

Electronic Supplementary Information

In Silico Modelling of Chelate Stabilized Tetrylene Derivatives

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PCPX systems

Table S1. Selection of the most relevant geometrical parameters computed for model $RP=C(Cl)-P(X)RR'$ derivatives incorporating the $P=C(Cl)-P=X$ ($X = O$ or S) moiety.

| R | R' | PCPO | | | | | PCPS | | | | |
|------|----|---------|---------|---------|-----------|-----------|---------|---------|---------|-----------|-----------|
| | | P=C (Å) | C-P (Å) | P=O (Å) | C-P=O (°) | P=C-P (°) | P=C (Å) | C-P (Å) | P=S (Å) | C-P=S (°) | P=C-P (°) |
| H | Me | 1.671 | 1.814 | 1.474 | 113.2 | 117.9 | 1.674 | 1.822 | 1.925 | 115.9 | 118.6 |
| | Cl | 1.673 | 1.802 | 1.463 | 114.6 | 117.1 | 1.675 | 1.811 | 1.903 | 117.1 | 116.9 |
| Me | Me | 1.672 | 1.815 | 1.477 | 111.7 | 117.4 | 1.673 | 1.818 | 1.934 | 113.0 | 118.8 |
| | Cl | 1.674 | 1.802 | 1.466 | 112.9 | 116.5 | 1.675 | 1.809 | 1.913 | 114.4 | 117.9 |
| t-Bu | Me | 1.674 | 1.827 | 1.481 | 110.5 | 114.2 | 1.674 | 1.834 | 1.942 | 112.4 | 116.2 |
| | Cl | 1.676 | 1.817 | 1.469 | 111.6 | 113.0 | 1.678 | 1.828 | 1.921 | 113.1 | 114.6 |
| Ph | Me | 1.676 | 1.819 | 1.479 | 111.0 | 115.1 | 1.677 | 1.826 | 1.937 | 112.5 | 116.9 |
| | Cl | 1.678 | 1.807 | 1.468 | 112.3 | 114.2 | 1.677 | 1.821 | 1.915 | 114.3 | 122.1 |
| Mes | Me | 1.674 | 1.827 | 1.480 | 111.0 | 120.9 | 1.675 | 1.833 | 1.941 | 113.0 | 118.1 |
| | Cl | 1.677 | 1.814 | 1.468 | 111.1 | 119.0 | 1.676 | 1.820 | 1.919 | 114.0 | 117.2 |
| Mes* | Me | 1.673 | 1.848 | 1.484 | 106.9 | 125.2 | 1.676 | 1.852 | 1.954 | 108.1 | 125.8 |
| | Cl | 1.675 | 1.836 | 1.471 | 107.8 | 123.7 | 1.677 | 1.842 | 1.928 | 109.0 | 124.2 |

PCPX-E(II) systems

Table S2. Selected geometrical features for the $RP=C(Si(II)-Cl)-P(X)RR'$ ($X = O$ or S) model systems. The sum of covalent radii for relevant bonds: $\Sigma_{Si-C}=1.87 \text{ \AA}$, $\Sigma_{Si-O}=1.77 \text{ \AA}$, $\Sigma_{Si-S}=2.16 \text{ \AA}$, $\Sigma_{P=O}=1.59 \text{ \AA}$, $\Sigma_{P=S}=1.96 \text{ \AA}$.

| R | R' | P=C (\AA) | C-P (\AA) | P=X (\AA) | X-Si(II) (\AA) | Si(II)-C (\AA) | C-P=X ($^{\circ}$) | P=C-P ($^{\circ}$) | X-Si(II)-C ($^{\circ}$) | dev. pln. ($^{\circ}$) |
|--------------------|----|--------------|--------------|--------------|----------------|----------------|-------------------------|-------------------------|---------------------------|-----------------------------|
| PCPO-Si(II) | | | | | | | | | | |
| H | Me | 1.656 | 1.743 | 1.544 | 1.900 | 2.009 | 97.0 | 130.42 | 78.29 | 10.87 |
| | Cl | 1.657 | 1.727 | 1.533 | 1.919 | 2.007 | 98.4 | 130.6 | 77.94 | 13.81 |
| Me | Me | 1.654 | 1.741 | 1.553 | 1.875 | 1.99 | 96.4 | 130.3 | 78.97 | 6.81 |
| | Cl | 1.655 | 1.732 | 1.534 | 1.914 | 1.993 | 97.5 | 129.22 | 78.0 | 2.19 |
| t-Bu | Me | 1.659 | 1.754 | 1.557 | 1.867 | 1.997 | 96.3 | 125.23 | 79.39 | 4.23 |
| | Cl | 1.661 | 1.74 | 1.542 | 1.893 | 1.998 | 97.6 | 125.45 | 78.85 | 1.9 |
| Ph | Me | 1.661 | 1.744 | 1.552 | 1.877 | 1.985 | 96.7 | 126.31 | 79.33 | 3.15 |
| | Cl | 1.663 | 1.727 | 1.540 | 1.897 | 1.988 | 98.0 | 127.43 | 78.88 | 5.58 |
| Mes | Me | 1.657 | 1.757 | 1.555 | 1.87 | 1.983 | 94.6 | 134.11 | 78.47 | 6.4 |
| | Cl | 1.658 | 1.74 | 1.542 | 1.893 | 1.987 | 96.0 | 134.04 | 77.98 | 9.59 |
| Mes* | Me | 1.661 | 1.773 | 1.562 | 1.877 | 2.003 | 93.6 | 133.69 | 77.68 | 18.73 |
| | Cl | 1.661 | 1.751 | 1.541 | 1.912 | 2.003 | 95.2 | 133.61 | 76.91 | 16.94 |
| PCPS-Si(II) | | | | | | | | | | |
| H | Me | 1.658 | 1.751 | 1.996 | 2.451 | 1.972 | 99.2 | 127.33 | 79.71 | 17.73 |
| | Cl | 1.658 | 1.733 | 1.98 | 2.44 | 1.981 | 100.52 | 128.81 | 79.89 | 20.65 |
| Me | Me | 1.659 | 1.751 | 2.009 | 2.405 | 1.962 | 99.22 | 125.88 | 81.42 | 10.88 |
| | Cl | 1.659 | 1.732 | 1.993 | 2.398 | 1.97 | 100.23 | 127.82 | 81.29 | 15.01 |
| t-Bu | Me | 1.666 | 1.768 | 2.015 | 2.39 | 1.967 | 99.58 | 120 | 82.63 | 0.27 |
| | Cl | 1.667 | 1.75 | 1.997 | 2.396 | 1.976 | 100.78 | 121.08 | 82.16 | 4.17 |
| Ph | Me | 1.665 | 1.754 | 2.006 | 2.412 | 1.961 | 99.92 | 122.45 | 81.6 | 9.07 |
| | Cl | 1.666 | 1.734 | 1.989 | 2.416 | 1.967 | 101.05 | 124.94 | 81.4 | 13.01 |
| Mes | Me | 1.663 | 1.768 | 2.023 | 2.400 | 1.962 | 94.69 | 124.32 | 78.98 | 14.98 |
| | Cl | 1.663 | 1.748 | 2.005 | 2.398 | 1.968 | 96.0 | 125.84 | 78.93 | 22.25 |
| Mes* | Me | 1.668 | 1.779 | 2.028 | 2.384 | 1.984 | 96.9 | 128.6 | 81.01 | 17.65 |
| | Cl | 1.669 | 1.757 | 1.998 | 2.405 | 1.982 | 98.43 | 129.17 | 80.31 | 15.12 |

Table S3. Selected geometrical features for the RP=C(Ge(II)-Cl)-P(X)RR' (X = O or S) model systems. The sum of covalent radii for relevant bonds: $\Sigma_{\text{Ge-C}}=1.96 \text{ \AA}$, $\Sigma_{\text{Ge-O}}=1.84 \text{ \AA}$, $\Sigma_{\text{Ge-S}}=2.24 \text{ \AA}$, $\Sigma_{\text{P=O}}=1.59 \text{ \AA}$ and $\Sigma_{\text{P=S}}=1.96 \text{ \AA}$.

| R | R' | P=C (Å) | C-P (Å) | P=X (Å) | X-Si(II) (Å) | Si(II)-C (Å) | C-P=X (°) | P=C-P (°) | X-Si(II)-C (°) | dev. pln. (°) |
|--------------------|----|------------|------------|------------|--------------|--------------|--------------|--------------|----------------|------------------|
| PCPO-Ge(II) | | | | | | | | | | |
| H | Me | 1.654 | 1.748 | 1.533 | 2.079 | 2.107 | 99.86 | 129.58 | 73.87 | 13.32 |
| | Cl | 1.654 | 1.734 | 1.519 | 2.112 | 2.110 | 101.40 | 129.44 | 73.32 | 15.47 |
| Me | Me | 1.651 | 1.750 | 1.542 | 2.047 | 2.103 | 99.29 | 128.75 | 74.48 | 8.78 |
| | Cl | 1.652 | 1.734 | 1.527 | 2.074 | 2.104 | 100.64 | 129.19 | 73.97 | 11.35 |
| t-Bu | Me | 1.653 | 1.761 | 1.544 | 2.045 | 2.117 | 97.39 | 125.30 | 74.65 | 3.17 |
| | Cl | 1.655 | 1.748 | 1.527 | 2.078 | 2.115 | 100.62 | 125.32 | 74.02 | 1.44 |
| Ph | Me | 1.656 | 1.749 | 1.539 | 2.057 | 2.097 | 99.71 | 127.10 | 74.56 | 5.09 |
| | Cl | 1.657 | 1.733 | 1.526 | 2.083 | 2.098 | 101.04 | 127.96 | 74.05 | 6.69 |
| Mes | Me | 1.654 | 1.761 | 1.543 | 2.048 | 2.086 | 97.32 | 134.02 | 73.87 | 9.11 |
| | Cl | 1.658 | 1.733 | 1.526 | 2.085 | 2.097 | 101.04 | 127.96 | 74.05 | 6.70 |
| Mes* | Me | 1.657 | 1.770 | 1.549 | 2.053 | 2.117 | 96.85 | 135.01 | 73.20 | 19.30 |
| | Cl | 1.659 | 1.751 | 1.529 | 2.095 | 2.121 | 98.51 | 134.09 | 73.39 | 18.26 |
| PCPS-Ge(II) | | | | | | | | | | |
| H | Me | 1.657 | 1.752 | 1.997 | 2.549 | 2.080 | 100.92 | 126.63 | 76.70 | 20.14 |
| | Cl | 1.656 | 1.733 | 1.980 | 2.548 | 2.091 | 102.58 | 128.20 | 76.73 | 22.38 |
| Me | Me | 1.655 | 1.753 | 2.010 | 2.506 | 2.078 | 100.92 | 124.88 | 78.06 | 13.52 |
| | Cl | 1.656 | 1.734 | 1.992 | 2.506 | 2.087 | 102.19 | 126.85 | 77.85 | 16.77 |
| t-Bu | Me | 1.656 | 1.770 | 2.014 | 2.500 | 2.092 | 101.65 | 119.93 | 78.99 | 1.41 |
| | Cl | 1.661 | 1.753 | 1.993 | 2.513 | 2.096 | 103.07 | 120.76 | 78.60 | 4.41 |
| Ph | Me | 1.660 | 1.753 | 2.005 | 2.526 | 2.076 | 101.68 | 123.39 | 78.04 | 11.10 |
| | Cl | 1.661 | 1.733 | 1.988 | 2.528 | 2.083 | 103.01 | 125.75 | 77.81 | 13.98 |
| Mes | Me | 1.659 | 1.766 | 2.018 | 2.504 | 2.069 | 96.38 | 128.72 | 75.65 | 18.95 |
| | Cl | 1.659 | 1.744 | 1.998 | 2.505 | 2.079 | 98.28 | 130.97 | 75.78 | 20.55 |
| Mes* | Me | 1.663 | 1.773 | 2.028 | 2.485 | 2.106 | 99.24 | 129.77 | 77.88 | 17.18 |
| | Cl | 1.664 | 1.752 | 1.997 | 2.511 | 2.101 | 100.88 | 130.02 | 77.19 | 15.54 |

Table S4. Selected geometrical features for the RP=C(Sn(II)-Cl)-P(X)RR' (X = O or S) model systems. The sum of covalent radii for relevant bonds $\Sigma_{\text{Sn-C}}=2.15 \text{ \AA}$ and $\Sigma_{\text{Sn-O}}=2.03 \text{ \AA}$, $\Sigma_{\text{Sn-S}}=2.43 \text{ \AA}$, $\Sigma_{\text{P-O}}=1.59 \text{ \AA}$ and $\Sigma_{\text{P-S}}=1.96 \text{ \AA}$.

