**GAUSSIAN 98 CALCULATIONS**

Compound 1 (Me2)

Basis set

Cu 6-31111+g augmented with f exponent= 0.5283
All other atoms 6-31G*

| | | | |
|---|---|---|---|
| Cu | 0.000000 | 0.000000 | 0.000000 |
| Cu | 3.235600 | 0.000000 | 0.000000 |
| N | -1.642350 | 0.592240 | -1.118070 |
| N | -0.772640 | -1.826580 | -0.159810 |
| N | 4.826950 | 0.584580 | -1.159290 |
| N | 4.151620 | -1.762140 | 0.084330 |
| O | 1.610240 | -0.576160 | 0.846840 |
| O | 2.704040 | 1.839230 | 0.000000 |
| O | 0.480650 | 1.861980 | 0.165190 |
| C | 1.567870 | 2.414380 | 0.143570 |
| C | 1.617400 | -1.582200 | 1.689910 |
| C | -2.182450 | -0.626960 | -1.727660 |
| C | -2.076670 | -1.764970 | -0.801810 |
| C | -2.562320 | 1.391930 | -0.414560 |
| C | -1.156050 | 1.339980 | -2.335350 |
| C | 5.547200 | -0.650950 | -1.554730 |
| C | 5.469910 | -1.708740 | -0.561310 |
| C | 5.725760 | 1.442250 | -0.369580 |
| C | 4.480980 | 1.275850 | -2.405040 |
| H | 1.627030 | 3.367430 | 0.242540 |
| H | -0.221150 | -2.347980 | -0.646140 |
| H | -0.856340 | -2.194010 | 0.656840 |
| H | 4.248900 | -2.007290 | 0.944300 |
| H | 3.642860 | -2.382050 | -0.325720 |
| H | -3.110000 | -0.487700 | -1.967400 |
| H | -1.688390 | -0.827080 | -2.540700 |
| H | -2.234310 | -2.587940 | -1.289070 |
| H | -2.764450 | -1.684990 | -0.121790 |
| H | -3.379850 | 1.448280 | -0.915010 |
| H | -2.195580 | 2.271380 | -0.300110 |
| H | -2.733830 | 0.999290 | 0.441270 |
| H | -1.904430 | 1.552190 | -2.898440 |
| H | -0.532960 | 0.794510 | -2.816220 |
| H | -0.725290 | 2.152690 | -2.056670 |
| H | 5.169840 | -0.976100 | -2.386940 |
| H | 6.475860 | -0.433850 | -1.711520 |
| H | 6.153080 | -1.562910 | 0.114130 |
| H | 5.652270 | -2.560250 | -0.989730 |
| H | 6.184640 | 2.049900 | -0.952240 |
| H | 6.367370 | 0.894970 | 0.093100 |
| H | 5.211570 | 1.941330 | 0.271680 |
| H | 5.065040 | 2.025870 | -2.528580 |
| H | 3.572270 | 1.585330 | -2.352660 |
| H | 4.569680 | 0.671820 | -3.142670 |
| H | 0.814890 | -1.569270 | 2.213690 |
| H | 2.380530 | -1.509810 | 2.269500 |
| H | 1.666000 | -2.408770 | 1.201320 |

| Total Energy | Triplet state | Broken symmetry state |
|---|---|---|
| UHF | -4114.366390 | -4114.366353 |
| U-B3LYP | -4122.688159 | -4122.688299 |

Electronic Supplementary Information for Dalton Transactions


Compound 2 (Me4)

