*Supporting Information*

# Evidence for Charge-shift Bonding in [1.1.1]propellanes $C_5H_6$ and $E_5Me_6$ (E=Si, Ge and Sn), A Theoretical Investigation

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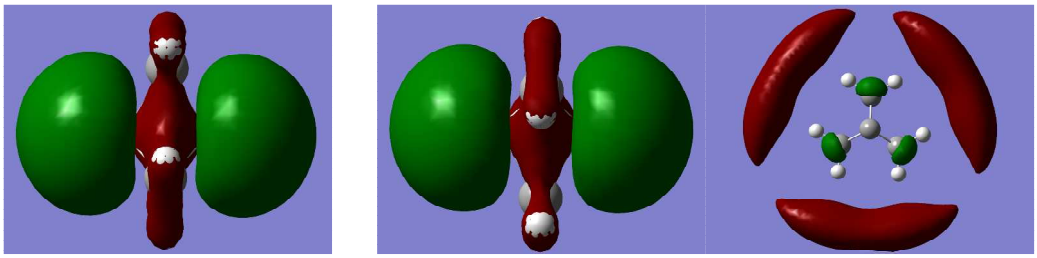

(1) (2)

Figure 1S HOMO of $C_5H_6$ (1) as well as HOMO-1 and HOMO of $C_5H_6^{2-}$ (2).

Table 1S Symmetries, state, total energy (E), energy of HOMO ($E_{HOMO}$) and LUMO ($E_{LUMO}$) and energy gap ($E_{gap}$) of [1.1.1]propellane $C_5H_6$, $E_5M_6$ (E=Si, Ge and Sn) and their dianions.

| species | symmetry | state | E (a.u.) | $E_{HOMO}$ (a.u.) | $E_{LUMO}$ (a.u.) | $E_{gap}$ (eV) |
|---|---|---|---|---|---|---|
| $C_5H_6$ | $D_{3h}$ | $^1A_1'$ | -194.05885 | -0.269 | -0.004 | 7.21 |
| $Si_5Me_6$ | $C_3$ | $^1A$ | -1687.19847 | -0.216 | -0.067 | 4.05 |
| $Ge_5Me_6$ | $C_3$ | $^1A$ | -258.49222 | -0.208 | -0.078 | 3.54 |
| $Sn_5Me_6$ | $C_3$ | $^1A$ | -256.53423 | -0.196 | -0.091 | 2.86 |
| $C_5H_6^{2-}$ | $D_{3h}$ | $^1A_1'$ | -193.91470 | 0.156 | 0.183 | 0.73 |
| $Si_5Me_6^{2-}$ | $C_1$ | $^1A$ | -1687.14936 | 0.119 | 0.164 | 1.22 |
| $Ge_5Me_6^{2-}$ | $C_3$ | $^1A$ | -258.46263 | 0.108 | 0.159 | 1.39 |
| $Sn_5Me_6^{2-}$ | $C_1$ | $^1A$ | -256.53904 | 0.087 | 0.151 | 1.74 |

Table 2S Symmetries, state, total energy (E), energy of HOMO ($E_{HOMO}$) and LUMO ($E_{LUMO}$), energy gap ($E_{gap}$) and the smallest frequencies ($\nu_{min}$) of compound **1**-**12**.

| species | symmetry | state | E(a.u.) | $E_{HOMO}$(a.u.) | $E_{LUMO}$(a.u.) | $E_{gap}$(eV) | $\nu_{min}$ ($cm^{-1}$) |
|---|---|---|---|---|---|---|---|
| **1** | $C_1$ | $^1A$ | -1281.40889 | -0.201 | -0.045 | 4.24 | 23 |
| **2** | $C_1$ | $^1A$ | -2774.45405 | -0.198 | -0.061 | 3.73 | 13 |
| **3** | $C_1$ | $^1A$ | -1345.82960 | -0.194 | -0.069 | 3.40 | 12 |
| **4** | $C_1$ | $^1A$ | -1343.87084 | -0.186 | -0.079 | 2.91 | 12 |
| **5** | $D_{3h}$ | $^1A_1'$ | -273.92129 | -0.297 | 0.006 | 8.25 | 201 |
| **6** | $C_1$ | $^1A$ | -1766.89960 | -0.209 | -0.032 | 4.82 | 32 |
| **7** | $C_1$ | $^1A$ | -338.25698 | -0.207 | -0.019 | 5.12 | 29 |
| **8** | $C_1$ | $^1A$ | -336.28401 | -0.196 | -0.042 | 4.19 | 49 |
| **9** | $C_s$ | $^1A'$ | -1026.27739 | -0.183 | -0.087 | 2.61 | 18 |
| **10** | $C_1$ | $^1A$ | -2597.93908 | -0.194 | -0.078 | 3.16 | 16 |
| **11** | $C_1$ | $^1A$ | -1169.31107 | -0.197 | -0.072 | 3.40 | 16 |
| **12** | $C_1$ | $^1A$ | -1167.35132 | -0.200 | -0.071 | 3.51 | 19 |

**Complete Reference for Ref (35):**

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T., Jr.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, *Revision C 02*; Gaussian, Inc.: Pittsburgh, PA, 2004.

## Cartesian coordinates for all the species calculated at the B3LYP level in this study

$C_5H_6$

E = -194.02279 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.299201 | 0.000000 |
| H | -0.915990 | 1.884903 | 0.000000 |
| H | 0.915990 | 1.884903 | 0.000000 |
| C | -1.125141 | -0.649601 | 0.000000 |
| H | -1.174379 | -1.735722 | 0.000000 |
| H | -2.090369 | -0.149181 | 0.000000 |
| C | 1.125141 | -0.649601 | 0.000000 |
| H | 2.090369 | -0.149181 | 0.000000 |
| H | 1.174379 | -1.735722 | 0.000000 |
| C | 0.000000 | 0.000000 | 0.788328 |
| C | 0.000000 | 0.000000 | -0.788328 |

$Si_5Me_6$

E=-1687.03180 a.u.

| | | | |
|---|---|---|---|
| Si | 0.000000 | 0.000000 | -1.376724 |
| Si | 0.000000 | 0.000000 | 1.380952 |
| Si | 0.000000 | 1.930790 | 0.001684 |
| Si | 1.672113 | -0.965395 | 0.001684 |
| Si | -1.672113 | -0.965395 | 0.001684 |
| C | 1.516118 | 3.075139 | 0.082936 |
| H | 1.330868 | 3.857418 | 0.828727 |
| H | 2.434604 | 2.557432 | 0.365342 |
| H | 1.679978 | 3.567622 | -0.882472 |
| C | -1.519419 | 3.069599 | -0.086835 |
| H | -2.437054 | 2.542727 | -0.354326 |
| H | -1.678886 | 3.578481 | 0.870717 |
| H | -1.342029 | 3.838922 | -0.847899 |
| C | 3.418060 | -0.218944 | -0.086835 |
| H | 3.938498 | -0.335282 | 0.870717 |
| H | 3.995619 | -0.757230 | -0.847899 |
| H | 3.420593 | 0.839187 | -0.354326 |
| C | 1.905090 | -2.850566 | 0.082936 |
| H | 2.675188 | -3.081275 | 0.828727 |
| H | 0.997499 | -3.387145 | 0.365342 |
| H | 2.249662 | -3.238715 | -0.882472 |
| C | -1.898641 | -2.850655 | -0.086835 |
| H | -0.983540 | -3.381914 | -0.354326 |

| | | | |
|---|---|---|---|
| H | -2.259612 | -3.243199 | 0.870717 |
| H | -2.653590 | -3.081692 | -0.847899 |
| C | -3.421208 | -0.224573 | 0.082936 |
| H | -4.006056 | -0.776143 | 0.828727 |
| H | -3.432103 | 0.829713 | 0.365342 |
| H | -3.929640 | -0.328908 | -0.882472 |

$Ge_5Me_6$

E=-258.41681 a.u.