| R | R' | P=C (Å) | C-P (Å) | P=X (Å) | X-Si(II) (Å) | Si(II)-C (Å) | C-P=X (°) | P=C-P (°) | X-Si(II)-C (°) | dev. pln. (°) |
|--------------------|----|------------|------------|------------|--------------|--------------|--------------|--------------|----------------|------------------|
| PCPO-Sn(II) | | | | | | | | | | |
| H | Me | 1.654 | 1.752 | 1.529 | 2.261 | 2.307 | 102.67 | 127.08 | 68.32 | 14.54 |
| | Cl | 1.655 | 1.736 | 1.515 | 2.294 | 2.314 | 104.21 | 127.09 | 67.76 | 16.39 |
| Me | Me | 1.650 | 1.754 | 1.537 | 2.229 | 2.305 | 102.11 | 126.14 | 68.83 | 10.72 |
| | Cl | 1.651 | 1.738 | 1.522 | 2.256 | 2.309 | 103.46 | 126.72 | 68.32 | 13.02 |
| t-Bu | Me | 1.652 | 1.763 | 1.540 | 2.229 | 2.316 | 102.22 | 124.60 | 68.98 | 2.03 |
| | Cl | 1.653 | 1.750 | 1.523 | 2.260 | 2.316 | 103.45 | 124.63 | 68.42 | 1.02 |
| Ph | Me | 1.654 | 1.751 | 1.534 | 2.249 | 2.295 | 102.55 | 126.96 | 68.76 | 6.11 |
| | Cl | 1.655 | 1.734 | 1.520 | 2.276 | 2.295 | 103.83 | 127.95 | 68.25 | 7.19 |
| Mes | Me | 1.653 | 1.761 | 1.537 | 2.241 | 2.279 | 99.93 | 133.42 | 68.03 | 10.15 |
| | Cl | 1.654 | 1.743 | 1.522 | 2.273 | 2.283 | 101.59 | 133.61 | 67.57 | 11.42 |
| Mes* | Me | 1.655 | 1.768 | 1.543 | 2.248 | 2.315 | 99.79 | 135.45 | 67.52 | 19.40 |
| | Cl | 1.657 | 1.749 | 1.522 | 2.291 | 2.316 | 101.45 | 134.41 | 66.79 | 19.17 |
| PCPS-Sn(II) | | | | | | | | | | |
| H | Me | 1.657 | 1.754 | 2.009 | 2.714 | 2.284 | 104.03 | 124.06 | 72.13 | 17.78 |
| | Cl | 1.656 | 1.733 | 1.982 | 2.722 | 2.298 | 105.42 | 126.23 | 77.96 | 24.15 |
| Me | Me | 1.654 | 1.756 | 2.013 | 2.677 | 2.285 | 103.58 | 122.77 | 72.91 | 16.17 |
| | Cl | 1.655 | 1.735 | 1.995 | 2.680 | 2.297 | 104.96 | 124.91 | 72.58 | 19.06 |
| t-Bu | Me | 1.658 | 1.771 | 2.017 | 2.672 | 2.298 | 104.48 | 118.98 | 73.81 | 3.35 |
| | Cl | 1.660 | 1.752 | 1.996 | 2.685 | 2.304 | 105.95 | 120.00 | 73.38 | 6.06 |
| Ph | Me | 1.658 | 1.753 | 2.007 | 2.705 | 2.277 | 104.38 | 123.37 | 72.77 | 12.30 |
| | Cl | 1.656 | 1.733 | 1.990 | 2.711 | 2.286 | 105.81 | 125.87 | 72.46 | 14.67 |
| Mes | Me | 1.659 | 1.764 | 2.019 | 2.684 | 2.268 | 98.89 | 128.01 | 70.52 | 20.23 |
| | Cl | 1.658 | 1.741 | 1.999 | 2.690 | 2.280 | 100.93 | 130.53 | 70.55 | 21.61 |
| Mes* | Me | 1.661 | 1.769 | 2.032 | 2.663 | 2.309 | 102.18 | 130.22 | 72.75 | 17.39 |
| | Cl | 1.663 | 1.751 | 2.000 | 2.690 | 2.308 | 103.67 | 129.93 | 71.98 | 16.97 |

Table S5. Selected geometrical features for the RP=C(Pb(II)-Cl)-P(X)RR' (X = O or S) model systems. The sum of covalent radii for relevant bonds $\Sigma_{\text{Pb-C}}=2.19 \text{ \AA}$, $\Sigma_{\text{Pb-O}}=2.07 \text{ \AA}$, $\Sigma_{\text{Pb-S}}=2.47 \text{ \AA}$, $\Sigma_{\text{P=O}}=1.59 \text{ \AA}$ and $\Sigma_{\text{P=S}}=1.96 \text{ \AA}$.

| R | R' | P=C (\AA) | C-P (\AA) | P=X (\AA) | X-Si(II) (\AA) | Si(II)-C (\AA) | C-P=X ($^\circ$) | P=C-P ($^\circ$) | X-Si(II)-C ($^\circ$) | dev. pln. ($^\circ$) |
|--------------------|----|-------------------------|-------------------------|-------------------------|---------------------------|---------------------------|-----------------------|-----------------------|-------------------------|---------------------------|
| PCPO-Pb(II) | | | | | | | | | | |
| H | Me | 1.654 | 1.754 | 1.523 | 2.390 | 2.404 | 104.58 | 126.22 | 65.61 | 15.88 |
| | Cl | 1.654 | 1.737 | 1.510 | 2.424 | 2.412 | 106.19 | 126.33 | 65.03 | 17.59 |
| Me | Me | 1.649 | 1.757 | 1.532 | 2.355 | 2.403 | 103.97 | 125.39 | 66.08 | 13.03 |
| | Cl | 1.650 | 1.740 | 1.517 | 2.382 | 2.409 | 105.39 | 126.08 | 65.55 | 15.18 |
| t-Bu | Me | 1.650 | 1.764 | 1.533 | 2.361 | 2.409 | 104.16 | 124.85 | 66.20 | 0.16 |
| | Cl | 1.651 | 1.750 | 1.517 | 2.389 | 2.409 | 105.40 | 124.97 | 65.69 | 0.73 |
| Ph | Me | 1.652 | 1.751 | 1.528 | 2.385 | 2.390 | 104.41 | 127.65 | 65.83 | 7.79 |
| | Cl | 1.653 | 1.734 | 1.514 | 2.412 | 2.390 | 105.68 | 128.72 | 65.32 | 8.57 |
| Mes | Me | 1.651 | 1.759 | 1.530 | 2.379 | 2.371 | 101.64 | 134.30 | 65.05 | 11.53 |
| | Cl | 1.652 | 1.741 | 1.514 | 2.414 | 2.374 | 103.39 | 134.57 | 64.58 | 12.45 |
| Mes* | Me | 1.652 | 1.766 | 1.535 | 2.391 | 2.406 | 101.87 | 137.12 | 64.71 | 14.23 |
| | Cl | 1.653 | 1.745 | 1.514 | 2.442 | 2.405 | 103.69 | 136.16 | 63.94 | 18.97 |
| PCPS-Pb(II) | | | | | | | | | | |
| H | Me | 1.657 | 1.753 | 2.000 | 2.805 | 2.386 | 105.06 | 123.68 | 69.60 | 24.37 |
| | Cl | 1.656 | 1.731 | 1.982 | 2.811 | 2.404 | 107.05 | 125.82 | 69.45 | 25.88 |
| Me | Me | 1.653 | 1.755 | 2.012 | 2.767 | 2.391 | 104.99 | 122.39 | 70.52 | 18.49 |
| | Cl | 1.653 | 1.733 | 1.995 | 2.770 | 2.405 | 106.48 | 124.88 | 70.19 | 21.17 |
| t-Bu | Me | 1.656 | 1.765 | 2.019 | 2.753 | 2.404 | 105.79 | 120.09 | 71.38 | 5.95 |
| | Cl | 1.657 | 1.744 | 1.999 | 2.763 | 2.413 | 107.26 | 121.46 | 70.94 | 8.75 |
| Ph | Me | 1.656 | 1.762 | 2.011 | 2.771 | 2.387 | 105.61 | 121.88 | 70.95 | 2.95 |
| | Cl | 1.655 | 1.740 | 1.987 | 2.809 | 2.404 | 106.79 | 124.16 | 69.66 | 19.48 |
| Mes | Me | 1.655 | 1.769 | 2.019 | 2.791 | 2.388 | 105.12 | 124.77 | 70.62 | 11.46 |
| | Cl | 1.657 | 1.752 | 1.988 | 2.822 | 2.385 | 106.61 | 125.64 | 69.84 | 13.42 |
| Mes* | Me | 1.658 | 1.765 | 2.031 | 2.757 | 2.409 | 103.86 | 131.45 | 70.44 | 16.26 |
| | Cl | 1.660 | 1.747 | 1.998 | 2.786 | 2.406 | 105.40 | 131.19 | 69.69 | 16.68 |

Table S6. Calculated *relaxed* BDE (kcal mol⁻¹) values for the O-E(II) and S-E(II) bonds of model PCPO-E(II) and PCPS-E(II) systems.

| R | R' | PCPO-E(II) | | | | PCPS-E(II) | | | |
|--------------|----|------------|--------|--------|--------|------------|--------|--------|--------|
| | | Si(II) | Ge(II) | Sn(II) | Pb(II) | Si(II) | Ge(II) | Sn(II) | Pb(II) |
| H | Me | -9.4 | -9.7 | -12.6 | -13.0 | -8.7 | -11.1 | -13.8 | -14.1 |
| Me | Me | -20.5 | -18.2 | -21.0 | -19.9 | -19.1 | -19.9 | -22.5 | -22.5 |
| <i>t</i> -Bu | Me | -21.0 | -18.6 | -21.6 | -20.4 | -19.0 | -19.6 | -22.5 | -22.3 |
| Ph | | -15.5 | -12.3 | -12.7 | -10.7 | -13.6 | -13.4 | -13.6 | -9.6 |
| Mes | Me | -15.1 | -12.4 | -12.3 | -10.1 | -12.3 | -11.2 | -10.8 | -9.7 |
| Mes* | Me | -15.7 | -12.0 | -12.6 | -10.9 | -16.0 | -19.4 | -19.8 | -19.0 |

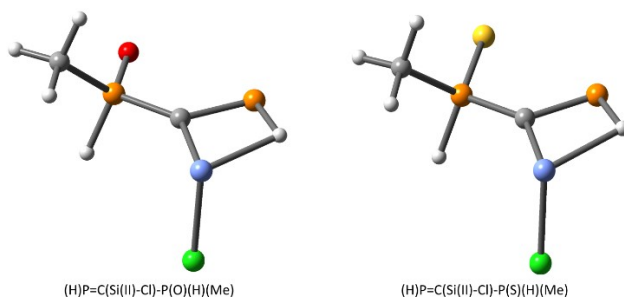


Figure S1. Equilibrium geometry of the (H)P=C(E(II)-Cl)-P(X)(H)(Me) model systems employed in the *relaxed* BDE approximation. The structures were obtained from the initial chelate geometry through rotation with 180° around the σ (P-C) bond. Following the geometry optimization the H atom bound to the P(sp²) atom migrates into a bridging coordination mode between the P(sp²) and the E atoms.

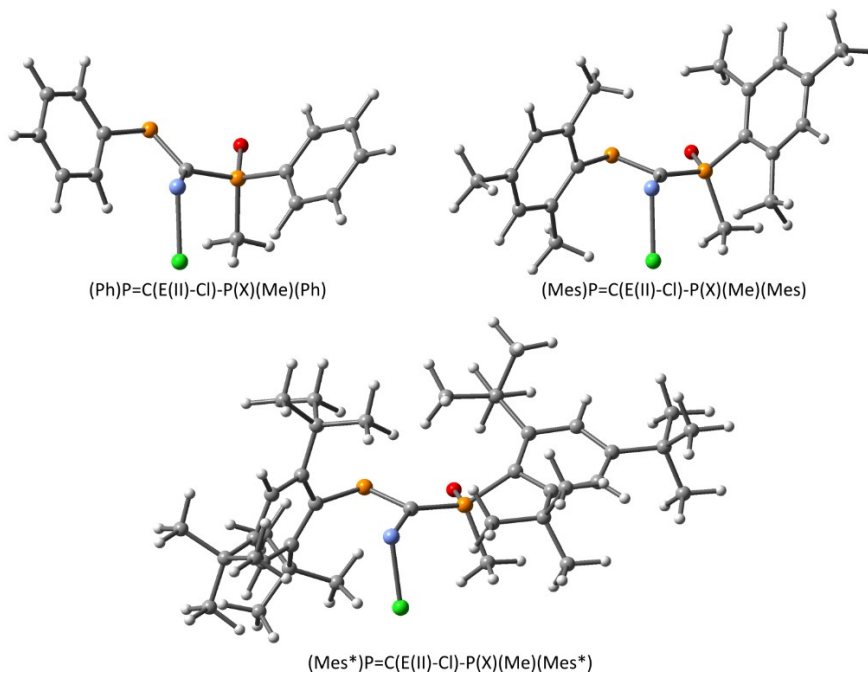


Figure S2. Equilibrium geometry of (Ph)P=C(E(II)-Cl)-P(X)(Ph)(Me), (Mes)P=C(E(II)-Cl)-P(X)(Ph)(Mes) and (Mes*)P=C(E(II)-Cl)-P(X)(Ph)(Mes*) model systems employed in the *relaxed* BDE approximation. The structures were obtained from the initial chelate geometry through rotation with 180° around the σ (P-C) bond.

Table S7. Atomic orbital (AO) composition of the $\sigma(\text{E-X})$, $\sigma(\text{E-C})$ and $\sigma(\text{E-Cl})$ sigma bonds, in the particular cases of $(\text{Me})\text{P}=\text{C}(\text{E}(\text{II})-\text{Cl})-\text{P}(\text{X})(\text{Me})(\text{Me})$ and $(\text{Mes}^*)\text{P}=\text{C}(\text{E}(\text{II})-\text{Cl})-\text{P}(\text{X})(\text{Mes}^*)(\text{Me})$ model systems.

| E(II) | R | (%) E(II) in $\sigma(\text{X-E})$ bond | % p of E(II) in $\sigma(\text{X-E})$ bond | (%) E(II) in $\sigma(\text{C-E})$ bond | % p of E(II) in $\sigma(\text{C-E})$ bond | (%) E(II) in $\sigma(\text{Cl-E})$ bond | % p of E(II) in $\sigma(\text{Cl-E})$ bond |
|-------------------|------|----------------------------------------|-------------------------------------------|----------------------------------------|-------------------------------------------|-----------------------------------------|--------------------------------------------|
| PCPO-E(II) | | | | | | | |
| Si(II) | Me | 11.12 | 90.22 | 20.01 | 88.13 | 19.97 | 89.97 |
| | Mes* | - | - | 19.96 | 85.93 | 20.01 | 88.54 |
| Ge(II) | Me | 8.83 | 94.06 | 18.53 | 92.30 | 17.67 | 94.03 |
| | Mes* | - | - | 18.84 | 89.42 | - | - |
| Sn(II) | Me | 7.56 | 95.29 | 16.82 | 93.49 | 16.19 | 94.58 |
| | Mes* | - | - | 16.28 | 91.23 | - | - |
| Pb(II) | Me | 6.70 | 96.72 | 16.43 | 95.63 | 15.23 | 96.55 |
| | Mes* | - | - | 14.92 | 94.19 | - | - |
| PCPS-E(II) | | | | | | | |
| Si(II) | Me | 19.84 | 93.59 | 20.73 | 87.49 | 20.07 | 90.33 |
| | Mes* | 20.02 | 93.92 | 20.17 | 87.17 | 19.95 | 89.97 |
| Ge(II) | Me | 18.07 | 96.21 | 19.29 | 91.68 | 18.24 | 94.12 |
| | Mes* | 18.46 | 96.39 | 19.03 | 91.42 | 18.52 | 93.78 |
| Sn(II) | Me | 15.88 | 96.60 | 17.43 | 93.18 | 16.57 | 94.71 |
| | Mes* | 15.41 | 96.58 | 16.35 | 92.14 | - | - |
| Pb(II) | Me | 14.58 | 97.92 | 16.75 | 95.53 | 15.55 | 96.65 |
| | Mes* | - | - | 15.10 | 94.47 | - | - |