Basis set

Cu 6-31111+g augmented with f exponent= 0.5283
All other atoms 6-31G*

| | | | |
|---|---|---|---|
| Cu | 0.000000 | 0.000000 | 0.000000 |
| Cu | 3.363100 | 0.000000 | 0.000000 |
| N | -1.862120 | 0.666590 | -0.521360 |
| N | -0.874800 | -1.879360 | 0.100140 |
| N | 5.234350 | 0.689060 | -0.383370 |
| N | 4.283040 | -1.807200 | 0.316380 |
| O | 2.802330 | 1.853840 | 0.000000 |
| O | 0.537940 | 1.869370 | -0.042750 |
| O | 1.683700 | -0.690470 | 0.569790 |
| C | 1.664190 | 2.425090 | -0.047190 |
| C | -2.702400 | -0.546390 | -0.778280 |
| C | -2.324850 | -1.611350 | 0.138580 |
| C | -2.404900 | 1.502800 | 0.572780 |
| C | -0.515680 | -2.623320 | 1.336550 |
| C | -1.883580 | 1.462980 | -1.746400 |
| C | -0.489570 | -2.688330 | -1.055240 |
| C | 6.134440 | -0.475760 | -0.462770 |
| C | 5.740630 | -1.560440 | 0.096160 |
| C | 5.703710 | 1.581570 | 0.684020 |
| C | 4.135950 | -2.241680 | 1.702240 |
| C | 5.322420 | 1.455500 | -1.651180 |
| C | 3.772530 | -2.823650 | -0.555550 |
| H | 1.680790 | 3.383770 | -0.094720 |
| H | 1.625520 | -0.656590 | 1.522110 |
| H | -3.640040 | -0.325120 | -0.658580 |
| H | -2.576500 | -0.842920 | -1.693970 |
| H | -2.807810 | -2.420920 | -0.092960 |
| H | -2.579970 | -1.362270 | 1.041310 |
| H | -2.400670 | 1.001160 | 1.390350 |
| H | -3.303650 | 1.763960 | 0.360520 |
| H | -1.860550 | 2.287080 | 0.675540 |
| H | -0.763510 | -2.104470 | 2.104300 |
| H | 0.430550 | -2.784700 | 1.351150 |
| H | -0.982970 | -3.462780 | 1.353310 |
| H | -1.534730 | 0.941790 | -2.473480 |
| H | -1.343820 | 2.247880 | -1.627290 |
| H | -2.787000 | 1.723540 | -1.943110 |
| H | 0.459370 | -2.837460 | -1.040240 |
| H | -0.727030 | -2.226250 | -1.862160 |
| H | -0.945720 | -3.532060 | -1.022570 |
| H | 6.296800 | -0.663030 | -1.399740 |
| H | 6.983550 | -0.226680 | -0.068130 |
| H | 6.176410 | -1.612500 | 0.960530 |
| H | 6.080570 | -2.296720 | -0.435660 |
| H | 5.122620 | 2.344060 | 0.741490 |
| H | 6.596270 | 1.873170 | 0.486200 |
| H | 5.698180 | 1.111150 | 1.520160 |
| H | 4.477370 | -1.562380 | 2.288730 |
| H | 4.624720 | -3.056230 | 1.835890 |
| H | 3.206900 | -2.391690 | 1.892900 |
| H | 5.023520 | 0.905550 | -2.378940 |
| H | 6.233620 | 1.719080 | -1.802790 |
| H | 4.768490 | 2.236500 | -1.592370 |
| H | 3.867140 | -2.540610 | -1.467780 |
| H | 2.843600 | -2.972980 | -0.361790 |
| H | 4.262480 | -3.636700 | -0.419240 |

| Total Energy | Triplet state | Broken symmetry state |
|---|---|---|
| UHF | -4231.360721 | -4231.360664 |
| U-B3LYP | -4240.530011 | -4240.529840 |

**CASPT2 CALCULATIONS**

Real structure compound (1):