| | | | |
|---|---|---|---|
| Ge | 0.000000 | 0.000000 | -1.543726 |
| Ge | 0.000000 | 0.000000 | 1.544461 |
| Ge | 0.000000 | 2.064359 | -0.000259 |
| Ge | 1.787787 | -1.032180 | -0.000259 |
| Ge | -1.787787 | -1.032180 | -0.000259 |
| C | 1.589534 | 3.254132 | 0.038629 |
| H | 1.479384 | 3.977945 | 0.852805 |
| H | 2.516597 | 2.699671 | 0.193505 |
| H | 1.666006 | 3.806977 | -0.903244 |
| C | -1.592389 | 3.250349 | -0.038640 |
| H | -2.518340 | 2.693394 | -0.191785 |
| H | -1.669429 | 3.803651 | 0.902913 |
| H | -1.485673 | 3.973728 | -0.853666 |
| C | 3.611079 | -0.246126 | -0.038640 |
| H | 4.128773 | -0.456058 | 0.902913 |
| H | 4.184185 | -0.700233 | -0.853666 |
| H | 3.591718 | 0.834249 | -0.191785 |
| C | 2.023393 | -3.003643 | 0.038629 |
| H | 2.705309 | -3.270157 | 0.852805 |
| H | 1.079685 | -3.529273 | 0.193505 |
| H | 2.463936 | -3.346292 | -0.903244 |
| C | -2.018691 | -3.004223 | -0.038640 |
| H | -1.073378 | -3.527643 | -0.191785 |
| H | -2.459344 | -3.347594 | 0.902913 |
| H | -2.698513 | -3.273494 | -0.853666 |
| C | -3.612928 | -0.250489 | 0.038629 |
| H | -4.184693 | -0.707788 | 0.852805 |
| H | -3.596282 | 0.829601 | 0.193505 |
| H | -4.129942 | -0.460685 | -0.903244 |

$Sn_5Me_6$

E=-256.46560 a.u.

| | | | |
|---|---|---|---|
| Sn | 0.000000 | 0.000000 | -1.782711 |
| Sn | 0.000000 | 0.000000 | 1.786211 |
| Sn | 0.000000 | 2.324592 | 0.000665 |

| | | | |
|---|---|---|---|
| Sn | 2.013155 | -1.162296 | 0.000665 |
| Sn | -2.013155 | -1.162296 | 0.000665 |
| C | 1.727678 | 3.627853 | -0.001250 |
| H | 1.657536 | 4.337473 | 0.828906 |
| H | 2.655055 | 3.059527 | 0.102463 |
| H | 1.766385 | 4.192736 | -0.937726 |
| C | -1.744521 | 3.605366 | -0.008036 |
| H | -2.664138 | 3.017928 | -0.064327 |
| H | -1.769929 | 4.209676 | 0.903967 |
| H | -1.706443 | 4.279710 | -0.869157 |
| C | 3.994599 | -0.291883 | -0.008036 |
| H | 4.530651 | -0.572034 | 0.903967 |
| H | 4.559559 | -0.662032 | -0.869157 |
| H | 3.945672 | 0.798247 | -0.064327 |
| C | 2.277974 | -3.310140 | -0.001250 |
| H | 2.927594 | -3.604205 | 0.828906 |
| H | 1.322100 | -3.829108 | 0.102463 |
| H | 2.747823 | -3.626103 | -0.937726 |
| C | -2.250078 | -3.313482 | -0.008036 |
| H | -1.281534 | -3.816176 | -0.064327 |
| H | -2.760722 | -3.637642 | 0.903967 |
| H | -2.853116 | -3.617678 | -0.869157 |
| C | -4.005652 | -0.317713 | -0.001250 |
| H | -4.585130 | -0.733268 | 0.828906 |
| H | -3.977155 | 0.769582 | 0.102463 |
| H | -4.514209 | -0.566634 | -0.937726 |

$C_5H_6^{2-}$

E=-193.81467 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.298084 | 0.000000 |
| H | -0.917168 | 1.892106 | 0.000000 |
| H | 0.917168 | 1.892106 | 0.000000 |
| C | -1.124173 | -0.649042 | 0.000000 |
| H | -1.180027 | -1.740344 | 0.000000 |
| H | -2.097196 | -0.151762 | 0.000000 |
| C | 1.124173 | -0.649042 | 0.000000 |
| H | 2.097196 | -0.151762 | 0.000000 |
| H | 1.180027 | -1.740344 | 0.000000 |
| C | 0.000000 | 0.000000 | 0.783628 |
| C | 0.000000 | 0.000000 | -0.783628 |

$Si_5Me_6^{2-}$

E=-1686.98167 a.u.

| | | | |
|---|---|---|---|
| Si | 0.002406 | -0.001741 | -1.760097 |

| | | | |
|---|---|---|---|
| Si | -0.000283 | 0.000391 | 1.760169 |
| Si | -1.206622 | -1.166486 | 0.000151 |
| Si | -0.407474 | 1.627259 | -0.001850 |
| Si | 1.615690 | -0.460535 | 0.002035 |
| C | -3.153088 | -1.025635 | 0.083431 |
| H | -3.526686 | -1.679030 | 0.887214 |
| H | -3.498321 | -0.009635 | 0.294477 |
| H | -3.610630 | -1.356620 | -0.861587 |
| C | -1.134487 | -3.116882 | -0.081120 |
| H | -0.128396 | -3.497941 | -0.277630 |
| H | -1.494107 | -3.561264 | 0.859807 |
| H | -1.789430 | -3.468679 | -0.893520 |
| C | -2.135938 | 2.532455 | -0.083207 |
| H | -2.357019 | 3.039442 | 0.868559 |
| H | -2.106149 | 3.296841 | -0.875433 |
| H | -2.961374 | 1.852209 | -0.310229 |
| C | 0.681924 | 3.245933 | 0.079855 |
| H | 0.303224 | 3.896531 | 0.883686 |
| H | 1.736111 | 3.041541 | 0.286740 |
| H | 0.617750 | 3.805781 | -0.865933 |
| C | 3.266162 | 0.580399 | -0.076690 |
| H | 3.092938 | 1.640048 | -0.284049 |
| H | 3.822066 | 0.500421 | 0.870203 |
| H | 3.906670 | 0.182752 | -0.879345 |
| C | 2.470130 | -2.214602 | 0.077543 |
| H | 3.212758 | -2.221382 | 0.890707 |
| H | 1.762390 | -3.026558 | 0.266304 |
| H | 2.997954 | -2.428885 | -0.864547 |

$Ge_5Me_6^{2-}$

E=-258.38276 a.u.

| | | | |
|---|---|---|---|
| Ge | 0.000000 | 0.000000 | 1.939009 |
| Ge | 0.000000 | 0.000000 | -1.938096 |
| Ge | -1.832883 | 0.138945 | -0.000097 |
| Ge | 0.796112 | -1.656796 | -0.000097 |
| Ge | 1.036771 | 1.517851 | -0.000097 |
| C | -3.313226 | -1.276861 | -0.004548 |
| H | -3.948799 | -1.152771 | -0.893605 |
| H | -2.901720 | -2.291156 | -0.014035 |
| H | -3.942918 | -1.166536 | 0.890417 |
| C | -3.068966 | 1.771868 | 0.003852 |
| H | -2.499854 | 2.706845 | 0.020268 |
| H | -3.703533 | 1.767776 | -0.894581 |
| H | -3.721346 | 1.747701 | 0.889080 |

| | | | |
|---|---|---|---|
| C | 0.000000 | -3.543736 | 0.003852 |
| H | 0.320827 | -4.091242 | -0.894581 |
| H | 0.347120 | -4.096630 | 0.889080 |
| H | -1.094269 | -3.518359 | 0.020268 |
| C | 2.762407 | -2.230907 | -0.004548 |
| H | 2.972729 | -2.843375 | -0.893605 |
| H | 3.435059 | -1.367385 | -0.014035 |
| H | 2.981709 | -2.831399 | 0.890417 |
| C | 3.068966 | 1.771868 | 0.003852 |
| H | 3.594123 | 0.811514 | 0.020268 |
| H | 3.382706 | 2.323465 | -0.894581 |
| H | 3.374226 | 2.348929 | 0.889080 |
| C | 0.550819 | 3.507768 | -0.004548 |
| H | 0.976070 | 3.996146 | -0.893605 |
| H | -0.533340 | 3.658541 | -0.014035 |
| H | 0.961209 | 3.997935 | 0.890417 |

$Sn_5Me_6^{2-}$

E=-256.46733 a.u.