Table S8. Calculated interaction-energies (kcal mol^{-1}) of $\text{LP}(\text{P}) \rightarrow \sigma^*(\text{E-R})$, $\text{LP}(\text{X}) \rightarrow p(\text{E})$ or $\pi(\text{C}=\text{P}) \rightarrow \sigma^*(\text{E-Cl})$ donations, as well as the total electron-donation energy, for several model PCPX-E(II) systems.

| E(II) | R | $\text{LP}(\text{P}) \rightarrow \sigma^*(\text{E-R})$ | $\text{LP}(\text{X}) \rightarrow \sigma^*(\text{E-Cl})$ | $\text{LP}(\text{X}) \rightarrow \text{LV}(\text{E})$ | $\pi(\text{C}=\text{P}) \rightarrow \sigma^*(\text{E-Cl})$ | Total donation |
|-------------------|------|--------------------------------------------------------|---------------------------------------------------------|-------------------------------------------------------|------------------------------------------------------------|----------------|
| PCPO-E(II) | | | | | | |
| Si(II) | Me | 7.07 | 5 | | 1.74 | 13.81 |
| | Mes* | 6.64 | 5.08 | 11.07 | 1.54 | 24.33 |
| Ge(II) | Me | 6.79 | 3.43 | | 1.56 | 11.78 |
| | Mes* | 6.9 | 6.33 | 9.4 | 2.94 | 25.57 |
| Sn(II) | Me | 6.52 | 2.34 | | 0.75 | 9.61 |
| | Mes* | 7.32 | 4.11 | 8.27 | 1.56 | 21.26 |
| Pb(II) | Me | 6.73 | 1.79 | | 0.57 | 9.09 |
| | Mes* | 7.39 | 2.8 | 7.63 | 1.22 | 19.04 |
| PCPS-E(II) | | | | | | |
| Si(II) | Me | 7.21 | 4.79 | | 2.13 | 14.13 |
| | Mes* | 7.94 | 4.23 | | 1.74 | 13.91 |
| Ge(II) | Me | 6.76 | 4.52 | | 1.84 | 13.12 |
| | Mes* | 6.92 | 4.22 | | 1.5 | 12.64 |
| Sn(II) | Me | 6.59 | 3.23 | | 0.83 | 10.65 |
| | Mes* | 7.39 | 5.01 | 3.52 | 1.69 | 17.61 |
| Pb(II) | Me | 6.68 | 2.84 | | 0.59 | 10.11 |
| | Mes* | 7.33 | 3.98 | 4.18 | 1.26 | 16.75 |

PCPX-E(II)-AuCl systems

Table S9. The most relevant geometrical data computed for the {RP=C(Si(II)-Cl)-P(X)(Me)R}AuCl model complexes obtained via Si→Au bonds.

| X | R | P=X (Å) | X-Si (Å) | Si-C (Å) | Au-Si (Å) | dev. pln. (°) |
|---|--------------|---------|----------|----------|-----------|---------------|
| O | H | 1.556 | 1.814 | 1.947 | 2.236 | 3.29 |
| | Me | 1.567 | 1.794 | 1.932 | 2.242 | 3.66 |
| | <i>t</i> -Bu | 1.572 | 1.787 | 1.939 | 2.247 | 3.48 |
| | Ph | 1.568 | 1.787 | 1.932 | 2.246 | 2.53 |
| | Mes | 1.570 | 1.786 | 1.925 | 2.246 | 0.57 |
| | Mes* | 1.581 | 1.782 | 1.926 | 2.256 | 14.37 |
| S | H | 2.012 | 2.328 | 1.919 | 2.240 | 13.72 |
| | Me | 2.026 | 2.296 | 1.911 | 2.248 | 9.46 |
| | <i>t</i> -Bu | 2.032 | 2.285 | 1.920 | 2.253 | 2.04 |
| | Ph | 2.030 | 2.282 | 1.911 | 2.253 | 4.80 |
| | Mes | 2.038 | 2.277 | 1.908 | 2.251 | 14.88 |
| | Mes* | 2.049 | 2.267 | 1.918 | 2.260 | 14.31 |

Table S10. The most relevant geometrical data computed for the {RP=C(Ge(II)-Cl)-P(X)(Me)R}AuCl model complexes obtained via Ge→Au bonds.

| X | R | P=X (Å) | X-Ge (Å) | Ge-C (Å) | Au-Ge (Å) | dev. pln. (°) |
|---|--------------|---------|----------|----------|-----------|---------------|
| O | H | 1.542 | 1.992 | 2.030 | 2.327 | 6.36 |
| | Me | 1.553 | 1.966 | 2.021 | 2.331 | 5.83 |
| | <i>t</i> -Bu | 1.556 | 1.958 | 2.030 | 2.336 | 3.27 |
| | Ph | 1.552 | 1.967 | 2.017 | 2.332 | 2.79 |
| | Mes | 1.555 | 1.960 | 2.010 | 2.335 | 6.88 |
| | Mes* | 1.564 | 1.958 | 2.024 | 2.340 | 16.76 |
| S | H | 2.008 | 2.439 | 2.011 | 2.332 | 16.20 |
| | Me | 2.023 | 2.401 | 2.006 | 2.338 | 12.27 |
| | <i>t</i> -Bu | 2.389 | 2.388 | 2.013 | 2.342 | 2.87 |
| | Ph | 2.021 | 2.408 | 2.004 | 2.339 | 9.69 |
| | Mes | 2.041 | 2.386 | 1.996 | 2.341 | 15.40 |
| | Mes* | 2.027 | 2.375 | 2.021 | 2.346 | 15.34 |

Table S11. The most relevant geometrical data computed for the {RP=C(Sn(II)-Cl)-P(X)(Me)R}AuCl model complexes obtained via Sn→Au bonds.

| X | R | P=X (Å) | X-Sn (Å) | Sn-C (Å) | Au-Sn (Å) | dev. pln. (°) |
|---|--------------|---------|----------|----------|-----------|---------------|
| O | H | 1.534 | 2.191 | 2.227 | 2.502 | 7.93 |
| | Me | 1.543 | 2.165 | 2.216 | 2.504 | 7.84 |
| | <i>t</i> -Bu | 1.547 | 2.161 | 2.221 | 2.507 | 2.19 |
| | Ph | 1.542 | 2.176 | 2.207 | 2.506 | 4.46 |
| | Mes | 1.545 | 2.174 | 2.194 | 2.508 | 8.47 |
| | Mes* | 1.552 | 2.173 | 2.209 | 2.512 | 17.13 |
| S | H | 2.008 | 2.622 | 2.210 | 2.506 | 18.12 |
| | Me | 2.023 | 2.584 | 2.584 | 2.509 | 14.98 |
| | <i>t</i> -Bu | 2.028 | 2.574 | 2.212 | 2.513 | 3.85 |
| | Ph | 2.019 | 2.602 | 2.197 | 2.511 | 11.34 |
| | Mes | 2.040 | 2.581 | 2.186 | 2.514 | 16.31 |
| | Mes* | 2.046 | 2.565 | 2.211 | 2.517 | 15.92 |

Table S12. The most relevant geometrical data computed for the {RP=C(Pb(II)-Cl)-P(X)(Me)R}AuCl model complexes obtained via Pb→Au bonds.

| X | R | P=X (Å) | X-Pb (Å) | Pb-C (Å) | Au-Pb (Å) | dev. pln. (°) |
|---|--------------|---------|----------|----------|-----------|---------------|
| O | H | 1.523 | 2.354 | 2.306 | 2.591 | 10.73 |
| | Me | 1.531 | 2.321 | 2.298 | 2.591 | 9.94 |
| | <i>t</i> -Bu | 1.534 | 2.319 | 2.302 | 2.594 | 0.80 |
| | Ph | 1.528 | 2.346 | 2.285 | 2.593 | 6.34 |
| | Mes | 1.529 | 2.354 | 2.267 | 2.593 | 7.00 |
| | Mes* | 1.535 | 2.352 | 2.287 | 2.598 | 16.92 |
| S | H | 2.000 | 2.743 | 2.297 | 2.595 | 21.04 |
| | Me | 2.015 | 2.702 | 2.294 | 2.596 | 16.91 |
| | <i>t</i> -Bu | 2.020 | 2.692 | 2.302 | 2.600 | 4.52 |
| | Ph | 2.009 | 2.732 | 2.282 | 2.597 | 13.26 |
| | Mes | 2.021 | 2.724 | 2.269 | 2.600 | 18.54 |
| | Mes* | 2.036 | 2.688 | 2.296 | 2.603 | 15.59 |

Table S13. Computed relative enthalpies (kcal mol⁻¹) of PCPO-Ge(II)-AuCl and PCPS-Ge(II)-AuCl coordination isomers obtained through Ge(II)→Au, X→Au (X = O or S), P(sp²)→Au and π(C=P)→Au donations. The relative enthalpies are calculated with respect to the coordination isomer displaying Ge(II)→Au bonds.

| R | R' | PCPO-Ge(II)-AuCl | | | | PCPS-Ge(II)-AuCl | | | |
|------|----|------------------|------|------|-----------|------------------|------|------|-----------|
| | | Ge(II)→Au | O→Au | P→Au | π(C=P)→Au | Ge(II)→Au | S→Au | P→Au | π(C=P)→Au |
| H | Me | 0.0 | 27.4 | 0.5 | 2.6 | 0.0 | 14.4 | 0.6 | 2.6 |
| | Cl | 0.0 | 27.5 | -0.5 | 0.9 | 0.0 | 13.8 | -0.4 | 0.4 |
| Me | Me | 0.0 | 28.1 | -1.7 | 4.1 | 0.0 | 15.8 | -1.4 | 4.5 |
| | Cl | 0.0 | 28.2 | -2.5 | 2.9 | 0.0 | 15.0 | -2.1 | 2.7 |
| t-Bu | Me | 0.0 | 29.3 | -1.1 | 6.1 | 0.0 | 19.0 | -0.8 | 6.8 |
| | Cl | 0.0 | 29.5 | -2.1 | 4.8 | 0.0 | 18.3 | -1.6 | 5.4 |
| Ph | Me | 0.0 | 28.5 | -2.1 | 6.4 | 0.0 | 16.4 | -1.8 | 6.4 |
| | Cl | 0.0 | 28.5 | -2.8 | 5.4 | 0.0 | 16.5 | -2.4 | 4.8 |
| Mes | Me | 0.0 | 30.4 | 1.0 | 10.7 | 0.0 | 21.4 | 1.0 | 12.6 |
| | Cl | 0.0 | 31.0 | 0.1 | 9.8 | 0.0 | 21.5 | 0.1 | 10.6 |
| Mes* | Me | 0.0 | 29.9 | 6.7 | 23.7 | 0.0 | 14.5 | 5.9 | 26.0 |
| | Cl | 0.0 | 29.0 | 3.9 | 23.4 | 0.0 | 14.5 | 3.7 | 25.4 |

Table S14. Computed relative enthalpies (kcal mol⁻¹) of PCPO-Sn(II)-AuCl and PCPS-Sn(II)-AuCl coordination isomers obtained through Sn(II)→Au, X→Au (X = O or S), P(sp²)→Au and π(C=P)→Au donations. The relative enthalpies are calculated with respect to the coordination isomer displaying Sn(II)→Au bonds.

| R | R' | PCPO-Sn(II)-AuCl | | | | PCPS-Sn(II)-AuCl | | | |
|------|----|------------------|------|-------|-----------|------------------|------|-------|-----------|
| | | Sn(II)→Au | O→Au | P→Au | π(C=P)→Au | Sn(II)→Au | S→Au | P→Au | π(C=P)→Au |
| H | Me | 0.0 | 16.2 | -10.4 | -8.2 | 0.0 | 4.4 | -9.7 | -7.5 |
| | Cl | 0.0 | 16.7 | -11.1 | -9.6 | 0.0 | 4.2 | -10.3 | -9.5 |
| Me | Me | 0.0 | 16.4 | -12.7 | -7.0 | 0.0 | 5.6 | -11.6 | -5.8 |
| | Cl | 0.0 | 17.0 | -13.3 | -8.0 | 0.0 | 5.1 | -12.1 | -7.4 |
| t-Bu | Me | 0.0 | 17.8 | -11.8 | -4.9 | 0.0 | 9.5 | -10.9 | -3.4 |
| | Cl | 0.0 | 18.5 | -12.5 | -6.0 | 0.0 | 8.9 | -11.6 | -4.9 |
| Ph | Me | 0.0 | 16.8 | -12.7 | -5.1 | 0.0 | 6.9 | -11.5 | -4.2 |
| | Cl | 0.0 | 17.2 | -13.3 | -5.9 | 0.0 | 6.5 | -12.0 | -5.6 |
| Mes | Me | 0.0 | 18.6 | -9.5 | -0.7 | 0.0 | 10.3 | -7.4 | 1.9 |
| | Cl | 0.0 | 19.5 | -10.4 | -1.5 | 0.0 | 9.4 | -9.8 | -1.0 |
| Mes* | Me | 0.0 | 18.2 | -4.2 | 12.4 | 0.0 | 4.4 | -4.2 | 15.5 |
| | Cl | 0.0 | 18.4 | -6.1 | 13.3 | 0.0 | 5.1 | -5.9 | 15.4 |

Table S15. Computed relative enthalpies (kcal mol⁻¹) of PCPO-Pb(II)-AuCl and PCPS-Pb(II)-AuCl coordination isomers obtained through Pb(II)→Au, X→Au (X = O or S), P(sp²)→Au and π(C=P)→Au donations. The relative enthalpies are calculated with respect to the coordination isomer displaying Pb(II)→Au bonds.