| | | | | |
|---|---|---|---|---|
| CU1 | 0.000000 | 0.000000 | 0.000000 | Angstrom |
| CU2 | 3.235600 | 0.000000 | 0.000000 | Angstrom |
| N1 | -1.642350 | 0.592240 | -1.118070 | Angstrom |
| N2 | -0.772640 | -1.826580 | -0.159810 | Angstrom |
| N3 | 4.826950 | 0.584580 | -1.159290 | Angstrom |
| N4 | 4.151620 | -1.762140 | 0.084330 | Angstrom |
| O1 | 1.610240 | -0.576160 | 0.846840 | Angstrom |
| O2 | 2.704040 | 1.839230 | 0.000000 | Angstrom |
| O3 | 0.480650 | 1.861980 | 0.165190 | Angstrom |
| C1 | 1.567870 | 2.414380 | 0.143570 | Angstrom |
| C2 | 1.617400 | -1.582200 | 1.689910 | Angstrom |
| C3 | -2.182450 | -0.626960 | -1.727660 | Angstrom |
| C4 | -2.076670 | -1.764970 | -0.801810 | Angstrom |
| C5 | -2.562320 | 1.391930 | -0.414560 | Angstrom |
| C6 | -1.156050 | 1.339980 | -2.335350 | Angstrom |
| C7 | 5.547200 | -0.650950 | -1.554730 | Angstrom |
| C8 | 5.469910 | -1.708740 | -0.561310 | Angstrom |
| C9 | 5.725760 | 1.442250 | -0.369580 | Angstrom |
| C10 | 4.480980 | 1.275850 | -2.405040 | Angstrom |
| H1 | 1.627030 | 3.367430 | 0.242540 | Angstrom |
| H2 | -0.221150 | -2.347980 | -0.646140 | Angstrom |
| H3 | -0.856340 | -2.194010 | 0.656840 | Angstrom |
| H4 | 4.248900 | -2.007290 | 0.944300 | Angstrom |
| H5 | 3.642860 | -2.382050 | -0.325720 | Angstrom |
| H6 | -3.110000 | -0.487700 | -1.967400 | Angstrom |
| H7 | -1.688390 | -0.827080 | -2.540700 | Angstrom |
| H8 | -2.234310 | -2.587940 | -1.289070 | Angstrom |
| H9 | -2.764450 | -1.684990 | -0.121790 | Angstrom |
| H10 | -3.379850 | 1.448280 | -0.915010 | Angstrom |
| H11 | -2.195580 | 2.271380 | -0.300110 | Angstrom |
| H12 | -2.733830 | 0.999290 | 0.441270 | Angstrom |
| H13 | -1.904430 | 1.552190 | -2.898440 | Angstrom |
| H14 | -0.532960 | 0.794510 | -2.816220 | Angstrom |
| H15 | -0.725290 | 2.152690 | -2.056670 | Angstrom |
| H16 | 5.169840 | -0.976100 | -2.386940 | Angstrom |
| H17 | 6.475860 | -0.433850 | -1.711520 | Angstrom |
| H18 | 6.153080 | -1.562910 | 0.114130 | Angstrom |
| H19 | 5.652270 | -2.560250 | -0.989730 | Angstrom |
| H20 | 6.184640 | 2.049900 | -0.952240 | Angstrom |
| H21 | 6.367370 | 0.894970 | 0.093100 | Angstrom |
| H22 | 5.211570 | 1.941330 | 0.271680 | Angstrom |
| H23 | 5.065040 | 2.025870 | -2.528580 | Angstrom |
| H24 | 3.572270 | 1.585330 | -2.352660 | Angstrom |
| H25 | 4.569680 | 0.671820 | -3.142670 | Angstrom |
| H26 | 0.814890 | -1.569270 | 2.213690 | Angstrom |
| H27 | 2.380530 | -1.509810 | 2.269500 | Angstrom |
| H28 | 1.666000 | -2.408770 | 1.201320 | Angstrom |

Total CASPT2 energies:
singlet -4116.7263317624 Hartree
triplet -4116.7262388399 Hartree

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Real structure compound (2):