| | | | |
|---|---|---|---|
| Sn | 0.000885 | -0.000817 | -2.226270 |
| Sn | 0.000430 | -0.001655 | 2.226366 |
| Sn | -0.578157 | 1.971413 | 0.001119 |
| Sn | 1.997135 | -0.487008 | -0.000514 |
| Sn | -1.421089 | -1.485418 | -0.000255 |
| C | 0.596330 | 3.866276 | 0.008338 |
| H | 0.299850 | 4.485850 | 0.865966 |
| H | 1.670143 | 3.660459 | 0.081322 |
| H | 0.409938 | 4.432786 | -0.914135 |
| C | -2.584251 | 2.944098 | -0.008124 |
| H | -3.384493 | 2.195436 | -0.022454 |
| H | -2.704418 | 3.567472 | 0.888452 |
| H | -2.687372 | 3.583146 | -0.895709 |
| C | 3.834143 | 0.777152 | -0.006458 |
| H | 4.390300 | 0.650041 | 0.931933 |
| H | 4.483682 | 0.482433 | -0.842078 |
| H | 3.577657 | 1.836366 | -0.119519 |
| C | 3.062043 | -2.445667 | 0.004551 |
| H | 3.717816 | -2.515873 | 0.883017 |
| H | 2.350841 | -3.278951 | 0.032580 |
| H | 3.677472 | -2.541047 | -0.900318 |
| C | -1.255604 | -3.708333 | -0.000736 |
| H | -0.205424 | -4.021351 | -0.007659 |
| H | -1.738478 | -4.123306 | 0.894496 |
| H | -1.750178 | -4.123521 | -0.889447 |

| | | | |
|---|---|---|---|
| C | -3.648840 | -1.415631 | 0.000571 |
| H | -4.041622 | -1.932649 | 0.886653 |
| H | -4.006717 | -0.380118 | 0.013655 |
| H | -4.042123 | -1.910328 | -0.897892 |

$C_5H_6[FeCp(CO)_2]_2$

E=-1281.40889 a.u.

| | | | |
|---|---|---|---|
| Fe | -2.970617 | -0.188609 | 0.031625 |
| Fe | 2.970560 | 0.188675 | 0.031585 |
| C | 2.796329 | 1.841746 | -0.529077 |
| C | 2.906099 | 0.603225 | 1.736194 |
| C | -2.796576 | -1.841456 | -0.529729 |
| C | -2.906051 | -0.603840 | 1.736070 |
| O | -2.878291 | -0.863011 | 2.861808 |
| O | -2.689921 | -2.926332 | -0.915005 |
| O | 2.878686 | 0.861906 | 2.862053 |
| O | 2.689583 | 2.926735 | -0.914010 |
| C | -2.999990 | 1.714437 | -1.025474 |
| H | -2.097911 | 2.244825 | -1.292119 |
| C | -3.702051 | 1.837708 | 0.203140 |
| H | -3.453209 | 2.505387 | 1.016231 |
| C | -4.824718 | 0.938595 | 0.157316 |
| H | -5.553011 | 0.792856 | 0.943681 |
| C | -3.641310 | 0.720905 | -1.811985 |
| H | -3.339955 | 0.393866 | -2.797484 |
| C | -4.787529 | 0.253247 | -1.078238 |
| H | -5.482450 | -0.508783 | -1.404254 |
| C | 4.788053 | -0.252861 | -1.077579 |
| H | 5.483414 | 0.509164 | -1.402664 |
| C | 4.824346 | -0.939050 | 0.157534 |
| H | 5.552197 | -0.794061 | 0.944446 |
| C | 3.701395 | -1.837877 | 0.202127 |
| H | 3.451887 | -2.505970 | 1.014674 |
| C | 3.642151 | -0.719752 | -1.812305 |
| H | 3.341511 | -0.391969 | -2.797777 |
| C | 3.000092 | -1.713618 | -1.026828 |
| H | 2.098003 | -2.243518 | -1.294402 |
| C | -0.000049 | 0.000821 | -1.178969 |
| H | -0.073513 | 0.902173 | -1.797760 |
| H | 0.073426 | -0.899549 | -1.799201 |
| C | -0.092678 | 1.070720 | 0.693408 |
| H | -0.172610 | 2.057747 | 0.224493 |
| H | -0.100906 | 1.148955 | 1.785852 |
| C | 0.936644 | 0.079762 | 0.067161 |

| | | | |
|---|---|---|---|
| C | -0.936681 | -0.080111 | 0.067032 |
| C | 0.092647 | -1.072073 | 0.691685 |
| H | 0.172560 | -2.058336 | 0.221171 |
| H | 0.100866 | -1.152070 | 1.784002 |

$Si_5Me_6[FeCp(CO)_2]_2$

E=-2774.45405 a.u.

| | | | |
|---|---|---|---|
| Si | -1.492742 | -0.074760 | 0.039700 |
| Si | 0.083295 | -1.600136 | 0.997053 |
| Si | -0.084080 | 1.618664 | 0.962051 |
| Si | 0.000717 | -0.018145 | -1.825217 |
| Fe | 3.861403 | 0.185914 | 0.007355 |
| Fe | -3.861144 | -0.186823 | 0.004495 |
| C | -3.647717 | -1.779960 | -0.696531 |
| C | -3.729205 | -0.749765 | 1.659633 |
| C | 3.647233 | 1.789846 | -0.668262 |
| C | 3.726924 | 0.720028 | 1.671921 |
| O | 3.684179 | 1.056660 | 2.778349 |
| O | 3.546364 | 2.843240 | -1.136894 |
| O | -3.688425 | -1.107024 | 2.759692 |
| O | -3.547340 | -2.826143 | -1.181118 |
| C | 3.885167 | -1.751233 | -0.952125 |
| H | 3.001688 | -2.302200 | -1.240310 |
| C | 4.543601 | -1.825476 | 0.308850 |
| H | 4.252373 | -2.448027 | 1.143233 |
| C | 5.675571 | -0.942731 | 0.267099 |
| H | 6.372178 | -0.766758 | 1.075492 |
| C | 4.577636 | -0.804497 | -1.757806 |
| H | 4.317907 | -0.517306 | -2.767226 |
| C | 5.696488 | -0.313250 | -1.001624 |
| H | 6.413112 | 0.425114 | -1.334313 |
| C | -5.694350 | 0.329938 | -0.999053 |
| H | -6.410465 | -0.402518 | -1.345621 |
| C | -5.675420 | 0.937332 | 0.280441 |
| H | -6.373370 | 0.747410 | 1.084500 |
| C | -4.543478 | 1.819180 | 0.339237 |
| H | -4.253677 | 2.427272 | 1.184726 |
| C | -4.574293 | 0.834096 | -1.744875 |
| H | -4.312700 | 0.564633 | -2.758676 |
| C | -3.883348 | 1.766889 | -0.921978 |
| H | -2.999895 | 2.323348 | -1.199547 |
| Si | 1.493282 | 0.072348 | 0.038700 |
| C | -0.102382 | 3.389266 | 0.239407 |
| H | -1.074746 | 3.870497 | 0.403275 |

| | | | |
|---|---|---|---|
| H | 0.649977 | 3.993889 | 0.760985 |
| H | 0.127589 | 3.432182 | -0.826864 |
| C | -0.175685 | 1.902687 | 2.848516 |
| H | 0.765856 | 2.319817 | 3.225045 |
| H | -0.968176 | 2.630929 | 3.062800 |
| H | -0.396635 | 0.996995 | 3.416148 |
| C | 0.174141 | -1.834750 | 2.890257 |
| H | -0.776830 | -2.214084 | 3.282435 |
| H | 0.947334 | -2.578108 | 3.122264 |
| H | 0.423430 | -0.919493 | 3.430433 |
| C | 0.097311 | -3.387534 | 0.318259 |
| H | 1.060968 | -3.873756 | 0.515066 |
| H | -0.672211 | -3.971618 | 0.838308 |
| H | -0.109972 | -3.454575 | -0.751481 |
| C | 0.138020 | -1.521274 | -2.999212 |
| H | -0.791218 | -1.651666 | -3.567127 |
| H | 0.941005 | -1.343887 | -3.726025 |
| H | 0.349435 | -2.462303 | -2.487570 |
| C | -0.132216 | 1.460281 | -3.030216 |
| H | 0.806096 | 1.592157 | -3.582682 |
| H | -0.918707 | 1.257956 | -3.768350 |
| H | -0.365896 | 2.407800 | -2.540878 |