| R | R' | PCPO-Pb(II)-AuCl | | | | PCPS-Pb(II)-AuCl | | | |
|------|----|------------------|------|-------|-----------|------------------|-------|-------|-----------|
| | | Pb(II)→Au | O→Au | P→Au | π(C=P)→Au | Pb(II)→Au | S→Au | P→Au | π(C=P)→Au |
| H | Me | 0.0 | -1.2 | -26.8 | -24.9 | 0.0 | -12.1 | -25.8 | -24.0 |
| | Cl | 0.0 | -0.2 | -27.1 | -26.0 | 0.0 | -12.0 | -26.2 | -25.8 |
| Me | Me | 0.0 | -1.3 | -29.2 | -24.0 | 0.0 | -11.4 | -27.9 | -22.8 |
| | Cl | 0.0 | -0.3 | -29.5 | -24.8 | 0.0 | -11.6 | -28.2 | -24.3 |
| t-Bu | Me | 0.0 | -0.6 | -28.7 | -22.3 | 0.0 | -7.9 | -27.8 | -20.8 |
| | Cl | 0.0 | 0.7 | -28.9 | -22.9 | 0.0 | -8.8 | -28.3 | -22.2 |
| Ph | Me | 0.0 | -1.0 | -28.9 | -22.3 | 0.0 | -10.2 | -27.7 | -21.3 |
| | Cl | 0.0 | -0.2 | -29.3 | -22.9 | 0.0 | -10.3 | -28.1 | -22.6 |
| Mes | Me | 0.0 | 0.6 | -26.1 | -17.8 | 0.0 | -8.7 | -25.7 | -16.6 |
| | Cl | 0.0 | 1.7 | -26.7 | -18.5 | 0.0 | -8.2 | -26.2 | -18.2 |
| Mes* | Me | 0.0 | -0.2 | -21.0 | -5.0 | 0.0 | -13.2 | -21.2 | -2.3 |
| | Cl | 0.0 | 0.7 | -22.7 | -3.5 | 0.0 | -12.1 | -22.8 | -2.2 |

Table S16. Relative energies (kcal mol⁻¹) of the PCPX-E(II)-AuCl complexes formed through the E(II)→Au donations, in which the X→E(II) donations are absent (i.e., geometries are obtained from the equilibrium chelate structures by rotating the σ(P-C) bond of the PCPX-E(II) ligand with 180°). The relative energies are calculated with respect to the complexes involving the chelate PCPX-E(II) ligands.

| X | R | E | | | |
|------|------|------|------|------|------|
| | | Si | Ge | Sn | Pb |
| O | H | 20.3 | 13.7 | 15.9 | 12.2 |
| | Me | 30.7 | 23.6 | 23.7 | 19.0 |
| | t-Bu | 31.5 | 23.8 | 24.4 | 19.7 |
| | Ph | 25.2 | 16.7 | 14.8 | 10.3 |
| | Mes | 24.8 | 17.3 | 14.4 | 9.3 |
| | Mes* | 26.1 | 17.6 | 15.3 | 11.6 |
| | S | H | 19.3 | 14.8 | 17.3 |
| Me | | 26.5 | 24.4 | 26.7 | 22.3 |
| t-Bu | | 27.1 | 24.8 | 26.1 | 22.2 |
| Ph | | 20.0 | 17.3 | 16.0 | 12.6 |
| Mes | | 17.8 | 17.5 | 15.2 | 9.7 |
| Mes* | | 23.1 | 20.4 | 19.0 | 19.0 |

Table S17. Total back-donation $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{Y})$ energy (kcal mol^{-1}) arising from $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{C})$, $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{Cl})$ and $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{X})$ interactions, for several $\{\text{RP}=\text{C}(\text{E}(\text{II})-\text{Cl})-\text{P}(\text{X})(\text{Me})\text{R}\}\text{AuCl}$ model complexes that involve the $\text{E}(\text{II}) \rightarrow \text{Au}$ dative bond.

| E | R' | PCPO-E(II)-AuCl | |
|----|------|------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
| | | $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{Y})$ (Y = C, Cl or O) (kcal/mol) | $d(\text{Au}) \rightarrow \sigma^*(\text{E}-\text{Y})$ (Y = C, Cl or S) (kcal/mol) |
| Si | Me | 21.0 | 15.5 |
| | Mes* | 18.0 | 12.9 |
| Ge | Me | 16.5 | 12.8 |
| | Mes* | 15.0 | 11.2 |
| Sn | Me | 12.8 | 10.5 |
| | Mes* | 10.9 | 8.9 |
| Pb | Me | 9.4 | 7.8 |
| | Mes* | 9.2 | 7.9 |

Table S18. Calculated EDA parameters (kcal mol^{-1}) for several model $\{\text{RP}=\text{C}(\text{Si}(\text{II})-\text{Cl})-\text{P}(\text{X})(\text{Me})\text{R}\}\text{AuCl}$ model complexes (R = Me or Mes*; X = O or S).

| R | coord.mode | Total int. energy | Electrostatic Int. | Exchange-Rep. | Exchange Int. | Repulsion | Orbital Relaxation |
|-------------------------|------------------------------------------------|-------------------|--------------------|---------------|---------------|-----------|--------------------|
| PCPO-Si(II)-AuCl | | | | | | | |
| Me | Si(II)→Au | -81.0 | -84.1 | 143.8 | -85.3 | 229.0 | -123.1 |
| | O→Au | -29.7 | -41.2 | 59.8 | -31.3 | 91.1 | -37.7 |
| | P→Au | -62.2 | -74.9 | 138.1 | -77.4 | 215.5 | -106.8 |
| | $\pi(\text{C}=\text{P}) \rightarrow \text{Au}$ | -57.8 | -75.7 | 154.3 | -82.4 | 236.7 | -110.3 |
| Mes* | Si(II)→Au | -88.4 | -93.1 | 154.4 | -91.6 | 245.9 | -129.2 |
| | O→Au | -32.9 | -45.0 | 65.7 | -34.8 | 100.5 | -39.7 |
| | P→Au | -60.9 | -76.8 | 144.2 | -80.8 | 225.0 | -105.0 |
| | $\pi(\text{C}=\text{P}) \rightarrow \text{Au}$ | -57.9 | -102.4 | 201.4 | -109.7 | 311.2 | -119.8 |
| PCPS-Si(II)-AuCl | | | | | | | |
| Me | Si(II)→Au | -77.7 | -79.5 | 139.3 | -82.5 | 221.9 | -119.8 |
| | S→Au | -43.2 | -51.5 | 96.8 | -53.4 | 150.3 | -71.8 |
| | P→Au | -61.5 | -74.2 | 138.5 | -77.5 | 215.9 | -106.8 |
| | $\pi(\text{C}=\text{P}) \rightarrow \text{Au}$ | -57.0 | -75.2 | 155.0 | -82.6 | 237.6 | -110.0 |
| Mes* | Si(II)→Au | -84.7 | -87.1 | 147.7 | -87.6 | 235.4 | -124.6 |
| | S→Au | -49.0 | -57.5 | 101.9 | -56.6 | 158.5 | -75.8 |
| | P→Au | -60.8 | -76.6 | 144.2 | -81.0 | 225.1 | -104.8 |
| | $\pi(\text{C}=\text{P}) \rightarrow \text{Au}$ | -54.5 | -93.6 | 189.5 | -102.4 | 291.8 | -113.6 |

Table S19. Calculated EDA parameters (kcal mol⁻¹) for several model {RP=C(Ge(II)-Cl)-P(X)(Me)R}AuCl model complexes (R = Me or Mes*; X = O or S).

| R | coord.mode | Total int. energy | Electrostatic Int. | Exchange-Rep. | Exchange Int. | Repulsion | Orbital Relaxation |
|-------------------------|------------|-------------------|--------------------|---------------|---------------|-----------|--------------------|
| PCPO-Ge(II)-AuCl | | | | | | | |
| Me | Ge(II)→Au | -62.2 | -61.3 | 106.4 | -64.2 | 170.6 | -90.8 |
| | O→Au | -32.1 | -44.2 | 63.0 | -33.0 | 96.0 | -40.0 |
| | P→Au | -62.3 | -74.8 | 138.3 | -77.4 | 215.7 | -107.0 |
| | π(C=P)→Au | -59.0 | -77.1 | 155.0 | -83.0 | 238.1 | -111.1 |
| Mes* | Ge(II)→Au | -67.8 | -68.2 | 113.2 | -68.6 | 181.9 | -94.2 |
| | O→Au | -35.5 | -48.1 | 68.9 | -36.4 | 105.3 | -42.2 |
| | P→Au | -57.0 | -89.0 | 177.0 | -95.6 | 272.6 | -111.0 |
| | π(C=P)→Au | -55.0 | -87.8 | 178.6 | -95.8 | 274.4 | -111.6 |
| PCPS-Ge(II)-AuCl | | | | | | | |
| Me | Ge(II)→Au | -61.4 | -59.2 | 104.7 | -63.0 | 167.7 | -90.1 |
| | S→Au | -43.6 | -52.2 | 97.6 | -53.9 | 151.5 | -72.4 |
| | P→Au | -61.6 | -74.2 | 138.6 | -77.6 | 216.2 | -106.9 |
| | π(C=P)→Au | -57.9 | -76.3 | 155.7 | -83.0 | 238.7 | -110.9 |
| Mes* | Ge(II)→Au | -66.8 | -65.6 | 111.2 | -67.2 | 178.4 | -93.3 |
| | S→Au | -49.7 | -58.3 | 102.7 | -57.1 | 159.8 | -76.4 |
| | P→Au | -60.8 | -76.2 | 143.6 | -80.7 | 224.2 | -104.7 |
| | π(C=P)→Au | -53.5 | -88.0 | 180.9 | -96.8 | 277.7 | -111.3 |

Table S20. Calculated EDA parameters (kcal mol⁻¹) for several model {RP=C(Sn(II)-Cl)-P(X)(Me)R}AuCl model complexes (R = Me or Mes*; X = O or S).

| R | coord.mode | Total int. energy | Electrostatic Int. | Exchange-Rep. | Exchange Int. | Repulsion | Orbital Relaxation |
|-------------------------|------------|-------------------|--------------------|---------------|---------------|-----------|--------------------|
| PCPO-Sn(II)-AuCl | | | | | | | |
| Me | Sn(II)→Au | -50.6 | -43.0 | 82.1 | -52.1 | 134.2 | -74.8 |
| | O→Au | -33.2 | -45.8 | 64.5 | -33.9 | 98.4 | -40.7 |
| | P→Au | -62.9 | -75.3 | 138.6 | -77.7 | 216.2 | -107.2 |
| | π(C=P)→Au | -59.5 | -77.8 | 154.6 | -83.1 | 237.7 | -110.4 |
| Mes* | Sn(II)→Au | -55.9 | -48.4 | 87.6 | -55.7 | 143.3 | -78.4 |
| | O→Au | -36.7 | -49.9 | 70.8 | -37.5 | 108.3 | -43.3 |
| | P→Au | -60.8 | -76.0 | 142.8 | -80.2 | 222.9 | -104.6 |
| | π(C=P)→Au | -55.7 | -88.0 | 177.4 | -95.6 | 273.0 | -110.9 |
| PCPS-Sn(II)-AuCl | | | | | | | |
| Me | Sn(II)→Au | -50.8 | -42.3 | 81.3 | -51.5 | 132.8 | -74.8 |
| | S→Au | -44.0 | -52.6 | 97.6 | -54.0 | 151.6 | -72.3 |
| | P→Au | -61.9 | -74.6 | 139.0 | -77.8 | 216.8 | -107.1 |
| | π(C=P)→Au | -58.3 | -76.8 | 155.3 | -83.1 | 238.4 | -110.3 |
| Mes* | Sn(II)→Au | -56.0 | -47.8 | 87.0 | -55.2 | 142.2 | -78.0 |
| | S→Au | -50.3 | -58.8 | 102.8 | -57.3 | 160.1 | -76.3 |
| | P→Au | -60.9 | -75.9 | 143.1 | -80.4 | 223.5 | -104.6 |
| | π(C=P)→Au | -54.2 | -87.6 | 178.7 | -96.2 | 275.0 | -110.3 |

Table S21. Calculated EDA parameters (kcal mol⁻¹) for several model {RP=C(Pb(II)-Cl)-P(X)(Me)R}AuCl model complexes (R = Me or Mes*; X = O or S).

| R | coord.mode | Total int. energy | Electrostatic Int. | Exchange-Rep. | Exchange Int. | Repulsion | Orbital Relaxation |
|-------------------------|------------|-------------------|--------------------|---------------|---------------|-----------|--------------------|
| PCPO-Pb(II)-AuCl | | | | | | | |
| Me | Pb(II)→Au | -33.7 | -24.1 | 58.7 | -36.6 | 95.4 | -55.8 |
| | O→Au | -34.8 | -47.6 | 66.0 | -34.7 | 100.7 | -41.9 |
| | P→Au | -63.3 | -75.5 | 138.3 | -77.6 | 215.9 | -107.1 |
| | π(C=P)→Au | -60.2 | -78.9 | 154.8 | -83.5 | 238.2 | -110.2 |
| Mes* | Pb(II)→Au | -38.1 | -27.7 | 62.3 | -39.0 | 101.3 | -58.7 |
| | O→Au | -38.6 | -52.0 | 72.6 | -38.5 | 111.0 | -44.9 |
| | P→Au | -61.0 | -75.8 | 142.2 | -79.9 | 222.1 | -104.4 |
| | π(C=P)→Au | -57.0 | -89.0 | 177.0 | -95.6 | 272.6 | -111.0 |
| PCPS-Pb(II)-AuCl | | | | | | | |
| Me | Pb(II)→Au | -33.8 | -23.6 | 58.0 | -36.1 | 94.2 | -55.7 |
| | S→Au | -45.0 | -53.7 | 98.4 | -54.5 | 152.8 | -72.8 |
| | P→Au | -62.2 | -74.7 | 138.7 | -77.7 | 216.3 | -106.9 |
| | π(C=P)→Au | -59.1 | -78.0 | 155.6 | -83.5 | 239.1 | -110.3 |
| Mes* | Pb(II)→Au | -38.1 | -27.5 | 61.9 | -38.7 | 100.6 | -58.0 |
| | S→Au | -51.4 | -59.6 | 103.2 | -57.7 | 160.8 | -76.8 |
| | P→Au | -61.1 | -75.7 | 142.3 | -80.1 | 222.4 | -104.4 |
| | π(C=P)→Au | -55.5 | -88.1 | 177.5 | -95.6 | 273.1 | -110.3 |

xyz coordinates

PCPX model systems 24

R-P=C(Cl)-P(O)ClR.....

