

**Synthesis and Structural Characterization of  
*Tris*(2-mercapto-1-methylbenzimidazolyl)hydroborato Cadmium Halide  
Complexes,  $\{[\text{Tm}^{\text{MeBenz}}]\text{Cd}(\mu\text{-Cl})\}_2$  and  $[\text{Tm}^{\text{MeBenz}}]\text{CdI}$ : A Rare Example of  
Cadmium in a Trigonal Bipyramidal  
Sulfur-Rich Coordination Environment**

Joshua H. Palmer and Gerard Parkin,\*

*Department of Chemistry,*

*Columbia University,*

*New York, New York 10027, USA.*

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**Table 1.** Cartesian coordinates for geometry optimized structures (energies in parentheses are for the geometry optimization basis set, and those not in parentheses are for the single point basis set)

| [Tm <sup>MeBenz</sup> ]CdCl  |              |             |              |
|------------------------------|--------------|-------------|--------------|
| -2984.80449484489 Hartrees   |              |             |              |
| (-2984.29328050069 Hartrees) |              |             |              |
| Atom                         | x            | y           | z            |
| Cl                           | 2.012679913  | 4.078327524 | 0.338754895  |
| Cd                           | 1.162000985  | 5.698978585 | -1.257690829 |
| B                            | -0.184159128 | 8.314195349 | -3.836603511 |
| H                            | -0.604838273 | 9.117372    | -4.625382861 |
| N                            | -1.453009734 | 7.628633127 | -3.243621822 |
| N                            | -3.054360115 | 6.261154966 | -2.540392282 |
| N                            | 0.714127581  | 7.354877068 | -4.675186454 |
| N                            | 2.319395924  | 6.096732392 | -5.550323387 |
| N                            | 0.618066236  | 9.150928124 | -2.796272653 |
| N                            | 1.521626206  | 10.11119302 | -1.010890174 |
| S                            | -0.722746154 | 4.949332158 | -3.005459071 |
| S                            | 2.870882889  | 6.816576903 | -2.99295455  |
| S                            | 0.018420773  | 7.946591617 | -0.355366867 |
| C                            | -1.741414829 | 6.332958645 | -2.931900765 |
| C                            | -2.608031058 | 8.392066744 | -3.02814587  |
| C                            | -3.619292853 | 7.527263881 | -2.59025359  |
| C                            | -4.907224826 | 7.97307909  | -2.297665351 |
| H                            | -5.683372812 | 7.292166589 | -1.964493109 |
| C                            | -5.152106139 | 9.336463739 | -2.45113573  |
| H                            | -6.140814739 | 9.72771249  | -2.231483936 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -4.142541157 | 10.21186493 | -2.882009231 |
| H | -4.366264889 | 11.26918462 | -2.987246714 |
| C | -2.857325488 | 9.758056295 | -3.175275201 |
| H | -2.082842308 | 10.44145559 | -3.501186383 |
| C | -3.764181632 | 5.068687229 | -2.107042052 |
| H | -3.050944964 | 4.248054853 | -2.040803616 |
| H | -4.212890527 | 5.247023173 | -1.125500186 |
| H | -4.55065814  | 4.813099959 | -2.824353336 |
| C | 1.917810544  | 6.766148905 | -4.422876066 |
| C | 1.361588861  | 6.24856916  | -6.542050296 |
| C | 0.344845333  | 7.037546614 | -5.989027098 |
| C | -0.78337325  | 7.370884728 | -6.741339052 |
| H | -1.583237962 | 7.970667287 | -6.324475389 |
| C | -0.843612993 | 6.899633672 | -8.052097005 |
| H | -1.708012411 | 7.144424627 | -8.662022241 |
| C | 0.183864083  | 6.115408842 | -8.600398554 |
| H | 0.10071772   | 5.766541577 | -9.625190279 |
| C | 1.309013711  | 5.775001117 | -7.851805642 |
| H | 2.105888979  | 5.169591669 | -8.27049694  |
| C | 3.536163653  | 5.316722636 | -5.704249116 |
| H | 4.033568617  | 5.259862947 | -4.736894029 |
| H | 3.28241987   | 4.309962774 | -6.047576145 |
| H | 4.202826875  | 5.791328039 | -6.431254739 |
| C | 0.729941637  | 9.076605027 | -1.439743098 |
| C | 1.367519944  | 10.25144393 | -3.232559732 |
| C | 1.933667848  | 10.85886071 | -2.104510128 |
| C | 2.73520921   | 11.99555007 | -2.194386426 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 3.1647945   | 12.4599401  | -1.312955739 |
| C | 2.961900159 | 12.50865146 | -3.470437697 |
| H | 3.58290652  | 13.39189632 | -3.585509319 |
| C | 2.403937025 | 11.90283153 | -4.60805402  |
| H | 2.603090969 | 12.32687409 | -5.587482864 |
| C | 1.601907235 | 10.76633387 | -4.509605796 |
| H | 1.179815614 | 10.30097401 | -5.391882209 |
| C | 1.915197755 | 10.3850739  | 0.361759112  |
| H | 1.476238993 | 11.32808879 | 0.702832444  |
| H | 1.559587424 | 9.569812089 | 0.990765925  |
| H | 3.005438167 | 10.44902055 | 0.423352534  |