$Ge_5Me_6[FeCp(CO)_2]_2$

E=-1345.82960 a.u.

| | | | |
|---|---|---|---|
| Ge | 1.605187 | -0.062186 | -0.036105 |
| Ge | -0.068673 | -1.707806 | -1.065325 |
| Ge | 0.068071 | 1.747480 | -1.006218 |
| Ge | -0.000067 | -0.030141 | 1.963568 |
| Fe | -4.060222 | 0.175538 | 0.004088 |
| Fe | 4.059629 | -0.180924 | 0.004623 |
| C | 3.845819 | -1.773062 | 0.717478 |
| C | 3.935349 | -0.752950 | -1.651958 |
| C | -3.856313 | 1.774728 | 0.703959 |
| C | -3.935384 | 0.733961 | -1.657171 |
| O | -3.902545 | 1.085429 | -2.758830 |
| O | -3.767809 | 2.821497 | 1.188545 |
| O | 3.902987 | -1.114037 | -2.750570 |
| O | 3.750919 | -2.815197 | 1.210743 |
| C | -4.064050 | -1.774385 | 0.940366 |
| H | -3.175114 | -2.320536 | 1.221217 |
| C | -4.719977 | -1.836516 | -0.322344 |
| H | -4.423660 | -2.446590 | -1.164019 |
| C | -5.857731 | -0.961775 | -0.269752 |

| | | | |
|---|---|---|---|
| H | -6.556375 | -0.780680 | -1.075239 |
| C | -4.761527 | -0.842145 | 1.757693 |
| H | -4.503167 | -0.566633 | 2.770634 |
| C | -5.882671 | -0.347649 | 1.006875 |
| H | -6.605858 | 0.380011 | 1.348765 |
| C | 5.882182 | 0.340236 | 1.008602 |
| H | 6.599370 | -0.388892 | 1.359889 |
| C | 5.865384 | 0.942119 | -0.273933 |
| H | 6.565512 | 0.748681 | -1.075235 |
| C | 4.733398 | 1.823590 | -0.338702 |
| H | 4.443709 | 2.427508 | -1.187091 |
| C | 4.761792 | 0.849056 | 1.750984 |
| H | 4.498581 | 0.585089 | 2.765747 |
| C | 4.073214 | 1.777910 | 0.922476 |
| H | 3.187009 | 2.332624 | 1.194769 |
| Ge | -1.606095 | 0.066032 | -0.032110 |
| C | 0.114191 | 3.569928 | -0.195607 |
| H | 1.076545 | 4.054985 | -0.393224 |
| H | -0.672358 | 4.187008 | -0.643484 |
| H | -0.050381 | 3.544655 | 0.883106 |
| C | 0.128044 | 2.049075 | -2.975310 |
| H | -0.819404 | 2.475293 | -3.321580 |
| H | 0.928953 | 2.758641 | -3.211032 |
| H | 0.314485 | 1.127022 | -3.528800 |
| C | -0.129241 | -1.919469 | -3.046050 |
| H | 0.826879 | -2.304519 | -3.415704 |
| H | -0.913598 | -2.636557 | -3.312654 |
| H | -0.341709 | -0.976967 | -3.554021 |
| C | -0.104200 | -3.565863 | -0.340216 |
| H | -1.059214 | -4.050286 | -0.571641 |
| H | 0.693208 | -4.152461 | -0.809476 |
| H | 0.049226 | -3.592121 | 0.740169 |
| C | -0.106594 | -1.629582 | 3.153616 |
| H | 0.824309 | -1.742183 | 3.719725 |
| H | -0.924788 | -1.500079 | 3.870963 |
| H | -0.279228 | -2.552213 | 2.596047 |
| C | 0.102813 | 1.518156 | 3.219423 |
| H | -0.845549 | 1.636891 | 3.754345 |
| H | 0.888499 | 1.334280 | 3.960773 |
| H | 0.324579 | 2.456228 | 2.706986 |

$Sn_5Me_6[FeCp(CO)_2]_2$

E=-1343.87084 a.u.

| | | | |
|---|---|---|---|
| Sn | 1.832254 | -0.067595 | -0.030338 |

| | | | |
|---|---|---|---|
| Sn | -0.070588 | -1.957292 | -1.152180 |
| Sn | 0.070227 | 1.959626 | -1.148420 |
| Sn | 0.000398 | -0.002015 | 2.230704 |
| Fe | -4.445790 | 0.172751 | 0.004397 |
| Fe | 4.445785 | -0.173087 | 0.004377 |
| C | 4.253301 | -1.786600 | 0.674680 |
| C | 4.330898 | -0.702015 | -1.667450 |
| C | -4.254000 | 1.787151 | 0.672737 |
| C | -4.330471 | 0.699584 | -1.668065 |
| O | -4.323338 | 1.026122 | -2.778493 |
| O | -4.190828 | 2.846483 | 1.135038 |
| O | 4.324092 | -1.029978 | -2.777460 |
| O | 4.189652 | -2.845333 | 1.138284 |
| C | -4.436231 | -1.764203 | 0.973066 |
| H | -3.554184 | -2.314537 | 1.268167 |
| C | -5.090717 | -1.848163 | -0.289753 |
| H | -4.791323 | -2.470857 | -1.121148 |
| C | -6.231294 | -0.977141 | -0.252829 |
| H | -6.929842 | -0.812306 | -1.061822 |
| C | -5.139201 | -0.821032 | 1.774350 |
| H | -4.885443 | -0.529150 | 2.783962 |
| C | -6.260284 | -0.342784 | 1.014359 |
| H | -6.986878 | 0.386970 | 1.344202 |
| C | 6.260366 | 0.343291 | 1.013756 |
| H | 6.986890 | -0.386195 | 1.344348 |
| C | 6.231417 | 0.976332 | -0.254089 |
| H | 6.929912 | 0.810554 | -1.062935 |
| C | 5.090930 | 1.847425 | -0.291915 |
| H | 4.791595 | 2.469275 | -1.123960 |
| C | 5.139353 | 0.822474 | 1.773272 |
| H | 4.885598 | 0.531694 | 2.783202 |
| C | 4.436468 | 1.764872 | 0.971021 |
| H | 3.554454 | 2.315581 | 1.265532 |
| Sn | -1.832213 | 0.067738 | -0.029464 |
| C | 0.184960 | 3.943543 | -0.273236 |
| H | 1.082839 | 4.462429 | -0.624462 |
| H | -0.690256 | 4.531913 | -0.566338 |
| H | 0.214576 | 3.891762 | 0.818182 |
| C | 0.110869 | 2.240026 | -3.298247 |
| H | -0.687443 | 2.925475 | -3.599546 |
| H | 1.070681 | 2.666701 | -3.606183 |
| H | -0.032220 | 1.290598 | -3.820213 |
| C | -0.112136 | -2.232477 | -3.302656 |
| H | 0.686572 | -2.916459 | -3.606208 |

| | | | |
|---|---|---|---|
| H | -1.071772 | -2.659188 | -3.611082 |
| H | 0.029767 | -1.281580 | -3.822249 |
| C | -0.184758 | -3.943274 | -0.281777 |
| H | -1.084614 | -4.460086 | -0.630979 |
| H | 0.688585 | -4.532018 | -0.579678 |
| H | -0.210216 | -3.894196 | 0.809855 |
| C | -0.066717 | -1.732569 | 3.542520 |
| H | 0.794380 | -1.723379 | 4.218528 |
| H | -0.978998 | -1.715559 | 4.147658 |
| H | -0.044014 | -2.662997 | 2.969594 |
| C | 0.067345 | 1.725928 | 3.545901 |
| H | -0.792623 | 1.714206 | 4.223301 |
| H | 0.980650 | 1.709033 | 4.149483 |
| H | 0.042371 | 2.657370 | 2.974726 |