R = H 24

R = Me 24

R = *t*-Bu 24

R = Ph 24

R = Mes 24

R = Mes* 25

R-P=C(Cl)-P(O)MeR.....

R = H 26

R = Me 26

R = *t*-Bu 26

R = Ph 26

R = Mes 26

R = Mes* 27

R-P=C(Cl)-P(S)ClR.....

R = H 28

R = Me 28

R = *t*-Bu 28

R = Ph 28

R = Mes 28

R = Mes* 29

R-P=C(Cl)-P(S)MeR.....

R = H 29

R = Me 30

R = *t*-Bu 30

R = Ph 30

R = Mes 30

R = Mes* 31

PCPX-E(II) model systems 31

E = Si(II).....

R-P=C(Si(II)Cl)-P(O)ClR 31

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes.....

R = Mes*.....

R-P=C(Si(II)Cl)-P(O)MeR34

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes.....

R = Mes*.....

R-P=C(Si(II)Cl)-P(S)ClR 36

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes*.....

R-P=C(Si(II)Cl)-P(S)MeR 37

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes.....

R = Mes*.....

E = Ge(II).....

R-P=C(Ge(II)Cl)-P(O)ClR 39

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes.....

R = Mes*.....

R-P=C(Ge(II)Cl)-P(O)MeR 42

R = H.....

R = Me.....

R = *t*-Bu.....

R = Ph.....

R = Mes.....

R = Mes*.....

| | | | |
|-------------------------|----|---------------------------------------|-------|
| R-P=C(Ge(II)Cl)-P(S)ClR | 44 | R = Ph..... | |
| R = H..... | | R = Mes..... | 44 |
| R = Me..... | | R = Mes*..... | 44 |
| R = <i>t</i> -Bu..... | | R-P=C(Pb.(II)Cl)-P(O)ClR56..... | 44 |
| R = Ph..... | | R = H..... | 44 |
| R = Mes..... | | R = Me..... | 44 |
| R = Mes*..... | | R = <i>t</i> -Bu..... | 45 |
| R-P=C(Ge(II)Cl)-P(S)MeR | 45 | R = Ph..... | |
| R = H..... | | R = Mes..... | 45 |
| R = Me..... | | R = Mes*..... | 46 |
| R = <i>t</i> -Bu..... | | R-P=C(Pb.(II)Cl)-P(O)MeR..... | 58 46 |
| R = Ph..... | | R = H..... | 46 |
| R = Mes..... | | R = Me..... | 46 |
| R = Mes*..... | | R = <i>t</i> -Bu..... | 47 |
| E = Sn (II)..... | | R = Ph..... | 48 |
| R-P=C(Sn(II)Cl)-P(O)ClR | 48 | R = Mes..... | |
| R = H..... | | R = Mes*..... | 48 |
| R = Me..... | | R-P=C(Pb.(II)Cl)-P(S)ClR 60..... | 48 |
| R = <i>t</i> -Bu..... | | R = H..... | 48 |
| R = Ph..... | | R = Me..... | 48 |
| R = Mes..... | | R = <i>t</i> -Bu..... | 48 |
| R = Mes*..... | | R = Ph..... | 49 |
| R-P=C(Sn(II)Cl)-P(O)MeR | 50 | R = Mes..... | |
| R = H..... | | R = Mes*..... | 50 |
| R = Me..... | | R-P=C(Pb.(II)Cl)-P(S)MeR..... | 62 50 |
| R = <i>t</i> -Bu..... | | R = H..... | 50 |
| R = Ph..... | | R = Me..... | 50 |
| R = Mes..... | | R = <i>t</i> -Bu..... | 51 |
| R = Mes*..... | | R = Ph..... | 51 |
| R-P=C(Sn(II)Cl)-P(S)ClR | 52 | R = Mes..... | |
| R = H..... | | R = Mes*..... | 52 |
| R = Me..... | | PCPX-E(II)-AuCl model systems..... | 64 52 |
| R = <i>t</i> -Bu..... | | E = Si(II)..... | 52 |
| R = Ph..... | | [R-P=C(Si(II)Cl)-P(O)ClR](AuCl)..... | 64 52 |
| R = Mes..... | | Coordination through Si(II) atom..... | 53 |
| R = Mes*..... | | R = H..... | 53 |
| R-P=C(Sn(II)Cl)-P(S)MeR | 54 | R = Me..... | |
| R = H..... | | R = <i>t</i> -Bu..... | 54 |
| R = Me..... | | R = Ph..... | 54 |
| R = <i>t</i> -Bu..... | | R = Mes..... | 54 |

| | | |
|----------------------------------------------------|----------------------------------------------------|----|
| R = Mes * | R = <i>t</i> -Bu | 65 |
| Coordination through O atom | R = Ph | 66 |
| R = H | R = Mes | 66 |
| R = Me | R = Mes* | 66 |
| R = <i>t</i> -Bu | Coordination through $\pi(\text{C}=\text{P})$ bond | 67 |
| R = Ph | R = H | 67 |
| R = Mes | R = Me | 67 |
| R = Mes* | R = <i>t</i> -Bu | 67 |
| Coordination through P (sp^2) atom | R = Ph | 68 |
| R = H | R = Mes | 68 |
| R = Me | R = Mes* | 68 |
| R = <i>t</i> -Bu | [R-P=C(Si(II)Cl)-P(S)ClR](AuCl) | 81 |
| R = Ph | Coordination through Si(II) atom | 69 |
| R = Mes | R = H | 69 |
| R = Mes* | R = Me | 69 |
| Coordination through $\pi(\text{C}=\text{P})$ bond | R = <i>t</i> -Bu | 70 |
| R = H | R = Ph | 70 |
| R = Me | R = Mes | 70 |
| R = <i>t</i> -Bu | R = Mes* | 70 |
| R = Ph | Coordination through S atom | 71 |
| R = Mes | R = H | 71 |
| R = Mes* | R = Me | 71 |
| [R-P=C(Si(II)Cl)-P(O)MeR](AuCl) 72 | R = <i>t</i> -Bu | |
| Coordination through Si(II) atom | R = Ph | 72 |
| R = H | R = Mes | 72 |
| R = Me | R = Mes* | 72 |
| R = <i>t</i> -Bu | Coordination through P(sp^2) atom | 72 |
| R = Ph | R = H | 73 |
| R = Mes | R = Me | 73 |
| R = Mes* | R = <i>t</i> -Bu | 73 |
| Coordination through O atom 74 | R = Ph | |
| R = H | R = Mes | 74 |
| R = Me | R = Mes* | 74 |
| R = <i>t</i> -Bu | Coordination through $\pi(\text{C}=\text{P})$ bond | 75 |
| R = Ph | R = H | 75 |
| R = Mes | R = Me | 75 |
| R = Mes* | R = <i>t</i> -Bu | 76 |
| Coordination through P(sp^2) atom | R = Ph | 76 |
| R = H | R = Mes | 76 |
| R = Me | R = Mes* | 77 |

| | | | | |
|-----------------------------------------------|----|-----------------------------------------------|-------|-----|
| [R-P=C(Si(II)Cl)-P(S)MeR](AuCl) | 89 | R = H | | 89 |
| Coordination through Si(II) atom | | R = Me | | 89 |
| R = H | | R = <i>t</i> -Bu | | 89 |
| R = Me | | R = Ph | | 89 |
| R = <i>t</i> -Bu | | R = Mes | | 89 |
| R = Ph | | R = Mes* | | 90 |
| R = Mes | | Coordination through P(sp ²) atom | | 90 |
| R = Mes* | | R = H | | 90 |
| Coordination through S atom | | R = Me | | 91 |
| R = H | | R = <i>t</i> -Bu | | 91 |
| R = Me | | R = Ph | | 91 |
| R = <i>t</i> -Bu | | R = Mes | | 91 |
| R = Ph | | R = Mes* | | 92 |
| R = Mes | | Coordination through π(C=P) bond | | 92 |
| R = Mes* | | R = H | | 92 |
| Coordination through P(sp ²) atom | | R = Me | | 93 |
| R = H | | R = <i>t</i> -Bu | | 93 |
| R = Me | | R = Ph | | 93 |
| R = <i>t</i> -Bu | | R = Mes | | 93 |
| R = Ph | | R = Mes* | | 94 |
| R = Mes | | [R-P=C(Ge(II)Cl)-P(O)MeR](AuCl) | 106 | 94 |
| R = Mes* | | Coordination through Ge(II) atom | | 94 |
| Coordination through π(C=P) bond | | R = H | | 96 |
| R = H | | R = Me | | 96 |
| R = Me | | R = <i>t</i> -Bu | | 96 |
| R = <i>t</i> -Bu | | R = Ph | | 96 |
| R = Ph | | R = Mes | | 96 |
| R = Mes | | R = Mes* | | 96 |
| R = Mes* | | Coordination through O atom | | 97 |
| PCPX-E(II)-AuCl model systems | 98 | R = H | | 98 |
| E = Ge(II) | | R = Me | | 98 |
| [R-P=C(Ge(II)Cl)-P(O)CIR](AuCl) | 98 | R = <i>t</i> -Bu | | 98 |
| Coordination through Ge(II) atom | | R = Ph | | 98 |
| R = H | | R = Mes | | 98 |
| R = Me | | R = Mes* | | 98 |
| R = <i>t</i> -Bu | | Coordination through P(sp ²) atom | | 98 |
| R = Ph | | R = H | | 98 |
| R = Mes | | R = Me | | 98 |
| R = Mes* | | R = <i>t</i> -Bu | | 99 |
| Coordination through O atom | | R = Ph | | 100 |

| | | |
|----------------------------------------------------------|----------------------------------------------------------|-----|
| R = Mes | R = H | 111 |
| R = Mes* | R = Me | 111 |
| Coordination through $\pi(\text{C}=\text{P})$ bond | R = <i>t</i> -Bu | 112 |
| R = H | R = Ph | 112 |
| R = Me | R = Mes | 112 |
| R = <i>t</i> -Bu | R = Mes* | 112 |
| R = Ph | Coordination through S atom | 113 |
| R = Mes | R = H | 113 |
| R = Mes* | R = Me | 113 |
| [R-P=C(Ge(II)Cl)-P(S)ClR](AuCl) 114 | R = <i>t</i> -Bu | |
| Coordination through Ge(II) atom | R = Ph | 114 |
| R = H | R = Mes | 114 |
| R = Me | R = Mes* | 114 |
| R = <i>t</i> -Bu | Coordination through P(sp ²) atom | 114 |
| R = Ph | R = H | 115 |
| R = Mes | R = Me | 115 |
| R = Mes* | R = <i>t</i> -Bu | 115 |
| Coordination through S atom | R = Ph | 116 |
| R = H | R = Mes | 116 |
| R = Me | R = Mes* | 116 |
| R = <i>t</i> -Bu | Coordination through $\pi(\text{C}=\text{P})$ bond | 116 |
| R = Ph | R = H | 117 |
| R = Mes | R = Me | 117 |
| R = Mes* | R = <i>t</i> -Bu | 117 |
| Coordination through P(sp ²) atom | R = Ph | 118 |
| R = H | R = Mes | 118 |
| R = Me | R = Mes* | 118 |
| R = <i>t</i> -Bu | E = Sn(II) | 118 |
| R = Ph | [R-P=C(Sn(II)Cl)-P(O)ClR](AuCl) ... 131 | 119 |
| R = Mes | Coordination through Sn(II) atom | 119 |
| R = Mes* | R = H | 119 |
| Coordination through $\pi(\text{C}=\text{P})$ bond | R = Me | 120 |
| R = H | R = <i>t</i> -Bu | 120 |
| R = Me | R = Ph | 120 |
| R = <i>t</i> -Bu | R = Mes | 120 |
| R = Ph | R = Mes* | 121 |
| R = Mes | Coordination through O atom | 121 |
| R = Mes* | R = H | 121 |
| [R-P=C(Ge(II)Cl)-P(S)MeR](AuCl) 122 | R = Me | |
| Coordination through Ge(II) atom | R = <i>t</i> -Bu | 122 |

| | | |
|-----------------------------------------------|-----------------------------------------------|---------|
| R = Ph | R = H | 133 |
| R = Mes | R = Me | 133 |
| R = Mes* | R = <i>t</i> -Bu | 134 |
| Coordination through P(sp ²) atom | R = Ph | 135 |
| R = H | R = Mes | 135 |
| R = Me | R = Mes* | 135 |
| R = <i>t</i> -Bu | [R-P=C(Sn(II)Cl)-P(S)ClR](AuCl) | 147 135 |
| R = Ph | Coordination through Sn(II) atom | 135 |
| R = Mes | R = H | 135 |
| R = Mes* | R = Me | 136 |
| Coordination through π(C=P) bond | R = <i>t</i> -Bu | 137 |
| R = H | R = Ph | 137 |
| R = Me | R = Mes | 137 |
| R = <i>t</i> -Bu | R = Mes* | 137 |
| R = Ph | Coordination through S atom | 137 |
| R = Mes | R = H | 137 |
| R = Mes* | R = Me | 138 |
| [R-P=C(Sn(II)Cl)-P(O)MeR](AuCl) 139 | R = <i>t</i> -Bu | |
| Coordination through Sn(II) atom | R = Ph | 139 |
| R = H | R = Mes | 139 |
| R = Me | R = Mes* | 139 |
| R = <i>t</i> -Bu | Coordination through P(sp ²) atom | 139 |
| R = Ph | R = H | 139 |
| R = Mes | R = Me | 139 |
| R = Mes* | R = <i>t</i> -Bu | 140 |
| Coordination through O atom | R = Ph | 141 |
| R = H | R = Mes | 141 |
| R = Me | R = Mes* | 141 |
| R = <i>t</i> -Bu | Coordination through π(C=P) bond | 141 |
| R = Ph | R = H | 141 |
| R = Mes | R = Me | 142 |
| R = Mes* | R = <i>t</i> -Bu | 142 |
| Coordination through P(sp ²) atom | R = Ph | 143 |
| R = H | R = Mes | 143 |
| R = Me | R = Mes* | 143 |
| R = <i>t</i> -Bu | [R-P=C(Sn(II)Cl)-P(S)MeR](AuCl) 155 | 143 |
| R = Ph | Coordination through Sn(II) atom | 143 |
| R = Mes | R = H | 144 |
| R = Mes* | R = Me | 144 |
| Coordination through π(C=P) bond | R = <i>t</i> -Bu | 145 |