| | | | | |
|---|---|---|---|---|
| CU1 | 0.000000 | 0.000000 | 0.000000 | Angstrom |
| CU2 | 3.363100 | 0.000000 | 0.000000 | Angstrom |
| N1 | -1.862120 | 0.666590 | -0.521360 | Angstrom |
| N2 | -0.874800 | -1.879360 | 0.100140 | Angstrom |
| N3 | 5.234350 | 0.689060 | -0.383370 | Angstrom |
| N4 | 4.283040 | -1.807200 | 0.316380 | Angstrom |
| O1 | 2.802330 | 1.853840 | 0.000000 | Angstrom |
| O2 | 0.537940 | 1.869370 | -0.042750 | Angstrom |
| O3 | 1.683700 | -0.690470 | 0.569790 | Angstrom |
| C1 | 1.664190 | 2.425090 | -0.047190 | Angstrom |
| C2 | -2.702400 | -0.546390 | -0.778280 | Angstrom |
| C3 | -2.324850 | -1.611350 | 0.138580 | Angstrom |
| C4 | -2.404900 | 1.502800 | 0.572780 | Angstrom |
| C5 | -0.515680 | -2.623320 | 1.336550 | Angstrom |
| C6 | -1.883580 | 1.462980 | -1.746400 | Angstrom |
| C7 | -0.489570 | -2.688330 | -1.055240 | Angstrom |
| C8 | 6.134440 | -0.475760 | -0.462770 | Angstrom |
| C9 | 5.740630 | -1.560440 | 0.096160 | Angstrom |
| C10 | 5.703710 | 1.581570 | 0.684020 | Angstrom |
| C11 | 4.135950 | -2.241680 | 1.702240 | Angstrom |
| C12 | 5.322420 | 1.455500 | -1.651180 | Angstrom |
| C13 | 3.772530 | -2.823650 | -0.555550 | Angstrom |
| H1 | 1.680790 | 3.383770 | -0.094720 | Angstrom |
| H2 | 1.625520 | -0.656590 | 1.522110 | Angstrom |
| H3 | -3.640040 | -0.325120 | -0.658580 | Angstrom |
| H4 | -2.576500 | -0.842920 | -1.693970 | Angstrom |
| H5 | -2.807810 | -2.420920 | -0.092960 | Angstrom |
| H6 | -2.579970 | -1.362270 | 1.041310 | Angstrom |
| H7 | -2.400670 | 1.001160 | 1.390350 | Angstrom |
| H8 | -3.303650 | 1.763960 | 0.360520 | Angstrom |
| H9 | -1.860550 | 2.287080 | 0.675540 | Angstrom |
| H10 | -0.763510 | -2.104470 | 2.104300 | Angstrom |
| H11 | 0.430550 | -2.784700 | 1.351150 | Angstrom |
| H12 | -0.982970 | -3.462780 | 1.353310 | Angstrom |
| H13 | -1.534730 | 0.941790 | -2.473480 | Angstrom |
| H14 | -1.343820 | 2.247880 | -1.627290 | Angstrom |
| H15 | -2.787000 | 1.723540 | -1.943110 | Angstrom |
| H16 | 0.459370 | -2.837460 | -1.040240 | Angstrom |
| H17 | -0.727030 | -2.226250 | -1.862160 | Angstrom |
| H18 | -0.945720 | -3.532060 | -1.022570 | Angstrom |
| H19 | 6.296800 | -0.663030 | -1.399740 | Angstrom |
| H20 | 6.983550 | -0.226680 | -0.068130 | Angstrom |
| H21 | 6.176410 | -1.612500 | 0.960530 | Angstrom |
| H22 | 6.080570 | -2.296720 | -0.435660 | Angstrom |
| H23 | 5.122620 | 2.344060 | 0.741490 | Angstrom |
| H24 | 6.596270 | 1.873170 | 0.486200 | Angstrom |
| H25 | 5.698180 | 1.111150 | 1.520160 | Angstrom |
| H26 | 4.477370 | -1.562380 | 2.288730 | Angstrom |
| H27 | 4.624720 | -3.056230 | 1.835890 | Angstrom |
| H28 | 3.206900 | -2.391690 | 1.892900 | Angstrom |
| H29 | 5.023520 | 0.905550 | -2.378940 | Angstrom |
| H30 | 6.233620 | 1.719080 | -1.802790 | Angstrom |
| H31 | 4.768490 | 2.236500 | -1.592370 | Angstrom |
| H32 | 3.867140 | -2.540610 | -1.467780 | Angstrom |
| H33 | 2.843600 | -2.972980 | -0.361790 | Angstrom |
| H34 | 4.262480 | -3.636700 | -0.419240 | Angstrom |

Total CASPT2 energies:
singlet -4233.9679832623 Hartree
triplet -4233.9680165331 Hartree