$C_5H_6Me_2$

E=-273.92129 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.238828 | 0.000000 |
| H | -0.905740 | 1.857495 | 0.000000 |
| H | 0.905740 | 1.857495 | 0.000000 |
| C | -1.072856 | -0.619414 | 0.000000 |
| H | -1.155768 | -1.713142 | 0.000000 |
| H | -2.061508 | -0.144354 | 0.000000 |
| C | 1.072856 | -0.619414 | 0.000000 |
| H | 2.061508 | -0.144354 | 0.000000 |
| H | 1.155768 | -1.713142 | 0.000000 |
| C | 0.000000 | 0.000000 | 0.948316 |
| C | 0.000000 | 0.000000 | -0.948316 |
| C | 0.000000 | 0.000000 | 2.457856 |
| H | 0.000000 | -1.023679 | 2.851417 |
| H | -0.886532 | 0.511840 | 2.851417 |
| H | 0.886532 | 0.511840 | 2.851417 |
| C | 0.000000 | 0.000000 | -2.457856 |
| H | -0.886532 | 0.511840 | -2.851417 |
| H | 0.000000 | -1.023679 | -2.851417 |
| H | 0.886532 | 0.511840 | -2.851417 |

$Si_5Me_8$

E=-1766.89960 a.u.

| | | | |
|---|---|---|---|
| C | -0.002239 | 0.003170 | 3.371935 |
| H | -1.015089 | 0.159671 | 3.757993 |
| H | 0.368377 | -0.950690 | 3.761973 |
| H | 0.638232 | 0.802668 | 3.759472 |
| C | 0.007867 | -0.001961 | -3.371839 |

| | | | |
|---|---|---|---|
| H | 0.627701 | 0.814243 | -3.758029 |
| H | 0.406087 | -0.945957 | -3.758821 |
| H | -1.007321 | 0.126145 | -3.762222 |
| Si | 1.862533 | -0.266258 | 0.002732 |
| Si | -1.161950 | -1.478020 | -0.001312 |
| Si | -0.701061 | 1.743043 | -0.002146 |
| Si | 0.003670 | -0.002411 | -1.462807 |
| Si | 0.000986 | 0.000572 | 1.462811 |
| C | -2.534832 | 2.275069 | 0.057026 |
| H | -2.668391 | 3.009454 | 0.861032 |
| H | -2.825069 | 2.760648 | -0.882493 |
| H | -3.227339 | 1.451974 | 0.241917 |
| C | 0.245394 | 3.400361 | -0.058294 |
| H | -0.148902 | 4.011986 | -0.879407 |
| H | 0.089742 | 3.960494 | 0.871666 |
| H | 1.320301 | 3.291179 | -0.212446 |
| C | -3.070581 | -1.475135 | -0.059950 |
| H | -3.504478 | -0.493719 | -0.260128 |
| H | -3.404492 | -2.154995 | -0.853675 |
| H | -3.485683 | -1.845775 | 0.885110 |
| C | -0.719075 | -3.334936 | 0.054592 |
| H | -1.255849 | -3.808602 | 0.885963 |
| H | -1.041181 | -3.831329 | -0.868879 |
| H | 0.345455 | -3.532128 | 0.191231 |
| C | 2.824319 | -1.915115 | -0.045200 |
| H | 3.398499 | -2.046876 | 0.880025 |
| H | 2.191373 | -2.793968 | -0.178649 |
| H | 3.540572 | -1.890198 | -0.875924 |
| C | 3.243262 | 1.052633 | 0.052625 |
| H | 2.878137 | 2.069747 | 0.204297 |
| H | 3.933461 | 0.820460 | 0.873158 |
| H | 3.822655 | 1.034083 | -0.878429 |

$Ge_5Me_8$

E=-338.25698 a.u.

| | | | |
|---|---|---|---|
| C | 0.004243 | 0.009477 | -3.564201 |
| H | -1.017364 | 0.110443 | -3.941032 |
| H | 0.600547 | 0.848344 | -3.933619 |
| H | 0.430774 | -0.922252 | -3.945975 |
| C | 0.011124 | -0.014555 | 3.564648 |
| H | 0.409962 | -0.963713 | 3.933215 |
| H | 0.633756 | 0.800965 | 3.942816 |
| H | -1.006023 | 0.112906 | 3.945489 |
| Ge | 1.992092 | -0.229476 | -0.001819 |

| | | | |
|---|---|---|---|
| Ge | -0.795814 | 1.830839 | 0.003807 |
| Ge | -1.199393 | -1.603177 | -0.002811 |
| Ge | 0.004448 | -0.003606 | 1.573113 |
| Ge | 0.003775 | -0.003784 | -1.572646 |
| C | -3.192340 | -1.620555 | -0.035564 |
| H | -3.533024 | -2.417988 | -0.704505 |
| H | -3.593066 | -1.818907 | 0.963657 |
| H | -3.606120 | -0.675641 | -0.392778 |
| C | -0.641005 | -3.516270 | 0.021691 |
| H | -1.152718 | -4.035054 | 0.839471 |
| H | -0.922150 | -4.001626 | -0.918898 |
| H | 0.435088 | -3.633676 | 0.161733 |
| C | -2.736807 | 2.277053 | 0.034630 |
| H | -3.365210 | 1.390868 | 0.139462 |
| H | -2.940827 | 2.945069 | 0.878431 |
| H | -3.018966 | 2.796281 | -0.887423 |
| C | 0.142361 | 3.587597 | -0.013051 |
| H | -0.104360 | 4.129687 | -0.932109 |
| H | -0.194365 | 4.188628 | 0.838249 |
| H | 1.227309 | 3.485665 | 0.044883 |
| C | 3.352172 | 1.228107 | 0.006110 |
| H | 4.010415 | 1.123819 | -0.862947 |
| H | 2.898590 | 2.220475 | -0.023521 |
| H | 3.967472 | 1.157495 | 0.909195 |
| C | 3.042992 | -1.921885 | -0.013250 |
| H | 2.410878 | -2.811619 | -0.018386 |
| H | 3.682638 | -1.948818 | -0.901803 |
| H | 3.686883 | -1.960630 | 0.871689 |

$Sn_5Me_8$

E=-336.28401 a.u.

| | | | |
|---|---|---|---|
| C | 0.005472 | 0.005865 | 3.967527 |
| H | 1.007183 | 0.249097 | 4.330627 |
| H | -0.702387 | 0.751561 | 4.337561 |
| H | -0.282869 | -0.979718 | 4.341567 |
| C | -0.003867 | -0.011650 | -3.965081 |
| H | -0.291946 | -1.000670 | -4.330109 |
| H | -0.714468 | 0.730101 | -4.338306 |
| H | 0.995669 | 0.230546 | -4.334834 |
| Sn | -2.193133 | -0.582101 | 0.003122 |
| Sn | 0.589659 | 2.184926 | -0.003622 |
| Sn | 1.603250 | -1.600080 | 0.001279 |
| Sn | -0.004512 | -0.002739 | -1.795341 |
| Sn | -0.002740 | -0.001379 | 1.798067 |

| | | | |
|---|---|---|---|
| C | 3.745055 | -1.252443 | 0.002874 |
| H | 4.236246 | -2.000186 | 0.633674 |
| H | 4.148278 | -1.334097 | -1.010923 |
| H | 3.981334 | -0.259776 | 0.393664 |
| C | 1.310272 | -3.747474 | -0.008465 |
| H | 1.795795 | -4.185510 | -0.886057 |
| H | 1.752502 | -4.188878 | 0.889845 |
| H | 0.247947 | -4.001215 | -0.035582 |
| C | 2.611025 | 2.969397 | -0.014943 |
| H | 3.342834 | 2.163038 | -0.111268 |
| H | 2.738066 | 3.656819 | -0.857265 |
| H | 2.811465 | 3.514752 | 0.912443 |
| C | -0.755613 | 3.884384 | 0.004744 |
| H | -0.584535 | 4.494789 | 0.896889 |
| H | -0.580772 | 4.504912 | -0.879633 |
| H | -1.798392 | 3.557223 | 0.000380 |
| C | -3.893690 | 0.762571 | -0.010554 |
| H | -4.604137 | 0.470026 | 0.768881 |
| H | -3.580291 | 1.793239 | 0.173247 |
| H | -4.402353 | 0.719594 | -0.978633 |
| C | -2.980494 | -2.602370 | 0.005333 |
| H | -2.175402 | -3.337014 | 0.090064 |
| H | -3.663105 | -2.735323 | 0.850558 |
| H | -3.531751 | -2.794333 | -0.920646 |