| | | |
|----------------------------------------------------|----------------------------------------------------|-----|
| R = Ph | R = H | 156 |
| R = Mes | R = Me | 156 |
| R = Mes* | R = <i>t</i> -Bu | 156 |
| Coordination through S atom | R = Ph | 157 |
| R = H | R = Mes | 157 |
| R = Me | R = Mes* | 157 |
| R = <i>t</i> -Bu | Coordination through $\pi(\text{C}=\text{P})$ bond | 157 |
| R = Ph | R = H | 158 |
| R = Mes | R = Me | 158 |
| R = Mes* | R = <i>t</i> -Bu | 158 |
| Coordination through P(sp ²) atom | R = Ph | 159 |
| R = H | R = Mes | 159 |
| R = Me | R = Mes* | 159 |
| R = <i>t</i> -Bu | [R-P=C(Pb(II)Cl)-P(O)MeR](AuCl) 172 | 160 |
| R = Ph | Coordination through Pb(II) atom | 160 |
| R = Mes | R = H | 160 |
| R = Mes* | R = Me | 161 |
| Coordination through $\pi(\text{C}=\text{P})$ bond | R = <i>t</i> -Bu | 161 |
| R = H | R = Ph | 161 |
| R = Me | R = Mes | 161 |
| R = <i>t</i> -Bu | R = Mes* | 162 |
| R = Ph | Coordination through O atom | 162 |
| R = Mes | R = H | 162 |
| R = Mes* | R = Me | 163 |
| [R-P=C(Pb(II)Cl)-P(O)CIR](AuCl) 164 | R = <i>t</i> -Bu | |
| Coordination through Pb(II) atom | R = Ph | 164 |
| R = H | R = Mes | 164 |
| R = Me | R = Mes* | 164 |
| R = <i>t</i> -Bu | Coordination through P(sp ²) atom | 164 |
| R = Ph | R = H | 164 |
| R = Mes | R = Me | 164 |
| R = Mes* | R = <i>t</i> -Bu | 165 |
| Coordination through O atom | R = Ph | 166 |
| R = H | R = Mes | 166 |
| R = Me | R = Mes* | 166 |
| R = <i>t</i> -Bu | Coordination through $\pi(\text{C}=\text{P})$ bond | 166 |
| R = Ph | R = H | 166 |
| R = Mes | R = Me | 166 |
| R = Mes* | R = <i>t</i> -Bu | 167 |
| Coordination through P(sp ²) atom | R = Ph | 168 |

| | | |
|-----------------------------------------------------|-----------------------------------------------------|-----|
| R = Mes | R = Mes* | 179 |
| R = Mes* | [R-P=C(Pb(II)Cl)-P(S)MeR](AuCl) | 179 |
| [R-P=C(Pb(II)Cl)-P(S)ClR](AuCl) 180 | Coordination through Pb(II) atom | |
| Coordination through Pb(II) atom | R = H | 180 |
| R = H | R = Me | 180 |
| R = Me | R = <i>t</i> -Bu | 180 |
| R = <i>t</i> -Bu | R = Ph | 180 |
| R = Ph | R = Mes | 181 |
| R = Mes | R = Mes* | 181 |
| R = Mes* | Coordination through S atom | 181 |
| Coordination through S atom | R = H | 182 |
| R = H | R = Me | 182 |
| R = Me | R = <i>t</i> -Bu | 182 |
| R = <i>t</i> -Bu | R = Ph | 182 |
| R = Ph | R = Mes | 183 |
| R = Mes | R = Mes* | 183 |
| R = Mes* | Coordination through P(sp ²) atom | 183 |
| Coordination through P(sp ²) atom | R = H | 184 |
| R = H | R = Me | 184 |
| R = Me | R = <i>t</i> -Bu | 184 |
| R = <i>t</i> -Bu | R = Ph | 184 |
| R = Ph | R = Mes | 185 |
| R = Mes | R = Mes* | 185 |
| R = Mes* | Coordination through π(C=P) bond | 185 |
| Coordination through π(C=P) bond | R = H | 186 |
| R = H | R = Me | 186 |
| R = Me | R = <i>t</i> -Bu | 186 |
| R = <i>t</i> -Bu | R = Ph | 186 |
| R = Ph | R = Mes | 187 |
| R = Mes | R = Mes* | 187 |

PCPX model systems

R-P=C(Cl)-P(O)CIR

R= H

| | | | |
|----|----------|----------|----------|
| P | 1.79405 | 0.09029 | -2.25367 |
| C | 0.31215 | -0.02845 | -1.48610 |
| P | -1.04264 | -0.75902 | -2.42456 |
| Cl | -0.09833 | 0.41754 | 0.11870 |
| O | -0.65622 | -1.31089 | -3.72351 |
| Cl | -2.43636 | 0.70450 | -2.48890 |
| H | 2.46714 | 0.68669 | -1.14569 |
| H | -1.65784 | -1.63561 | -1.50952 |

R= Me

| | | | |
|----|----------|----------|----------|
| P | 1.77770 | 0.04145 | -2.18154 |
| C | 0.27617 | -0.02102 | -1.44367 |
| P | -1.05425 | -0.77986 | -2.39304 |
| Cl | -0.12714 | 0.54600 | 0.13283 |
| O | -0.62108 | -1.23927 | -3.71641 |
| C | -1.82992 | -2.02023 | -1.35494 |
| H | -2.11693 | -1.60938 | -0.38776 |
| H | -2.71261 | -2.38967 | -1.87876 |
| H | -1.11927 | -2.83833 | -1.22257 |
| C | 2.81082 | 0.86042 | -0.90554 |
| H | 2.82660 | 0.27547 | 0.01723 |
| H | 3.82783 | 0.95642 | -1.28691 |
| H | 2.41973 | 1.85301 | -0.66912 |
| Cl | -2.46933 | 0.68703 | -2.45700 |

R= t-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.16488 | -1.27309 | -0.56412 |
| C | 0.59535 | -0.01290 | -1.51112 |
| P | -0.98752 | -0.39204 | -2.31823 |
| Cl | 1.27291 | 1.54587 | -1.81101 |
| O | -1.60410 | -1.60355 | -1.75911 |
| C | 2.79754 | -0.77278 | 0.21508 |
| C | -0.81468 | -0.46707 | -4.15116 |
| C | 3.19493 | -2.00439 | 1.03587 |
| H | 3.31943 | -2.88879 | 0.40514 |
| H | 4.14619 | -1.81511 | 1.54263 |
| H | 2.44823 | -2.24089 | 1.79862 |
| C | 3.87046 | -0.51008 | -0.83869 |
| H | 3.65473 | 0.37387 | -1.43757 |
| H | 4.83353 | -0.35381 | -0.34007 |
| H | 3.98609 | -1.36313 | -1.51283 |
| C | 2.62332 | 0.41701 | 1.15621 |
| H | 2.36716 | 1.33242 | 0.62442 |
| H | 1.84771 | 0.22612 | 1.90252 |
| H | 3.56204 | 0.58953 | 1.69430 |
| C | -0.27165 | 0.80300 | -4.79466 |
| H | 0.75657 | 1.01001 | -4.49737 |
| H | -0.28498 | 0.67291 | -5.88120 |
| H | -0.88243 | 1.67454 | -4.55408 |
| C | -2.21666 | -0.77153 | -4.68685 |
| H | -2.90149 | 0.06186 | -4.51864 |
| H | -2.14805 | -0.93995 | -5.76554 |
| H | -2.63603 | -1.66432 | -4.22120 |
| C | 0.11373 | -1.65142 | -4.43525 |
| H | 1.12855 | -1.46710 | -4.07566 |
| H | -0.25676 | -2.56832 | -3.97363 |

| | | | |
|----|----------|----------|----------|
| H | 0.16420 | -1.80646 | -5.51687 |
| Cl | -2.08643 | 1.29560 | -1.97265 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 1.06821 | -1.05973 | -0.36084 |
| C | 0.80585 | -0.30830 | -1.83838 |
| P | -0.79193 | -0.69339 | -2.59101 |
| Cl | 1.81880 | 0.76739 | -2.71673 |
| O | -1.60898 | -1.57138 | -1.74487 |
| C | -0.50386 | -1.33437 | -4.24480 |
| C | -0.66944 | -2.71034 | -4.39650 |
| C | -0.12116 | -0.55349 | -5.33284 |
| C | -0.44557 | -3.29986 | -5.63062 |
| H | -0.98924 | -3.30230 | -3.54680 |
| C | 0.10256 | -1.15043 | -6.56237 |
| H | -0.01113 | 0.51805 | -5.22186 |
| C | -0.05710 | -2.52159 | -6.71104 |
| H | -0.58124 | -4.36860 | -5.74910 |
| H | 0.39621 | -0.54213 | -7.40995 |
| H | 0.11509 | -2.98362 | -7.67663 |
| C | 2.73669 | -0.57428 | 0.15890 |
| C | 3.87674 | -0.64990 | -0.64379 |
| C | 2.87740 | -0.22199 | 1.50333 |
| C | 5.12195 | -0.35347 | -0.11580 |
| H | 3.79209 | -0.95008 | -1.68073 |
| C | 4.12177 | 0.09849 | 2.02221 |
| H | 2.00306 | -0.19423 | 2.14650 |
| C | 5.24580 | 0.03155 | 1.21269 |
| H | 6.00202 | -0.42130 | -0.74521 |
| H | 4.21466 | 0.38806 | 3.06257 |
| H | 6.22225 | 0.26896 | 1.61931 |
| Cl | -1.59855 | 1.14800 | -2.90187 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.64974 | -1.72979 | -1.07216 |
| C | 0.86245 | -0.53173 | -1.94196 |
| P | -0.77366 | -0.88482 | -2.64264 |
| Cl | 1.31459 | 1.11891 | -2.06143 |
| O | -1.82859 | -0.17986 | -1.90401 |
| C | 3.05446 | -0.86528 | -0.30122 |
| C | 4.32397 | -0.96292 | -0.88336 |
| C | 2.88031 | -0.19781 | 0.92006 |
| C | 5.40517 | -0.37731 | -0.23579 |
| C | 3.98942 | 0.37033 | 1.53150 |
| C | 5.26004 | 0.29134 | 0.97234 |
| H | 6.38887 | -0.44623 | -0.69122 |
| H | 3.85592 | 0.89113 | 2.47542 |
| C | -0.94608 | -2.67638 | -2.79894 |
| C | -1.93266 | -3.32061 | -2.01589 |
| C | -0.13058 | -3.43693 | -3.66485 |
| C | -2.07935 | -4.69736 | -2.13987 |
| C | -0.32644 | -4.80960 | -3.73628 |
| C | -1.29906 | -5.46089 | -2.99388 |
| H | -2.83365 | -5.18876 | -1.53340 |
| H | 0.31255 | -5.38820 | -4.39654 |
| C | 4.52321 | -1.65336 | -2.19950 |
| H | 4.03723 | -2.63440 | -2.21970 |
| H | 4.09676 | -1.06788 | -3.01972 |
| H | 5.58361 | -1.79967 | -2.40928 |
| C | 1.52881 | -0.07976 | 1.55787 |
| H | 0.85442 | 0.52986 | 0.94985 |

| | | | |
|----|----------|----------|----------|
| H | 1.05338 | -1.05824 | 1.67895 |
| H | 1.60241 | 0.38035 | 2.54393 |
| C | 6.44284 | 0.88843 | 1.67169 |
| H | 6.81097 | 0.21819 | 2.45480 |
| H | 7.26636 | 1.06824 | 0.97884 |
| H | 6.18501 | 1.83527 | 2.15057 |
| C | -1.51003 | -6.93705 | -3.12115 |
| H | -1.89035 | -7.36671 | -2.19288 |
| H | -2.24186 | -7.15359 | -3.90580 |
| H | -0.58461 | -7.45080 | -3.38716 |
| C | 0.94942 | -2.87451 | -4.54502 |
| H | 0.53495 | -2.53299 | -5.49642 |
| H | 1.47447 | -2.03081 | -4.10149 |
| H | 1.68311 | -3.65256 | -4.76165 |
| C | -2.83943 | -2.63211 | -1.03583 |
| H | -2.28245 | -2.06416 | -0.29014 |
| H | -3.49693 | -1.91451 | -1.52602 |
| H | -3.44833 | -3.37782 | -0.52338 |
| Cl | -0.66768 | -0.15822 | -4.54839 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 2.29541 | -1.92892 | -0.69160 |
| C | 1.33217 | -1.01845 | -1.71583 |
| P | -0.25305 | -1.61620 | -2.42336 |
| Cl | 1.51248 | 0.67005 | -2.00997 |
| O | -1.34611 | -0.90380 | -1.74264 |
| C | 3.51219 | -0.73546 | 0.01625 |
| C | 4.76688 | -0.52942 | -0.60954 |
| C | 3.19276 | -0.01400 | 1.20091 |
| C | 5.57995 | 0.49855 | -0.13356 |
| C | 4.06079 | 0.99263 | 1.60229 |
| C | 5.23782 | 1.30085 | 0.93774 |
| H | 6.52224 | 0.67651 | -0.62489 |
| H | 3.81316 | 1.56505 | 2.48338 |
| C | -0.65204 | -3.39253 | -2.66553 |
| C | -1.78556 | -3.83160 | -1.91852 |
| C | -0.32440 | -4.09761 | -3.86406 |
| C | -2.70574 | -4.65972 | -2.55825 |
| C | -1.28704 | -4.93192 | -4.41109 |
| C | -2.52806 | -5.15729 | -3.83409 |
| H | -3.60576 | -4.91647 | -2.01980 |
| H | -1.05363 | -5.43065 | -5.34273 |
| C | 5.32016 | -1.35948 | -1.78740 |
| C | 1.96817 | -0.27992 | 2.10358 |
| C | 6.11043 | 2.45357 | 1.42477 |
| C | -3.58224 | -5.97800 | -4.56608 |
| C | 1.04292 | -4.18044 | -4.57807 |
| C | -2.09136 | -3.59526 | -0.42158 |
| C | 4.64884 | -0.93789 | -3.09783 |
| H | 3.57245 | -1.09057 | -3.07806 |
| H | 4.83188 | 0.12077 | -3.29516 |
| H | 5.05788 | -1.51586 | -3.93180 |
| C | 6.82817 | -1.15183 | -1.98188 |
| H | 7.07377 | -0.14459 | -2.32425 |
| H | 7.39370 | -1.35895 | -1.07014 |
| H | 7.17548 | -1.84189 | -2.75428 |
| C | 5.15036 | -2.86208 | -1.54237 |
| H | 5.63999 | -3.16117 | -0.61227 |
| H | 4.10762 | -3.18283 | -1.48465 |
| C | 0.68821 | 0.29822 | 1.49011 |
| H | 0.79277 | 1.37485 | 1.33798 |