-5969.62804739330 Hartrees

(-5968.60556835470 Hartrees)

| Atom | x            | y            | z            |
|------|--------------|--------------|--------------|
| Cd   | 1.206354173  | -0.84881315  | 1.296814525  |
| Cl   | -0.861485331 | -1.537178306 | -0.353825966 |
| B    | 2.935422292  | -3.226488295 | 4.00783582   |
| H    | 3.396615228  | -4.008765525 | 4.797266238  |
| N    | 4.154821698  | -2.484445557 | 3.395663089  |
| N    | 5.62638538   | -1.032788167 | 2.586430029  |
| N    | 2.027330983  | -2.281001371 | 4.855447966  |
| N    | 0.445386334  | -1.004176977 | 5.744870844  |
| N    | 2.149404548  | -4.094188097 | 2.979638861  |
| N    | 1.245295021  | -5.072578729 | 1.20439791   |
| S    | 3.19093642   | 0.091558007  | 2.985452755  |
| S    | -0.242507286 | -1.920977267 | 3.283426877  |

|   |             |              |             |
|---|-------------|--------------|-------------|
| S | 2.75636007  | -2.913227437 | 0.532393209 |
| C | 4.324378718 | -1.188637144 | 2.998986096 |
| C | 5.366339109 | -3.1595689   | 3.208010264 |
| C | 6.29618798  | -2.240580878 | 2.702770812 |
| C | 7.612132758 | -2.59511382  | 2.413240888 |
| H | 8.32331892  | -1.872759513 | 2.026302144 |
| C | 7.973680862 | -3.922666991 | 2.639500166 |
| H | 8.988797574 | -4.242442778 | 2.423622847 |
| C | 7.047331686 | -4.851772352 | 3.137412755 |
| H | 7.35936232  | -5.879550408 | 3.29820146  |
| C | 5.731917395 | -4.488922306 | 3.427049374 |
| H | 5.02036015  | -5.214009645 | 3.803114971 |
| C | 6.222712121 | 0.184343531  | 2.065870433 |
| H | 5.438121077 | 0.934152614  | 1.967522218 |
| H | 6.666165036 | -0.015317502 | 1.086051142 |
| H | 6.998192468 | 0.551750485  | 2.74620506  |
| C | 0.794076955 | -1.741996938 | 4.640475786 |
| C | 1.470534822 | -1.05564432  | 6.676201759 |
| C | 2.471183168 | -1.859252576 | 6.11431507  |
| C | 3.65841129  | -2.101917783 | 6.808068282 |
| H | 4.44637231  | -2.71126566  | 6.382374276 |
| C | 3.795070829 | -1.52480019  | 8.070114016 |
| H | 4.707949222 | -1.695954124 | 8.633029814 |
| C | 2.784554676 | -0.725315735 | 8.627525593 |
| H | 2.929116063 | -0.290380531 | 9.612041178 |
| C | 1.599325235 | -0.47670374  | 7.937333953 |
| H | 0.815599828 | 0.142119675  | 8.361751301 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -0.777970906 | -0.241270304 | 5.920579654  |
| H  | -1.352266009 | -0.297251913 | 4.996420889  |
| H  | -0.531134175 | 0.802089777  | 6.137641372  |
| H  | -1.368807403 | -0.65349068  | 6.745132747  |
| C  | 2.037858109  | -4.034920065 | 1.621484529  |
| C  | 1.407558612  | -5.193613483 | 3.425813459  |
| C  | 0.837824128  | -5.810960881 | 2.304751484  |
| C  | 0.036878139  | -6.946992936 | 2.406690665  |
| H  | -0.398444617 | -7.416014668 | 1.530635662  |
| C  | -0.183371289 | -7.450505584 | 3.687180325  |
| H  | -0.80434717  | -8.332410952 | 3.813158595  |
| C  | 0.380652194  | -6.835928432 | 4.816846041  |
| H  | 0.18647394   | -7.253013139 | 5.800666399  |
| C  | 1.180890839  | -5.699634276 | 4.707445397  |
| H  | 1.606541892  | -5.226198452 | 5.584016302  |
| C  | 0.837898146  | -5.350586556 | -0.163423121 |
| H  | 1.265458276  | -6.300581177 | -0.500580545 |