(NHC)$C_5H_6AgCl$

E=-1026.27739 a.u.

| | | | |
|---|---|---|---|
| C | -1.185666 | 0.853575 | 0.000000 |
| H | -1.800556 | 0.896279 | 0.905434 |
| H | -1.800556 | 0.896279 | -0.905434 |
| C | 0.675399 | 0.784409 | 1.078709 |
| H | 1.766471 | 0.745459 | 1.167649 |
| H | 0.192339 | 0.797025 | 2.063057 |
| C | 0.675399 | 0.784409 | -1.078709 |
| H | 0.192339 | 0.797025 | -2.063057 |
| H | 1.766471 | 0.745459 | -1.167649 |
| C | 0.014912 | -0.183976 | 0.000000 |
| C | 0.105615 | 1.731135 | 0.000000 |
| C | 0.153854 | 3.211535 | 0.000000 |
| C | 0.157224 | 5.358273 | -0.680298 |
| C | 0.157224 | 5.358273 | 0.680298 |
| H | 0.162603 | 6.171976 | -1.387566 |
| H | 0.162603 | 6.171976 | 1.387566 |
| N | 0.157224 | 4.026308 | 1.071798 |

| | | | |
|---|---|---|---|
| H | 0.165541 | 3.676499 | 2.021828 |
| N | 0.157224 | 4.026308 | -1.071798 |
| H | 0.165541 | 3.676499 | -2.021828 |
| Ag | -0.087762 | -2.303598 | 0.000000 |
| Cl | -0.210170 | -4.709381 | 0.000000 |

(NHC)$Si_5Me_6AgCl$

E=-2597.93908 a.u.

| | | | |
|---|---|---|---|
| Si | -0.301294 | -0.533881 | 1.766306 |
| Si | -0.255719 | -1.244690 | -1.389030 |
| Si | -0.231876 | 1.838487 | -0.428003 |
| C | -0.315464 | -2.312377 | 2.456248 |
| H | -1.225785 | -2.501212 | 3.038350 |
| H | -0.220215 | -3.089274 | 1.696466 |
| H | 0.536336 | -2.418753 | 3.139405 |
| C | -0.420143 | 0.540014 | 3.338177 |
| H | -0.595720 | 1.599141 | 3.143146 |
| H | -1.232718 | 0.173391 | 3.977532 |
| H | 0.512401 | 0.453635 | 3.909004 |
| C | -0.351289 | -3.148347 | -1.256091 |
| H | -1.158903 | -3.536685 | -1.889972 |
| H | 0.586181 | -3.574321 | -1.633744 |
| H | -0.496555 | -3.525479 | -0.242183 |
| C | -0.233645 | -0.946776 | -3.271375 |
| H | -1.156271 | -1.308363 | -3.741244 |
| H | -0.091106 | 0.097838 | -3.551102 |
| H | 0.600150 | -1.517413 | -3.698845 |
| C | -0.298016 | 2.669393 | -2.144465 |
| H | -0.462104 | 1.974414 | -2.969462 |
| H | -1.096134 | 3.422122 | -2.172044 |
| H | 0.648835 | 3.191314 | -2.328397 |
| C | -0.212297 | 3.317451 | 0.777337 |
| H | -1.098188 | 3.954003 | 0.656651 |
| H | -0.134249 | 3.030210 | 1.826766 |
| H | 0.663150 | 3.935030 | 0.541470 |
| Si | -1.739422 | 0.039012 | -0.037853 |
| Si | 1.247695 | 0.001543 | 0.007353 |
| Ag | 3.674084 | -0.012934 | 0.022058 |
| Cl | 6.096561 | -0.026384 | 0.033931 |
| C | -5.816966 | -0.755506 | 0.024670 |
| C | -5.871202 | 0.603678 | 0.030720 |
| H | -6.603827 | -1.493406 | 0.038986 |
| H | -6.714084 | 1.276822 | 0.048794 |
| N | -4.479247 | -1.103582 | -0.013726 |

| | | | |
|---|---|---|---|
| N | -4.564407 | 1.057939 | -0.000523 |
| C | -3.694925 | 0.010006 | -0.024933 |
| C | -3.989591 | -2.483357 | 0.020174 |
| H | -3.963987 | -2.850739 | 1.049588 |
| H | -4.651797 | -3.110634 | -0.579544 |
| H | -2.983692 | -2.512460 | -0.397040 |
| C | -4.201457 | 2.476542 | 0.005976 |

(NHC)$Ge_5Me_6AgCl$

E=-1169.31107 a.u.

| | | | |
|---|---|---|---|
| Ge | -0.228500 | -0.552515 | 1.906229 |
| Ge | -0.191163 | -1.354478 | -1.461673 |
| Ge | -0.152071 | 1.962358 | -0.476069 |
| C | -0.309905 | -2.410588 | 2.621878 |
| H | -1.232612 | -2.566117 | 3.191255 |
| H | -0.244256 | -3.166879 | 1.837994 |
| H | 0.535546 | -2.558139 | 3.302783 |
| C | -0.377679 | 0.612005 | 3.515143 |
| H | -0.543984 | 1.659418 | 3.258085 |
| H | -1.206071 | 0.271209 | 4.145474 |
| H | 0.545986 | 0.544784 | 4.099891 |
| C | -0.353302 | -3.332464 | -1.259116 |
| H | -1.188439 | -3.710817 | -1.859645 |
| H | 0.563127 | -3.805911 | -1.627517 |
| H | -0.496560 | -3.640010 | -0.221430 |
| C | -0.246176 | -1.042173 | -3.427095 |
| H | -1.190480 | -1.399773 | -3.851004 |
| H | -0.122921 | 0.011597 | -3.682454 |
| H | 0.571640 | -1.601643 | -3.894331 |
| C | -0.261458 | 2.780683 | -2.289522 |
| H | -0.428125 | 2.039290 | -3.072935 |
| H | -1.073920 | 3.514657 | -2.326261 |
| H | 0.676719 | 3.302477 | -2.506512 |
| C | -0.212863 | 3.502349 | 0.786491 |
| H | -1.120327 | 4.099635 | 0.642667 |
| H | -0.163361 | 3.183554 | 1.828757 |
| H | 0.648703 | 4.149850 | 0.590280 |
| Ge | -1.794501 | 0.042695 | -0.030036 |
| Ge | 1.443810 | -0.005317 | 0.012438 |
| Ag | 3.977205 | -0.025361 | 0.021870 |
| Cl | 6.388860 | -0.043464 | 0.028796 |
| C | -5.970094 | -0.770105 | 0.016876 |
| C | -6.028646 | 0.588367 | 0.028989 |
| H | -6.754639 | -1.510576 | 0.023526 |

| | | | |
|---|---|---|---|
| H | -6.873675 | 1.258872 | 0.045425 |
| N | -4.629101 | -1.113236 | -0.014956 |
| N | -4.721374 | 1.046091 | 0.007514 |
| C | -3.850232 | 0.001917 | -0.017891 |
| C | -4.136456 | -2.491609 | 0.012451 |
| H | -4.124847 | -2.869368 | 1.038446 |
| H | -4.787866 | -3.115332 | -0.602773 |
| H | -3.124066 | -2.515399 | -0.390355 |
| C | -4.359644 | 2.464176 | 0.022023 |
| H | -4.817866 | 2.970506 | -0.831104 |
| H | -4.701613 | 2.924544 | 0.952496 |
| H | -3.275677 | 2.547283 | -0.045909 |

(NHC)$Sn_5Me_6AgCl$

E=-1167.35132 a.u.

