1.534200 M |

Optimized coordinates for compound **18b**.

HF=0.0073822

```
%chk=CU_onium.chk
```

```
%mem=1000mb
%nproclinda=1
%nprocshared=8
#p opt=gdiis oniom(upbepbe/geneadmp/auto:b3lyp/6 31+g(d):uff) guess=read

Cu and oniom

1 2 1 2 1 2 1 2 1 2 1 2
 C C_3            0    2.690643    3.086689    1.879244 L
 C C_3            0    1.192364    3.327709    1.611328 L
 C C_3            0    0.621698    1.885362    1.532059 L H H_      5
0.0000
 C C_3            0    2.777676    1.535126    1.946603 L
 C C_3            0    1.107561    1.236878    0.193882 M
 C C_3            0    2.634125    1.036254    0.468033 L H H_      5
0.0000
 C C_3            0    1.438661    1.151950    2.619605 L
 C C_3            0    1.223398    1.721098    4.061889 L
 C C_3            0    1.145830    0.376368    2.747639 L
 O O_3            0    0.476736    0.004201    0.006553 M H H_     27
0.0000
 C C_R            0    0.764720    2.083310    1.062457 M
 O O_3            0    3.033725    0.320467    0.348347 L
 C C_3            0    3.359292    0.630324    0.991684 L
 C C_R            0    3.489436    2.120267    1.128777 L
 C C_R            0    2.374974    2.944321    0.897911 L
 C C_R            0    2.487125    4.332487    1.021179 L
 C C_R            0    3.710206    4.907463    1.376559 L
 C C_R            0    4.823251    4.094930    1.609482 L
 C C_R            0    4.715857    2.705851    1.487002 L
 C C_R            0    1.544642    3.033903    1.731217 M
 C C_R            0    1.045097    3.655600    2.874605 M
 C C_R            0    0.223552    3.329337    3.342080 M
 C C_R            0    0.977952    2.384123    2.645658 M
 N N_R            0    0.480601    1.802444    1.534251 M
 C C_3            0    4.045272    1.041262    2.659234 L
 C C_3            0    2.348500    1.968629    3.109960 M
 Cu               0    1.339909    0.182178    0.516430 H
 O O_R            0    1.790234    1.761163    0.080639 M
 O O_R            0    3.353311    0.470146    0.327771 M
 H H_             0    3.320711    3.519132    1.071794 L
 H H_             0    3.009775    3.564832    2.829982 L
 H H_             0    0.717314    3.896616    2.437938 L
 H H_             0    1.025583    3.930316    0.698179 L
 H H_             0    0.479784    1.840321    1.676456 L
 H H_             0    3.281049    1.670894    0.176279 L
 H H_             0    0.165834    1.570374    4.367702 L
 H H_             0    1.870887    1.185868    4.788776 L
 H H_             0    1.447218    2.793914    4.195302 L
 H H_             0    1.702303    0.806920    3.607534 L
 H H_             0    1.429874    1.001849    1.889835 L
 H H_             0    0.061145    0.533273    2.930180 L
 H H_             0    4.316087    0.132541    1.267740 L
 H H_             0    2.569577    0.287079    1.698656 L
```

| | | | | | |
|---|---|---|---|---|---|
| H | H_ | 0 | 1.421230 | 2.512210 | 0.622407 L |
| H | H_ | 0 | 1.625536 | 4.962419 | 0.841247 L |
| H | H_ | 0 | 3.795503 | 5.982248 | 1.471591 L |
| H | H_ | 0 | 5.769912 | 4.541649 | 1.884732 L |
| H | H_ | 0 | 5.588227 | 2.090798 | 1.669623 L |
| H | H_ | 0 | 2.528818 | 3.319320 | 1.379042 M |
| H | H_ | 0 | 1.651421 | 4.388606 | 3.399173 M |
| H | H_ | 0 | 0.630188 | 3.793750 | 4.234391 M |
| H | H_ | 0 | 4.038585 | 0.064957 | 2.750471 L |
| H | H_ | 0 | 4.944301 | 1.345346 | 2.082521 L |
| H | H_ | 0 | 4.114936 | 1.477237 | 3.677813 L |
| H | H_ | 0 | 2.359440 | 0.907260 | 3.389063 M |
| H | H_ | 0 | 3.093836 | 2.113259 | 2.321557 M |
| H | H_ | 0 | 2.653878 | 2.546294 | 3.986034 M |
| C | C_R | 0 | 5.892008 | 1.601554 | 0.089568 M |
| H | H_ | 0 | 5.115335 | 2.289520 | 0.230631 M |
| H | H_ | 0 | 6.894117 | 1.998052 | 0.220243 M |
| C | C_R | 0 | 4.266415 | 0.227758 | 0.148513 M |
| N | N_R | 0 | 4.050422 | 1.542567 | 0.539626 M |
| C | C_R | 0 | 2.827013 | 2.214404 | 0.374298 M |
| O | O_R | 0 | 2.935444 | 3.469002 | 0.785511 M |
| C | C_3 | 0 | 4.220151 | 3.707522 | 1.417348 M |
| C | C_3 | 0 | 5.073892 | 2.474321 | 1.061734 M |
| H | H_ | 0 | 4.614546 | 4.640545 | 1.015982 M |
| H | H_ | 0 | 4.040972 | 3.807265 | 2.489857 M |
| H | H_ | 0 | 5.571142 | 2.059585 | 1.940283 M |
| H | H_ | 0 | 5.815165 | 2.693026 | 0.287654 M |
| C | C_R | 0 | 5.627314 | 0.307530 | 0.325503 M |
| H | H_ | 0 | 6.414856 | 0.361139 | 0.653887 M |