| H  | 1.192656008  | -4.539669064 | -0.797670028 |
| H  | -0.253033372 | -5.399067532 | -0.215215691 |
| Cd | -1.206354173 | 0.84881315   | -1.296814525 |
| Cl | 0.861485331  | 1.537178306  | 0.353825966  |
| B  | -2.935422292 | 3.226488295  | -4.00783582  |
| H  | -3.396615228 | 4.008765525  | -4.797266238 |
| N  | -4.154821698 | 2.484445557  | -3.395663089 |
| N  | -5.62638538  | 1.032788167  | -2.586430029 |
| N  | -2.027330983 | 2.281001371  | -4.855447966 |
| N  | -0.445386334 | 1.004176977  | -5.744870844 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -2.149404548 | 4.094188097  | -2.979638861 |
| N | -1.245295021 | 5.072578729  | -1.20439791  |
| S | -3.19093642  | -0.091558007 | -2.985452755 |
| S | 0.242507286  | 1.920977267  | -3.283426877 |
| S | -2.75636007  | 2.913227437  | -0.532393209 |
| C | -4.324378718 | 1.188637144  | -2.998986096 |
| C | -5.366339109 | 3.1595689    | -3.208010264 |
| C | -6.29618798  | 2.240580878  | -2.702770812 |
| C | -7.612132758 | 2.59511382   | -2.413240888 |
| H | -8.32331892  | 1.872759513  | -2.026302144 |
| C | -7.973680862 | 3.922666991  | -2.639500166 |
| H | -8.988797574 | 4.242442778  | -2.423622847 |
| C | -7.047331686 | 4.851772352  | -3.137412755 |
| H | -7.35936232  | 5.879550408  | -3.29820146  |
| C | -5.731917395 | 4.488922306  | -3.427049374 |
| H | -5.02036015  | 5.214009645  | -3.803114971 |
| C | -6.222712121 | -0.184343531 | -2.065870433 |
| H | -5.438121077 | -0.934152614 | -1.967522218 |
| H | -6.666165036 | 0.015317502  | -1.086051142 |
| H | -6.998192468 | -0.551750485 | -2.74620506  |
| C | -0.794076955 | 1.741996938  | -4.640475786 |
| C | -1.470534822 | 1.05564432   | -6.676201759 |
| C | -2.471183168 | 1.859252576  | -6.11431507  |
| C | -3.65841129  | 2.101917783  | -6.808068282 |
| H | -4.44637231  | 2.71126566   | -6.382374276 |
| C | -3.795070829 | 1.52480019   | -8.070114016 |
| H | -4.707949222 | 1.695954124  | -8.633029814 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.784554676 | 0.725315735  | -8.627525593 |
| H | -2.929116063 | 0.290380531  | -9.612041178 |
| C | -1.599325235 | 0.47670374   | -7.937333953 |
| H | -0.815599828 | -0.142119675 | -8.361751301 |
| C | 0.777970906  | 0.241270304  | -5.920579654 |
| H | 1.352266009  | 0.297251913  | -4.996420889 |
| H | 0.531134175  | -0.802089777 | -6.137641372 |
| H | 1.368807403  | 0.65349068   | -6.745132747 |
| C | -2.037858109 | 4.034920065  | -1.621484529 |
| C | -1.407558612 | 5.193613483  | -3.425813459 |
| C | -0.837824128 | 5.810960881  | -2.304751484 |
| C | -0.036878139 | 6.946992936  | -2.406690665 |
| H | 0.398444617  | 7.416014668  | -1.530635662 |
| C | 0.183371289  | 7.450505584  | -3.687180325 |
| H | 0.80434717   | 8.332410952  | -3.813158595 |
| C | -0.380652194 | 6.835928432  | -4.816846041 |
| H | -0.18647394  | 7.253013139  | -5.800666399 |
| C | -1.180890839 | 5.699634276  | -4.707445397 |
| H | -1.606541892 | 5.226198452  | -5.584016302 |
| C | -0.837898146 | 5.350586556  | 0.163423121  |
| H | -1.265458276 | 6.300581177  | 0.500580545  |
| H | -1.192656008 | 4.539669064  | 0.797670028  |
| H | 0.253033372  | 5.399067532  | 0.215215691  |