| | | | |
|---|---|---|---|
| Sn | -0.190011 | -0.640526 | 2.159356 |
| Sn | -0.166209 | -1.532436 | -1.652129 |
| Sn | -0.077291 | 2.220707 | -0.526159 |
| C | -0.358245 | -2.671804 | 2.902697 |
| H | -1.249210 | -2.777230 | 3.529794 |
| H | -0.412202 | -3.394133 | 2.084091 |
| H | 0.520121 | -2.909560 | 3.511245 |
| C | -0.328157 | 0.645867 | 3.898093 |
| H | -0.348289 | 1.698733 | 3.606695 |
| H | -1.234986 | 0.419338 | 4.467325 |
| H | 0.538511 | 0.483530 | 4.546671 |
| C | -0.378839 | -3.679218 | -1.409958 |
| H | -1.271789 | -4.038835 | -1.931917 |
| H | 0.492556 | -4.182690 | -1.840671 |
| H | -0.447310 | -3.958648 | -0.355527 |
| C | -0.304376 | -1.168018 | -3.784288 |
| H | -1.246531 | -1.562897 | -4.176975 |
| H | -0.250340 | -0.099736 | -4.007752 |
| H | 0.522779 | -1.670029 | -4.296188 |
| C | -0.210494 | 3.095481 | -2.505808 |
| H | -0.304971 | 2.324209 | -3.273992 |
| H | -1.074332 | 3.764642 | -2.570723 |
| H | 0.693701 | 3.677526 | -2.710379 |
| C | -0.201798 | 3.883108 | 0.861929 |
| H | -1.072051 | 4.509355 | 0.640255 |
| H | -0.272844 | 3.532944 | 1.894488 |
| H | 0.697170 | 4.501060 | 0.770239 |
| Sn | -1.976115 | 0.062587 | -0.025128 |
| Sn | 1.715174 | -0.031861 | 0.015928 |

| | | | |
|---|---|---|---|
| Ag | 4.392139 | -0.045026 | 0.017658 |
| Cl | 6.804738 | -0.056175 | 0.024505 |
| C | -6.373439 | -0.766577 | 0.011393 |
| C | -6.433210 | 0.591553 | 0.033108 |
| H | -7.157394 | -1.507760 | 0.010929 |
| H | -7.278922 | 1.261210 | 0.052158 |
| N | -5.030916 | -1.106644 | -0.021113 |
| N | -5.125184 | 1.048628 | 0.016571 |
| C | -4.249536 | 0.007582 | -0.014474 |
| C | -4.540954 | -2.485849 | -0.007194 |
| H | -4.504940 | -2.867768 | 1.016879 |
| H | -5.207922 | -3.107485 | -0.607779 |
| H | -3.538993 | -2.513424 | -0.436737 |
| C | -4.766333 | 2.466987 | 0.038245 |
| H | -5.239703 | 2.980666 | -0.802225 |
| H | -5.092053 | 2.919978 | 0.978274 |
| H | -3.683548 | 2.556042 | -0.048725 |

$C_5H_6$(NHC)

E=-420.17158 a.u.

| | | | |
|---|---|---|---|
| C | -1.436785 | -1.355489 | 0.000000 |
| H | -1.998504 | -1.101336 | 0.907059 |
| H | -1.998504 | -1.101336 | -0.907059 |
| C | 0.324278 | -1.976156 | 1.084914 |
| H | 1.340438 | -2.374520 | 1.176642 |
| H | -0.128665 | -1.800841 | 2.069019 |
| C | 0.324278 | -1.976156 | -1.084914 |
| H | -0.128665 | -1.800841 | -2.069019 |
| H | 1.340438 | -2.374520 | -1.176642 |
| C | 0.440840 | 0.554596 | 0.000000 |
| C | 0.135885 | 2.701268 | -0.679937 |
| C | 0.135885 | 2.701268 | 0.679937 |
| H | 0.019196 | 3.511470 | -1.382409 |
| H | 0.019196 | 3.511470 | 1.382409 |
| N | 0.324278 | 1.383114 | 1.075873 |
| H | 0.376408 | 1.045430 | 2.026952 |
| N | 0.324278 | 1.383114 | -1.075873 |
| H | 0.376408 | 1.045430 | -2.026952 |
| C | -0.635184 | -2.697688 | 0.000000 |
| C | 0.084529 | -0.938975 | 0.000000 |

$Si_5Me_6$(NHC)

E=-1991.86342 a.u.

| | | | |
|---|---|---|---|
| Si | 1.204992 | -0.259719 | 1.845660 |

| | | | |
|---|---|---|---|
| Si | 1.371831 | -1.445333 | -1.078953 |
| Si | 1.414756 | 1.671300 | -0.647338 |
| C | 0.993477 | -1.885231 | 2.839172 |
| H | 0.143421 | -1.798713 | 3.528075 |
| H | 0.838799 | -2.770693 | 2.219132 |
| H | 1.891103 | -2.057764 | 3.446489 |
| C | 1.134306 | 1.060176 | 3.231298 |
| H | 1.308048 | 2.077618 | 2.875812 |
| H | 0.171549 | 1.035006 | 3.757040 |
| H | 1.916413 | 0.831251 | 3.966662 |
| C | 1.349016 | -3.312660 | -0.643688 |
| H | 0.457652 | -3.819878 | -1.036401 |
| H | 2.218908 | -3.777965 | -1.124939 |
| H | 1.422809 | -3.516504 | 0.426240 |
| C | 1.346146 | -1.482216 | -2.995136 |
| H | 0.633272 | -2.239450 | -3.346088 |
| H | 1.068437 | -0.527159 | -3.445926 |
| H | 2.336410 | -1.760742 | -3.376810 |
| C | 1.562005 | 2.202381 | -2.481536 |
| H | 1.810078 | 1.376847 | -3.151611 |
| H | 0.644114 | 2.680556 | -2.845740 |
| H | 2.370067 | 2.941375 | -2.557707 |
| C | 1.274272 | 3.363462 | 0.247988 |
| H | 0.591523 | 4.030985 | -0.294962 |
| H | 0.930021 | 3.292613 | 1.282211 |
| H | 2.257835 | 3.849597 | 0.257904 |
| Si | -0.181777 | 0.020884 | -0.053552 |
| Si | 2.924190 | -0.042998 | 0.146031 |
| C | -4.329831 | -0.664631 | -0.106798 |
| C | -4.339444 | 0.695592 | -0.101563 |
| H | -5.140856 | -1.376275 | -0.112424 |
| H | -5.160364 | 1.395843 | -0.103282 |
| N | -3.001700 | -1.055161 | -0.112320 |
| N | -3.016429 | 1.104765 | -0.101813 |
| C | -2.179870 | 0.030555 | -0.106215 |
| C | -2.557206 | -2.448999 | -0.065256 |
| H | -2.651507 | -2.840792 | 0.951292 |
| H | -3.166042 | -3.044413 | -0.749173 |
| H | -1.511981 | -2.493111 | -0.370401 |
| C | -2.596847 | 2.506617 | -0.066299 |
| H | -3.069209 | 3.052192 | -0.886975 |
| H | -2.882002 | 2.956556 | 0.888489 |
| H | -1.513629 | 2.547637 | -0.175646 |

$Ge_5Me_6$(NHC)

E=-563.24968 a.u.

| | | | |
|---|---|---|---|
| Ge | -0.797248 | -0.050891 | 2.003506 |
| Ge | -1.019086 | 1.734871 | -0.923884 |
| Ge | -0.991318 | -1.694936 | -1.002206 |
| C | -0.545454 | 1.479759 | 3.268995 |
| H | 0.399436 | 1.371431 | 3.813418 |
| H | -0.543944 | 2.443679 | 2.756010 |
| H | -1.360283 | 1.485038 | 4.001888 |
| C | -0.570638 | -1.650165 | 3.187336 |
| H | -0.643796 | -2.589051 | 2.634224 |
| H | 0.397084 | -1.617537 | 3.700377 |
| H | -1.357394 | -1.644641 | 3.950511 |
| C | -0.853566 | 3.575275 | -0.147474 |
| H | 0.031528 | 4.091257 | -0.538668 |
| H | -1.732755 | 4.162433 | -0.436579 |
| H | -0.800480 | 3.563702 | 0.943159 |
| C | -0.974469 | 2.084291 | -2.894888 |
| H | -0.128510 | 2.732293 | -3.150503 |
| H | -0.893941 | 1.164133 | -3.477173 |
| H | -1.896016 | 2.597322 | -3.192578 |
| C | -0.976837 | -1.938885 | -2.988785 |
| H | -1.124734 | -0.996909 | -3.520609 |
| H | -0.031760 | -2.383264 | -3.320296 |
| H | -1.789008 | -2.619041 | -3.270137 |
| C | -0.754267 | -3.568780 | -0.330319 |
| H | 0.087728 | -4.058535 | -0.834356 |
| H | -0.589849 | -3.608853 | 0.748553 |
| H | -1.656621 | -4.148142 | -0.556427 |
| Ge | 0.687566 | 0.013134 | -0.080279 |
| Ge | -2.695437 | -0.019765 | 0.146053 |
| C | 4.963009 | 0.691593 | -0.101386 |
| C | 4.960381 | -0.668094 | -0.108490 |
| H | 5.780235 | 1.396136 | -0.094068 |
| H | 5.774915 | -1.375777 | -0.107702 |
| N | 3.636125 | 1.092725 | -0.111359 |
| N | 3.632126 | -1.064228 | -0.124011 |
| C | 2.805300 | 0.015877 | -0.123808 |
| C | 3.207779 | 2.491105 | -0.081107 |
| H | 3.493526 | 2.948926 | 0.869832 |
| H | 3.671322 | 3.036885 | -0.906857 |
| H | 2.123669 | 2.525252 | -0.185925 |
| C | 3.197661 | -2.460886 | -0.095253 |
| H | 3.733290 | -3.025952 | -0.861921 |