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Model structure compound (1)

| | | | | |
|---|---|---|---|---|
| Cu1 | 0.000000 | 1.617850 | 0.000000 | Angstrom |
| Cu2 | 0.000000 | -1.617850 | 0.000000 | Angstrom |
| N1 | 0.589701 | 3.234804 | -1.139984 | Angstrom |
| N2 | 0.589701 | -3.234804 | -1.139984 | Angstrom |
| N3 | -1.793371 | 2.464544 | -0.041681 | Angstrom |
| N4 | -1.793371 | -2.464544 | -0.041681 | Angstrom |
| O1 | 1.852080 | 1.112760 | 0.082388 | Angstrom |
| O2 | 1.852080 | -1.112760 | 0.082388 | Angstrom |
| O3 | -0.576508 | 0.000000 | 0.846397 | Angstrom |
| C1 | 2.414113 | 0.000000 | 0.143488 | Angstrom |
| C2 | -1.582408 | 0.000000 | 1.691780 | Angstrom |
| H1 | 3.307583 | 0.000000 | 0.236491 | Angstrom |
| H2 | -1.536771 | 0.782342 | 2.242898 | Angstrom |
| H3 | -1.536771 | -0.782342 | 2.242898 | Angstrom |
| H4 | -2.409115 | 0.000000 | 1.204688 | Angstrom |
| H5 | 1.110541 | 3.802499 | -0.674745 | Angstrom |
| H6 | 1.110541 | -3.802499 | -0.674745 | Angstrom |
| H7 | 1.024812 | 2.981920 | -1.886126 | Angstrom |
| H8 | 1.024812 | -2.981920 | -1.886126 | Angstrom |
| H9 | -0.171047 | 3.621750 | -1.425530 | Angstrom |
| H11 | -0.171047 | -3.621750 | -1.425530 | Angstrom |
| H12 | -1.752365 | 3.269532 | -0.442072 | Angstrom |
| H13 | -1.752365 | -3.269532 | -0.442072 | Angstrom |
| H14 | -2.365797 | 1.934096 | -0.486389 | Angstrom |
| H15 | -2.365797 | -1.934096 | -0.486389 | Angstrom |
| H16 | -2.099013 | 2.561387 | 0.797430 | Angstrom |
| H17 | -2.099013 | -2.561387 | 0.797430 | Angstrom |

Total CASPT2 energies:
singlet -3806.3867061103 Hartree
triplet -3806.3866281605 Hartree

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Model structure compound (2)

| | | | | |
|---|---|---|---|---|
| Cu1 | 0.000000 | 1.681500 | 0.000000 | Angstrom |
| Cu2 | 0.000000 | -1.681500 | 0.000000 | Angstrom |
| N1 | 0.742600 | 3.549000 | -0.335000 | Angstrom |
| N2 | 0.742600 | -3.549000 | -0.335000 | Angstrom |
| N3 | -1.853100 | 2.578600 | -0.096500 | Angstrom |
| N4 | -1.853100 | -2.578600 | -0.096500 | Angstrom |
| O1 | -0.774300 | 0.000000 | 0.449500 | Angstrom |
| O2 | 1.839300 | 1.132500 | 0.283500 | Angstrom |
| O3 | 1.839300 | -1.132500 | 0.283500 | Angstrom |
| C1 | 2.400100 | 0.000000 | 0.350500 | Angstrom |
| H1 | -0.896900 | 0.000000 | 1.394500 | Angstrom |
| H2 | 3.298900 | 0.000000 | 0.453500 | Angstrom |
| H3 | 0.008801 | 4.106238 | -0.566355 | Angstrom |
| H4 | 0.008801 | -4.106238 | -0.566355 | Angstrom |
| H5 | 1.178333 | 3.875268 | 0.443579 | Angstrom |
| H6 | 1.178333 | -3.875268 | 0.443579 | Angstrom |
| H7 | 1.371834 | 3.583979 | -1.045873 | Angstrom |
| H8 | 1.371834 | -3.583979 | -1.045873 | Angstrom |
| H9 | -1.680386 | 3.512281 | -0.126677 | Angstrom |
| H10 | -1.680386 | -3.512281 | -0.126677 | Angstrom |
| H11 | -2.370870 | 2.414388 | 0.682890 | Angstrom |
| H12 | -2.370870 | -2.414388 | 0.682890 | Angstrom |
| H13 | -2.338815 | 2.281955 | -0.857146 | Angstrom |
| H14 | -2.338815 | -2.281955 | -0.857146 | Angstrom |

```
Total CASPT2 energies:
singlet   -3767.5342625177 Hartree
triplet   -3767.5343700582 Hartree
```