[Tm<sup>MeBenz</sup>]CdI

-2535.96145310647 Hartrees

(-2535.49139235569 Hartrees)

| Atom | x            | y           | z            |
|------|--------------|-------------|--------------|
| I    | 2.115512847  | 3.87454761  | 0.519138203  |
| Cd   | 1.147659871  | 5.734995577 | -1.300100215 |
| B    | -0.203640575 | 8.363084068 | -3.877053326 |
| H    | -0.620717307 | 9.16800436  | -4.666041338 |
| N    | -1.473718116 | 7.677216118 | -3.289291908 |
| N    | -3.069468523 | 6.309365248 | -2.575566986 |
| N    | 0.693725833  | 7.40277845  | -4.714659852 |
| N    | 2.295213329  | 6.138457971 | -5.588596967 |
| N    | 0.596304916  | 9.197457548 | -2.832011457 |
| N    | 1.495170828  | 10.15026786 | -1.040616765 |
| S    | -0.740588242 | 4.998979773 | -3.053693712 |
| S    | 2.851752182  | 6.866123122 | -3.034069993 |
| S    | -0.007702792 | 7.980921628 | -0.399497608 |
| C    | -1.75919593  | 6.382116871 | -2.974116141 |
| C    | -2.629517383 | 8.439185847 | -3.072954817 |
| C    | -3.637164918 | 7.574070005 | -2.627650938 |
| C    | -4.924839957 | 8.018073232 | -2.331908642 |
| H    | -5.697872819 | 7.336820231 | -1.992273885 |
| C    | -5.173914737 | 9.380063084 | -2.491401009 |
| H    | -6.162874727 | 9.770045005 | -2.270326983 |
| C    | -4.168051857 | 10.25596302 | -2.930665602 |
| H    | -4.395115869 | 11.31213022 | -3.041262669 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -2.882551257 | 9.803960922 | -3.225769354 |
| H | -2.110983541 | 10.48774502 | -3.558011804 |
| C | -3.77427264  | 5.117140408 | -2.1332757   |
| H | -3.058435572 | 4.298860893 | -2.065544391 |
| H | -4.219453273 | 5.299606172 | -1.150907944 |
| H | -4.562868363 | 4.855362752 | -2.846014399 |
| C | 1.897208754  | 6.813777088 | -4.463212007 |
| C | 1.333654406  | 6.284814934 | -6.57760043  |
| C | 0.319796735  | 7.078393341 | -6.025497002 |
| C | -0.811589185 | 7.406655275 | -6.775362153 |
| H | -1.609175669 | 8.010293338 | -6.35969252  |
| C | -0.878480769 | 6.924598828 | -8.082016155 |
| H | -1.745937036 | 7.164247383 | -8.68979154  |
| C | 0.145982279  | 6.135260314 | -8.629175059 |
| H | 0.057221648  | 5.777415898 | -9.650507403 |
| C | 1.274855206  | 5.800828798 | -7.883436094 |
| H | 2.069256369  | 5.191262193 | -8.301006626 |
| C | 3.512232496  | 5.358486095 | -5.74383618  |
| H | 4.015336683  | 5.308897068 | -4.778993782 |
| H | 3.258168203  | 4.348943879 | -6.0788044   |
| H | 4.174094561  | 5.828854498 | -6.478048072 |
| C | 0.705091852  | 9.117098247 | -1.47595726  |
| C | 1.346334875  | 10.30027201 | -3.261704374 |
| C | 1.909746468  | 10.90324799 | -2.12972121  |
| C | 2.711194729  | 12.04082321 | -2.21151034  |
| H | 3.138129215  | 12.50138075 | -1.326809148 |
| C | 2.941115985  | 12.55944083 | -3.484427132 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 3.562163664 | 13.44324328 | -3.595193779 |
| C | 2.385842324 | 11.95785581 | -4.62532309  |
| H | 2.587501931 | 12.38649242 | -5.602495661 |
| C | 1.583736371 | 10.82106386 | -4.535659202 |
| H | 1.164308998 | 10.36016904 | -5.42161991  |
| C | 1.884876167 | 10.4212961  | 0.333704885  |
| H | 1.445545437 | 11.36431467 | 0.674433526  |
| H | 1.527053462 | 9.605329779 | 0.960422352  |
| H | 2.975022844 | 10.48484923 | 0.398175351  |