| | | | |
|---|---|---|---|
| H | 3.394667 | -2.895770 | 0.888588 |

$Sn_5Me_6$(NHC)

E=-561.29996a.u.

| | | | |
|---|---|---|---|
| Sn | -0.636631 | -0.000217 | 2.254794 |
| Sn | -0.840002 | 1.938841 | -1.100938 |
| Sn | -0.839855 | -1.938667 | -1.101305 |
| C | -0.367780 | 1.709723 | 3.578615 |
| H | 0.576306 | 1.621009 | 4.126452 |
| H | -0.361202 | 2.647736 | 3.016808 |
| H | -1.184833 | 1.750300 | 4.306933 |
| C | -0.367680 | -1.710371 | 3.578322 |
| H | -0.361032 | -2.648290 | 3.016359 |
| H | 0.576391 | -1.621684 | 4.126191 |
| H | -1.184740 | -1.751127 | 4.306623 |
| C | -0.597771 | 3.957217 | -0.311505 |
| H | 0.311762 | 4.421258 | -0.708671 |
| H | -1.451377 | 4.574463 | -0.611977 |
| H | -0.544807 | 3.954805 | 0.780640 |
| C | -0.767370 | 2.235502 | -3.257906 |
| H | 0.127665 | 2.800241 | -3.539385 |
| H | -0.758474 | 1.278042 | -3.785636 |
| H | -1.646871 | 2.801063 | -3.584080 |
| C | -0.767187 | -2.234859 | -3.258337 |
| H | -0.758407 | -1.277281 | -3.785855 |
| H | 0.127920 | -2.799423 | -3.539938 |
| H | -1.646617 | -2.800458 | -3.584635 |
| C | -0.597457 | -3.957185 | -0.312286 |
| H | 0.312174 | -4.421027 | -0.709462 |
| H | -0.544604 | -3.955003 | 0.779866 |
| H | -1.450956 | -4.574471 | -0.612979 |
| Sn | 1.098420 | 0.000057 | -0.085304 |
| Sn | -2.761383 | -0.000100 | 0.136356 |
| C | 5.613192 | 0.679844 | -0.095823 |
| C | 5.613195 | -0.679686 | -0.095816 |
| H | 6.429076 | 1.386027 | -0.089520 |
| H | 6.429082 | -1.385865 | -0.089503 |
| N | 4.284437 | 1.076518 | -0.110505 |
| N | 4.284442 | -1.076366 | -0.110495 |
| C | 3.451884 | 0.000074 | -0.118136 |
| C | 3.855187 | 2.474289 | -0.094901 |
| H | 4.134913 | 2.943066 | 0.852540 |
| H | 4.320558 | 3.013869 | -0.923835 |
| H | 2.771254 | 2.507719 | -0.206580 |

| | | | |
|---|---|---|---|
| C | 3.855191 | -2.474136 | -0.094851 |
| H | 4.320762 | -3.013791 | -0.923623 |
| H | 4.134690 | -2.942825 | 0.852701 |
| H | 2.771284 | -2.507580 | -0.206788 |

$C_5H_6AgCl$

E=-800.06091 a.u.

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.309474 | -2.356788 |
| H | -0.919090 | 1.888051 | -2.351365 |
| H | 0.919090 | 1.888051 | -2.351365 |
| C | -1.134038 | -0.654737 | -2.356788 |
| H | -1.175555 | -1.739980 | -2.351365 |
| H | -2.094645 | -0.148070 | -2.351365 |
| C | 1.134038 | -0.654737 | -2.356788 |
| H | 2.094645 | -0.148070 | -2.351365 |
| H | 1.175555 | -1.739980 | -2.351365 |
| Ag | 0.000000 | 0.000000 | 0.684324 |
| Cl | 0.000000 | 0.000000 | 3.052860 |
| C | 0.000000 | 0.000000 | -1.511726 |
| C | 0.000000 | 0.000000 | -3.076852 |

$Si_5Me_6AgCl$

E=-2293.07015 a.u.

| | | | |
|---|---|---|---|
| Si | 1.558161 | -0.122626 | 1.949582 |
| Si | 1.529065 | 1.742756 | -0.905739 |
| Si | 1.447818 | -1.666534 | -1.090982 |
| C | 1.631920 | 1.331113 | 3.161629 |
| H | 2.489083 | 1.200203 | 3.832089 |
| H | 1.722424 | 2.306691 | 2.683442 |
| H | 0.724893 | 1.338163 | 3.776934 |
| C | 1.559569 | -1.701386 | 2.995474 |
| H | 1.551283 | -2.622228 | 2.412108 |
| H | 2.449454 | -1.711445 | 3.635410 |
| H | 0.679174 | -1.706134 | 3.648286 |
| C | 1.615680 | 3.435755 | -0.060801 |
| H | 2.498819 | 3.975762 | -0.421448 |
| H | 0.731296 | 4.023252 | -0.332778 |
| H | 1.667824 | 3.389582 | 1.027294 |
| C | 1.493272 | 2.070325 | -2.770820 |
| H | 2.401346 | 2.608391 | -3.066076 |
| H | 1.417313 | 1.170092 | -3.380697 |
| H | 0.635018 | 2.710109 | -3.006320 |
| C | 1.425996 | -1.786516 | -2.981245 |
| H | 1.474820 | -0.823824 | -3.490403 |

| | | | |
|---|---|---|---|
| H | 2.279286 | -2.389377 | -3.313019 |
| H | 0.511429 | -2.296157 | -3.305258 |
| C | 1.424365 | -3.442920 | -0.434755 |
| H | 2.260376 | -4.001273 | -0.871550 |
| H | 1.496816 | -3.517801 | 0.650368 |
| H | 0.495726 | -3.934276 | -0.746751 |
| Si | 2.828527 | -0.047972 | -0.050590 |
| Si | 0.167844 | 0.018399 | 0.018535 |
| Ag | -2.297874 | 0.027542 | 0.026454 |
| Cl | -4.695937 | 0.035955 | 0.039815 |

$Ge_5Me_6AgCl$

E=-864.44765 a.u.

| | | | |
|---|---|---|---|
| Ge | -1.122762 | -0.664800 | 1.977707 |
| Ge | -1.094242 | -1.368047 | -1.583109 |
| Ge | -1.011351 | 2.069908 | -0.411047 |
| C | -1.195541 | -2.554975 | 2.559918 |
| H | -2.077409 | -2.709694 | 3.189648 |
| H | -1.241176 | -3.249567 | 1.720288 |
| H | -0.304549 | -2.785557 | 3.152462 |
| C | -1.119038 | 0.475711 | 3.594215 |
| H | -1.107084 | 1.539610 | 3.355031 |
| H | -2.009641 | 0.262504 | 4.193889 |
| H | -0.234787 | 0.246054 | 4.197158 |
| C | -1.174849 | -3.336988 | -1.402951 |
| H | -2.051183 | -3.716947 | -1.937656 |
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| H | -0.989006 | 0.142598 | -3.698362 |
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| H | -1.065049 | 2.162117 | -3.008690 |
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