| | | | |
|----|----------|----------|----------|
| H | 0.43235 | -0.14638 | 0.53142 |
| H | -0.15408 | 0.13263 | 2.16797 |
| C | 2.12029 | 0.37891 | 3.48147 |
| H | 3.04437 | 0.08035 | 3.98265 |
| H | 2.08450 | 1.46925 | 3.43202 |
| H | 1.28323 | 0.06384 | 4.10850 |
| C | 1.81492 | -1.77690 | 2.39028 |
| H | 1.60078 | -2.37378 | 1.50074 |
| H | 2.72180 | -2.17834 | 2.84971 |
| H | 0.98064 | -1.93706 | 3.07821 |
| C | 7.35509 | 2.64475 | 0.56220 |
| H | 7.93333 | 3.49161 | 0.93967 |
| H | 8.00582 | 1.76688 | 0.58423 |
| H | 7.09868 | 2.85744 | -0.47872 |
| C | 5.29574 | 3.75197 | 1.38479 |
| H | 4.96573 | 3.97463 | 0.36721 |
| H | 4.40845 | 3.69284 | 2.01818 |
| H | 5.90370 | 4.58978 | 1.73773 |
| C | 6.56124 | 2.18276 | 2.86508 |
| H | 7.18309 | 3.00658 | 3.22676 |
| H | 5.71183 | 2.08346 | 3.54382 |
| H | 7.14740 | 1.26232 | 2.92419 |
| C | -3.34172 | -2.73154 | -0.23129 |
| H | -4.21182 | -3.17626 | -0.72055 |
| H | -3.56888 | -2.64649 | 0.83557 |
| H | -3.18306 | -1.73428 | -0.63874 |
| C | -2.34624 | -4.98019 | 0.21191 |
| H | -2.48922 | -4.85203 | 1.28786 |
| H | -3.23522 | -5.47777 | -0.17495 |
| H | -1.49244 | -5.64591 | 0.06145 |
| C | -0.93487 | -3.00877 | 0.37833 |
| H | -0.01132 | -3.56566 | 0.20067 |
| H | -0.77213 | -1.95773 | 0.16152 |
| H | -1.16605 | -3.08771 | 1.44372 |
| C | 0.95085 | -3.80867 | -6.06203 |
| H | 1.92930 | -3.94546 | -6.53086 |
| H | 0.23895 | -4.43412 | -6.60317 |
| H | 0.65462 | -2.76816 | -6.19299 |
| C | 1.49158 | -5.65219 | -4.46782 |
| H | 2.47809 | -5.76428 | -4.92635 |
| H | 1.56614 | -5.95847 | -3.42152 |
| H | 0.80886 | -6.33789 | -4.97038 |
| C | 2.15580 | -3.36819 | -3.94150 |
| H | 2.26006 | -3.60634 | -2.88229 |
| H | 3.10107 | -3.61589 | -4.43106 |
| H | 2.01239 | -2.29620 | -4.04995 |
| C | -3.89338 | -5.30176 | -5.90677 |
| H | -3.00466 | -5.22386 | -6.53621 |
| H | -4.64311 | -5.87972 | -6.45424 |
| H | -4.28414 | -4.29297 | -5.75414 |
| C | -3.04827 | -7.39225 | -4.82259 |
| H | -2.14468 | -7.38080 | -5.43542 |
| H | -2.81121 | -7.89737 | -3.88303 |
| H | -3.79977 | -7.98716 | -5.34913 |
| C | -4.88123 | -6.09071 | -3.77276 |
| H | -4.73825 | -6.62198 | -2.82838 |
| H | -5.30878 | -5.10895 | -3.55484 |
| H | -5.61643 | -6.65110 | -4.35525 |
| Cl | -0.15977 | -0.93409 | -4.35504 |
| H | 5.60303 | -3.42295 | -2.36445 |

R-P=C(Cl)-P(O)MeR

R = H

| | | | |
|----|----------|----------|----------|
| P | 1.81869 | 0.09240 | -2.16926 |
| C | 0.30915 | -0.04938 | -1.46467 |
| P | -1.04359 | -0.70280 | -2.48218 |
| Cl | -0.13776 | 0.33233 | 0.15530 |
| O | -0.60076 | -1.16767 | -3.80972 |
| H | 2.46307 | 0.61837 | -1.00869 |
| H | -1.57582 | -1.69304 | -1.61876 |
| C | -2.31618 | 0.56978 | -2.48485 |
| H | -3.19857 | 0.16483 | -2.98378 |
| H | -2.57549 | 0.87559 | -1.47051 |
| H | -1.95047 | 1.42776 | -3.05119 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 1.77521 | 0.03941 | -2.15795 |
| C | 0.26259 | -0.00627 | -1.44631 |
| P | -1.09488 | -0.72326 | -2.41541 |
| Cl | -0.14433 | 0.56673 | 0.13637 |
| O | -0.63639 | -1.17748 | -3.74482 |
| C | -1.77001 | -2.03378 | -1.37427 |
| H | -2.03890 | -1.67148 | -0.38137 |
| H | -2.65474 | -2.44081 | -1.86810 |
| H | -1.02240 | -2.82345 | -1.28755 |
| C | 2.81069 | 0.82309 | -0.85696 |
| H | 2.80446 | 0.22696 | 0.05870 |
| H | 3.83437 | 0.90225 | -1.22455 |
| H | 2.44031 | 1.82142 | -0.61202 |
| C | -2.36174 | 0.56123 | -2.46497 |
| H | -1.98359 | 1.39446 | -3.05890 |
| H | -3.24510 | 0.15087 | -2.95850 |
| H | -2.62932 | 0.91225 | -1.46767 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.13042 | -1.26021 | -0.55769 |
| C | 0.57279 | -0.00127 | -1.50930 |
| P | -1.04478 | -0.31754 | -2.29831 |
| Cl | 1.28064 | 1.55518 | -1.80953 |
| O | -1.65905 | -1.54843 | -1.74796 |
| C | -2.00651 | 1.17735 | -1.97136 |
| H | -1.51650 | 2.08521 | -2.32096 |
| H | -2.98153 | 1.07377 | -2.44986 |
| H | -2.15570 | 1.23748 | -0.89199 |
| C | 2.78438 | -0.78688 | 0.20026 |
| C | -0.80323 | -0.45033 | -4.12944 |
| C | 3.17283 | -2.02362 | 1.01718 |
| H | 3.27229 | -2.91061 | 0.38561 |
| H | 4.13445 | -1.85127 | 1.51071 |
| H | 2.43227 | -2.24671 | 1.78996 |
| C | 3.84887 | -0.54367 | -0.86642 |
| H | 3.64168 | 0.34393 | -1.46304 |
| H | 4.82189 | -0.40522 | -0.38151 |
| H | 3.93875 | -1.39843 | -1.54228 |
| C | 2.64667 | 0.40597 | 1.14327 |
| H | 2.39868 | 1.32538 | 0.61417 |
| H | 1.87853 | 0.22876 | 1.90079 |
| H | 3.59577 | 0.56329 | 1.66809 |
| C | -0.30585 | 0.82393 | -4.80414 |
| H | 0.69162 | 1.10918 | -4.46910 |
| H | -0.25768 | 0.65524 | -5.88488 |
| H | -0.97832 | 1.66856 | -4.63726 |
| C | -2.17771 | -0.82878 | -4.69239 |
| H | -2.90307 | -0.01862 | -4.58182 |
| H | -2.07823 | -1.03538 | -5.76244 |
| H | -2.57555 | -1.71732 | -4.20046 |

| | | | |
|---|----------|----------|----------|
| C | 0.17365 | -1.59958 | -4.37638 |
| H | 1.18152 | -1.35285 | -4.03551 |
| H | -0.14954 | -2.50810 | -3.86416 |
| H | 0.22239 | -1.80838 | -5.44947 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 1.05272 | -1.10621 | -0.37323 |
| C | 0.75340 | -0.29653 | -1.81014 |
| P | -0.85670 | -0.65742 | -2.57778 |
| Cl | 1.74257 | 0.85345 | -2.63450 |
| O | -1.64248 | -1.59577 | -1.74729 |
| C | -1.63165 | 0.95062 | -2.82682 |
| H | -0.99828 | 1.63976 | -3.38508 |
| H | -2.56876 | 0.79367 | -3.36364 |
| H | -1.84789 | 1.37219 | -1.84381 |
| C | -0.49131 | -1.32374 | -4.21953 |
| C | -0.68999 | -2.69324 | -4.38325 |
| C | -0.04924 | -0.55944 | -5.29783 |
| C | -0.44197 | -3.29134 | -5.60891 |
| H | -1.05385 | -3.27171 | -3.54144 |
| C | 0.19675 | -1.16111 | -6.52198 |
| H | 0.10736 | 0.50709 | -5.18878 |
| C | 0.00276 | -2.52660 | -6.67753 |
| H | -0.60129 | -4.35663 | -5.73102 |
| H | 0.53878 | -0.56177 | -7.35802 |
| H | 0.19449 | -2.99419 | -7.63681 |
| C | 2.72079 | -0.59776 | 0.13933 |
| C | 3.84958 | -0.66404 | -0.67944 |
| C | 2.87940 | -0.24058 | 1.47981 |
| C | 5.10050 | -0.35462 | -0.17196 |
| H | 3.75080 | -0.96656 | -1.71490 |
| C | 4.12903 | 0.09081 | 1.97975 |
| H | 2.01475 | -0.21867 | 2.13618 |
| C | 5.24169 | 0.03284 | 1.15394 |
| H | 5.97115 | -0.41489 | -0.81524 |
| H | 4.23507 | 0.38242 | 3.01841 |
| H | 6.22207 | 0.27921 | 1.54561 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.61470 | -1.72697 | -1.06597 |
| C | 0.84404 | -0.53944 | -1.96016 |
| P | -0.77665 | -0.85553 | -2.74245 |
| Cl | 1.33187 | 1.10948 | -2.10002 |
| O | -1.86427 | -0.18032 | -1.99892 |
| C | -0.65692 | -0.16442 | -4.41140 |
| H | 0.32186 | -0.26021 | -4.87482 |
| H | -1.41492 | -0.63484 | -5.04030 |
| H | -0.90310 | 0.89229 | -4.29825 |
| C | 3.02176 | -0.86803 | -0.28814 |
| C | 4.30050 | -0.99690 | -0.84366 |
| C | 2.83873 | -0.17220 | 0.91629 |
| C | 5.37981 | -0.41420 | -0.18998 |
| C | 3.94579 | 0.39225 | 1.53527 |
| C | 5.22457 | 0.28244 | 1.00082 |
| H | 6.37018 | -0.50838 | -0.62621 |
| H | 3.80390 | 0.93467 | 2.46578 |
| C | -0.92460 | -2.66936 | -2.83615 |
| C | -1.83675 | -3.32234 | -1.97740 |
| C | -0.17214 | -3.43365 | -3.75170 |
| C | -1.99291 | -4.70008 | -2.09284 |
| C | -0.36814 | -4.80673 | -3.81733 |
| C | -1.28440 | -5.46134 | -3.00838 |
| H | -2.69381 | -5.19405 | -1.42685 |
| H | 0.22629 | -5.38320 | -4.52008 |
| C | 4.51431 | -1.72000 | -2.14010 |

| | | | |
|---|----------|----------|----------|
| H | 4.01945 | -2.69657 | -2.14505 |
| H | 4.10592 | -1.15034 | -2.98043 |
| H | 5.57671 | -1.87997 | -2.32929 |
| C | 1.47956 | -0.02207 | 1.53091 |
| H | 0.81895 | 0.57449 | 0.89569 |
| H | 0.99304 | -0.99206 | 1.67353 |
| H | 1.54443 | 0.46632 | 2.50399 |
| C | 6.40432 | 0.87630 | 1.70836 |
| H | 6.74564 | 0.22004 | 2.51513 |
| H | 7.24407 | 1.02436 | 1.02748 |
| H | 6.15442 | 1.83939 | 2.15833 |
| C | -1.50486 | -6.93747 | -3.12505 |
| H | -1.82832 | -7.36801 | -2.17581 |
| H | -2.28262 | -7.15391 | -3.86431 |
| H | -0.59746 | -7.45220 | -3.44637 |
| C | 0.86717 | -2.86069 | -4.67455 |
| H | 0.41490 | -2.41812 | -5.56550 |
| H | 1.47847 | -2.09709 | -4.19210 |
| H | 1.53563 | -3.65365 | -5.01227 |
| C | -2.64776 | -2.63783 | -0.91402 |
| H | -2.02208 | -2.05719 | -0.23538 |
| H | -3.35740 | -1.92830 | -1.33842 |
| H | -3.19053 | -3.38631 | -0.33474 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 2.28599 | -1.92738 | -0.66353 |
| C | 1.34620 | -1.04792 | -1.73311 |
| P | -0.28626 | -1.58908 | -2.41086 |
| Cl | 1.60612 | 0.62133 | -2.12121 |
| O | -1.33400 | -0.94877 | -1.57591 |
| C | -0.38904 | -0.87627 | -4.07369 |
| H | 0.48893 | -1.00495 | -4.70052 |
| H | -1.25904 | -1.32113 | -4.55835 |
| H | -0.57276 | 0.18728 | -3.92301 |
| C | 3.52016 | -0.73516 | 0.02285 |
| C | 4.80780 | -0.58965 | -0.55439 |
| C | 3.17289 | 0.04292 | 1.16440 |
| C | 5.63059 | 0.43181 | -0.08062 |
| C | 4.04930 | 1.04577 | 1.55821 |
| C | 5.26351 | 1.29094 | 0.93705 |
| H | 6.60072 | 0.56205 | -0.52984 |
| H | 3.77931 | 1.66448 | 2.40042 |
| C | -0.65624 | -3.38640 | -2.67354 |
| C | -1.74717 | -3.89236 | -1.90859 |
| C | -0.37132 | -4.02855 | -3.91738 |
| C | -2.67317 | -4.71744 | -2.54778 |
| C | -1.33347 | -4.86222 | -4.46911 |
| C | -2.54052 | -5.15286 | -3.85103 |
| H | -3.54319 | -5.02113 | -1.98505 |
| H | -1.12753 | -5.30902 | -5.43349 |
| C | 5.38736 | -1.48801 | -1.67240 |
| C | 1.91569 | -0.16341 | 2.04099 |
| C | 6.14697 | 2.43978 | 1.41420 |
| C | -3.60213 | -5.97375 | -4.57311 |
| C | 0.96394 | -4.03007 | -4.69497 |
| C | -2.00862 | -3.72293 | -0.39400 |
| C | 4.70943 | -1.15653 | -3.00497 |
| H | 3.64028 | -1.35094 | -2.98144 |
| H | 4.85070 | -0.09942 | -3.24078 |
| H | 5.14509 | -1.74119 | -3.81897 |
| C | 6.88623 | -1.24899 | -1.88254 |
| H | 7.09516 | -0.23961 | -2.24191 |
| H | 7.46709 | -1.42385 | -0.97324 |
| H | 7.25193 | -1.93106 | -2.65076 |
| C | 5.21295 | -2.97052 | -1.27443 |
| H | 5.66723 | -3.10644 | -0.28677 |