-5071.92613801334 Hartrees

(-5070.98501474896 Hartrees)

| Atom | x            | y            | z           |
|------|--------------|--------------|-------------|
| Cd   | 1.377980583  | -0.903813839 | 1.501914178 |
| I    | 1.07478818   | 1.782669557  | 0.4015631   |
| B    | 3.05812055   | -3.341307386 | 4.189343337 |
| H    | 3.503509893  | -4.138331571 | 4.972944925 |
| N    | 4.292517622  | -2.61527647  | 3.588829804 |
| N    | 5.790096656  | -1.178879429 | 2.800306512 |
| N    | 2.163607241  | -2.389359003 | 5.043156475 |
| N    | 0.604742558  | -1.085511401 | 5.933945282 |
| N    | 2.264207034  | -4.191924827 | 3.151592001 |
| N    | 1.417973253  | -5.191633803 | 1.359591266 |
| S    | 3.373328114  | -0.019036974 | 3.214051482 |
| S    | -0.092954345 | -1.974403706 | 3.463841591 |
| S    | 2.882525508  | -2.991864212 | 0.716064335 |
| C    | 4.485360216  | -1.317442216 | 3.209561024 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 5.492731113  | -3.308877889 | 3.394795571 |
| C | 6.438731069  | -2.399709383 | 2.901784474 |
| C | 7.748992281  | -2.773334499 | 2.609776946 |
| H | 8.472933965  | -2.058828121 | 2.231922812 |
| C | 8.087598481  | -4.10938371  | 2.821563578 |
| H | 9.097501085  | -4.443783866 | 2.603356678 |
| C | 7.145121906  | -5.028122286 | 3.308253545 |
| H | 7.439784782  | -6.062571106 | 3.458612356 |
| C | 5.835556404  | -4.646396339 | 3.600097894 |
| H | 5.111701986  | -5.363191874 | 3.968583064 |
| C | 6.407892396  | 0.034063884  | 2.294341157 |
| H | 5.639550232  | 0.802943319  | 2.217448592 |
| H | 6.836607918  | -0.157433377 | 1.306253665 |
| H | 7.198364375  | 0.371476869  | 2.972923297 |
| C | 0.943341799  | -1.823425792 | 4.827206396 |
| C | 1.624644877  | -1.164078876 | 6.869278545 |
| C | 2.61087112   | -1.984751155 | 6.306621093 |
| C | 3.789593649  | -2.257101895 | 7.00424602  |
| H | 4.566548013  | -2.880125333 | 6.578048179 |
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| H | 4.83851139   | -1.885133034 | 8.836736322 |
| C | 2.935689269  | -0.874356267 | 8.828689835 |
| H | 3.08453654   | -0.449205522 | 9.816816013 |
| C | 1.759438389  | -0.596358847 | 8.134907394 |
| H | 0.987012384  | 0.036060334  | 8.559822935 |
| C | -0.603687563 | -0.298450667 | 6.109603459 |
| H | -1.182058525 | -0.34741134  | 5.18763104  |

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| H  | -0.336552245 | 0.741042067  | 6.321001586  |
| H  | -1.198887601 | -0.696283324 | 6.937961809  |
| C  | 2.177766214  | -4.135637702 | 1.791796017  |
| C  | 1.531644859  | -5.302791593 | 3.584711051  |
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| C  | 0.219053054  | -7.085782433 | 2.540507556  |
| H  | -0.186968795 | -7.56583843  | 1.656359951  |
| C  | -0.021461885 | -7.589112109 | 3.817458452  |
| H  | -0.628628968 | -8.482175203 | 3.932433779  |
| C  | 0.504036247  | -6.959622541 | 4.957866212  |
| H  | 0.29425267   | -7.376695687 | 5.938548371  |
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| C  | 1.062562504  | -5.496498787 | -0.01737777  |
| H  | 1.510636893  | -6.448758843 | -0.319697475 |
| H  | 1.43412361   | -4.694794086 | -0.653519089 |
| H  | -0.025125067 | -5.555801862 | -0.109998085 |
| Cd | -1.377980583 | 0.903813839  | -1.501914178 |
| I  | -1.07478818  | -1.782669557 | -0.4015631   |
| B  | -3.05812055  | 3.341307386  | -4.189343337 |
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| S | -3.373328114 | 0.019036974  | -3.214051482 |
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| C | -0.943341799 | 1.823425792  | -4.827206396 |
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| H | -3.08453654  | 0.449205522  | -9.816816013 |

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| H | -0.987012384 | -0.036060334 | -8.559822935 |
| C | 0.603687563  | 0.298450667  | -6.109603459 |
| H | 1.182058525  | 0.34741134   | -5.18763104  |
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| H | 0.025125067  | 5.555801862  | 0.109998085  |