| | | | |
|---|----------|----------|----------|
| H | 4.14808 | -3.18858 | -1.13772 |
| C | 0.65257 | 0.38570 | 1.36787 |
| H | 0.77657 | 1.44607 | 1.13590 |
| H | 0.39003 | -0.12761 | 0.44617 |
| H | -0.19729 | 0.28770 | 2.04948 |
| C | 2.03298 | 0.56931 | 3.38512 |
| H | 2.93858 | 0.29263 | 3.93072 |
| H | 2.00714 | 1.65571 | 3.27516 |
| H | 1.17460 | 0.29397 | 4.00188 |
| C | 1.74707 | -1.64191 | 2.40764 |
| H | 1.56223 | -2.28794 | 1.54690 |
| H | 2.63630 | -2.01658 | 2.92131 |
| H | 0.88906 | -1.75980 | 3.07470 |
| C | 7.43617 | 2.55680 | 0.60543 |
| H | 8.02114 | 3.40361 | 0.97267 |
| H | 8.05844 | 1.66300 | 0.69779 |
| H | 7.23568 | 2.72847 | -0.45517 |
| C | 5.37453 | 3.75730 | 1.27759 |
| H | 5.10031 | 3.94259 | 0.23619 |
| H | 4.45648 | 3.75097 | 1.86843 |
| H | 5.98950 | 4.59324 | 1.62296 |
| C | 6.52152 | 2.22315 | 2.88522 |
| H | 7.15065 | 3.04474 | 3.23950 |
| H | 5.63855 | 2.17913 | 3.52586 |
| H | 7.07575 | 1.29005 | 3.01346 |
| C | -3.25979 | -2.87866 | -0.13263 |
| H | -4.13960 | -3.31077 | -0.61655 |
| H | -3.45806 | -2.84086 | 0.94285 |
| H | -3.11640 | -1.86418 | -0.50147 |
| C | -2.23351 | -5.13242 | 0.19444 |
| H | -2.32896 | -5.04642 | 1.27984 |
| H | -3.13860 | -5.61829 | -0.17016 |
| H | -1.38612 | -5.78926 | -0.01866 |
| C | -0.83268 | -3.15578 | 0.39033 |
| H | 0.08482 | -3.71168 | 0.18150 |
| H | -0.67522 | -2.10195 | 0.18242 |
| H | -1.04075 | -3.25299 | 1.45924 |
| C | 0.79552 | -3.55135 | -6.14166 |
| H | 1.75352 | -3.61907 | -6.66472 |
| H | 0.07702 | -4.15965 | -6.69351 |
| H | 0.45841 | -2.51548 | -6.19363 |
| C | 5.76464 | -4.01631 | -2.23215 |
| H | 5.49068 | -5.01510 | -1.88418 |
| H | 5.35958 | -3.90389 | -3.24041 |
| H | 6.85365 | -3.98917 | -2.30198 |
| C | 1.45201 | -5.49283 | -4.72466 |
| H | 2.42180 | -5.54233 | -5.22797 |
| H | 1.57470 | -5.87992 | -3.71043 |
| H | 0.76631 | -6.15372 | -5.25523 |
| C | 2.09092 | -3.25008 | -4.04172 |
| H | 2.25717 | -3.57786 | -3.01468 |
| H | 3.01304 | -3.42196 | -4.60243 |
| H | 1.92872 | -2.17525 | -4.02828 |
| C | -3.99725 | -5.24990 | -5.86579 |
| H | -3.14103 | -5.11186 | -6.52930 |
| H | -4.75114 | -5.82848 | -6.40702 |
| H | -4.41551 | -4.26401 | -5.64878 |
| C | -3.03810 | -7.35682 | -4.91932 |
| H | -2.16478 | -7.28784 | -5.57112 |
| H | -2.74137 | -7.89507 | -4.01586 |
| H | -3.79438 | -7.95254 | -5.43821 |
| C | -4.85871 | -6.16531 | -3.72817 |
| H | -4.65473 | -6.73231 | -2.81644 |
| H | -5.30628 | -5.20922 | -3.44570 |
| H | -5.60239 | -6.72379 | -4.30184 |

R-P=C(Cl)-P(S)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.78600 | -1.26507 | -0.12928 |
| C | 0.59073 | -0.53053 | -1.62238 |
| P | -0.99972 | -0.77462 | -2.45350 |
| Cl | 1.72803 | 0.37958 | -2.50890 |
| Cl | -1.87263 | 1.06120 | -2.30019 |
| S | -0.96161 | -1.55533 | -4.18878 |
| H | 2.13914 | -0.86803 | 0.06859 |
| H | -1.70798 | -1.45674 | -1.44477 |

R= Me

| | | | |
|----|----------|----------|----------|
| P | 0.89882 | -1.24252 | -0.11834 |
| C | 0.57027 | -0.53669 | -1.60142 |
| P | -1.03159 | -0.79997 | -2.41045 |
| Cl | 1.65894 | 0.39830 | -2.53883 |
| Cl | -1.84078 | 1.08664 | -2.32588 |
| S | -0.92491 | -1.55145 | -4.16566 |
| C | -2.07525 | -1.68330 | -1.23663 |
| H | -1.69574 | -2.69881 | -1.12077 |
| H | -2.11629 | -1.17571 | -0.27336 |
| H | -3.07028 | -1.72178 | -1.68248 |
| C | 2.64323 | -0.78074 | 0.19477 |
| H | 2.75132 | 0.30502 | 0.24548 |
| H | 2.95503 | -1.21842 | 1.14364 |
| H | 3.28936 | -1.15075 | -0.60444 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.66990 | 0.09407 | -2.03934 |
| C | 0.25258 | -0.11062 | -1.16484 |
| P | -1.20006 | -0.57774 | -2.17125 |
| Cl | -0.01184 | 0.07542 | 0.53067 |
| S | -0.72702 | -1.30178 | -3.88617 |
| C | 3.04598 | 0.61564 | -0.87014 |
| C | -2.39204 | 0.85455 | -2.25226 |
| C | 4.25342 | 0.77278 | -1.80130 |
| H | 4.07995 | 1.53618 | -2.56462 |
| H | 5.12895 | 1.07262 | -1.21732 |
| H | 4.49436 | -0.16259 | -2.31349 |
| C | 3.35059 | -0.47460 | 0.15465 |
| H | 4.24904 | -0.19708 | 0.71708 |
| H | 2.53827 | -0.61496 | 0.86631 |
| H | 3.55061 | -1.43377 | -0.33019 |
| C | 2.75685 | 1.95845 | -0.20457 |
| H | 2.53693 | 2.73210 | -0.94532 |
| H | 1.92281 | 1.90463 | 0.49376 |
| H | 3.64329 | 2.28157 | 0.35257 |
| C | -1.71450 | 1.94540 | -3.08199 |
| H | -2.41184 | 2.78105 | -3.19168 |
| H | -0.81171 | 2.32368 | -2.59747 |
| H | -1.44872 | 1.58359 | -4.07604 |
| C | -2.77325 | 1.39921 | -0.87965 |
| H | -3.19160 | 0.62703 | -0.23264 |
| H | -1.92774 | 1.85948 | -0.36849 |
| H | -3.53715 | 2.17009 | -1.01940 |
| C | -3.64010 | 0.35191 | -2.97815 |
| H | -4.32198 | 1.19603 | -3.11651 |
| H | -3.39358 | -0.05917 | -3.95791 |
| H | -4.16226 | -0.41313 | -2.40084 |
| Cl | -2.15981 | -1.92014 | -0.94819 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.93403 | -1.11657 | -0.07923 |
| C | 0.56811 | -0.43887 | -1.56960 |
| P | -1.03963 | -0.70289 | -2.38310 |
| Cl | 1.57159 | 0.52824 | -2.57804 |
| S | -0.94574 | -1.71286 | -4.00755 |
| C | 2.68023 | -0.72975 | 0.21975 |
| C | 3.00693 | -0.25000 | 1.48954 |
| C | 3.70604 | -1.00667 | -0.68583 |
| C | 4.32749 | -0.00498 | 1.83163 |
| H | 2.22029 | -0.06370 | 2.21427 |
| C | 5.02586 | -0.78175 | -0.33291 |
| H | 3.47209 | -1.40653 | -1.66500 |
| C | 5.33832 | -0.27180 | 0.92042 |
| H | 4.56749 | 0.38322 | 2.81479 |
| H | 5.81613 | -1.00486 | -1.04063 |
| H | 6.37289 | -0.09250 | 1.18994 |
| C | -1.78602 | 0.93771 | -2.50415 |
| C | -2.28049 | 1.36657 | -3.72943 |
| C | -1.86101 | 1.76729 | -1.38730 |
| C | -2.85498 | 2.62446 | -3.83661 |
| H | -2.20829 | 0.70806 | -4.58763 |
| C | -2.43171 | 3.02260 | -1.50164 |
| H | -1.47521 | 1.43025 | -0.43150 |
| C | -2.92979 | 3.45076 | -2.72600 |
| H | -3.24237 | 2.95892 | -4.79193 |
| H | -2.49017 | 3.66937 | -0.63394 |
| H | -3.37730 | 4.43448 | -2.81220 |
| Cl | -2.13927 | -1.58699 | -0.90122 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.76949 | -0.04887 | -2.16118 |
| C | 0.35569 | 0.29532 | -1.32760 |
| P | -1.19456 | -0.36989 | -2.01081 |
| Cl | 0.21438 | 1.09254 | 0.19099 |
| S | -0.99357 | -1.22131 | -3.71869 |
| C | 3.07178 | 0.58089 | -1.05245 |
| C | 3.72258 | 1.77687 | -1.38073 |
| C | 3.51343 | -0.19234 | 0.03226 |
| C | 4.79067 | 2.19844 | -0.59794 |
| C | 4.58632 | 0.26660 | 0.78401 |
| C | 5.23455 | 1.46154 | 0.49167 |
| H | 5.29297 | 3.12722 | -0.85290 |
| H | 4.93184 | -0.33369 | 1.62091 |
| C | -2.52143 | 0.86974 | -1.91224 |
| C | -3.85556 | 0.47573 | -1.68753 |
| C | -2.23314 | 2.22141 | -2.19227 |
| C | -4.83323 | 1.45974 | -1.59873 |
| C | -3.25419 | 3.15713 | -2.08868 |
| C | -4.55413 | 2.80768 | -1.75657 |
| H | -5.85835 | 1.14794 | -1.42231 |
| H | -3.02223 | 4.19617 | -2.30221 |
| C | 3.27218 | 2.61168 | -2.54238 |
| H | 3.10332 | 2.00330 | -3.43712 |
| H | 2.33001 | 3.12244 | -2.32250 |
| H | 4.01360 | 3.37283 | -2.78936 |
| C | 2.85645 | -1.49314 | 0.38417 |
| H | 1.83290 | -1.33960 | 0.73737 |
| H | 2.79873 | -2.16330 | -0.47902 |
| H | 3.41023 | -2.00739 | 1.17059 |
| C | 6.37167 | 1.94398 | 1.33943 |

| | | | |
|----|----------|----------|----------|
| H | 6.00004 | 2.45341 | 2.23411 |
| H | 6.99752 | 1.11471 | 1.67543 |
| H | 7.00155 | 2.65082 | 0.79689 |
| C | -4.32517 | -0.94893 | -1.60581 |
| H | -5.36817 | -0.99717 | -1.92274 |
| H | -3.74881 | -1.61415 | -2.24912 |
| H | -4.26776 | -1.34034 | -0.58837 |
| C | -5.62169 | 3.84548 | -1.60453 |
| H | -5.66180 | 4.20686 | -0.57207 |
| H | -5.43304 | 4.70899 | -2.24495 |
| H | -6.60661 | 3.44343 | -1.84817 |
| C | -0.90108 | 2.71868 | -2.67473 |
| H | -0.18810 | 2.84305 | -1.85736 |
| H | -0.45782 | 2.04558 | -3.41011 |
| H | -1.03034 | 3.69236 | -3.14910 |
| Cl | -1.55506 | -1.68003 | -0.45398 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 2.26179 | -1.89753 | -0.67438 |
| C | 1.32041 | -0.98120 | -1.71769 |
| P | -0.24491 | -1.57246 | -2.48747 |
| Cl | 1.56203 | 0.69359 | -2.03773 |
| C | 3.49195 | -0.71162 | 0.02426 |
| C | 4.75141 | -0.52617 | -0.59800 |
| C | 3.17556 | 0.02706 | 1.19932 |
| C | 5.57088 | 0.50222 | -0.13403 |
| C | 4.04983 | 1.03264 | 1.58937 |
| C | 5.23059 | 1.32349 | 0.92331 |
| H | 6.51656 | 0.66512 | -0.62415 |
| H | 3.80450 | 1.61862 | 2.46214 |
| C | -0.65627 | -3.36996 | -2.67472 |
| C | -1.77638 | -3.83255 | -1.92156 |
| C | -0.33893 | -4.06923 | -3.88147 |
| C | -2.72001 | -4.61864 | -2.57735 |
| C | -1.33352 | -4.84472 | -4.45849 |
| C | -2.57889 | -5.05044 | -3.88282 |
| H | -3.60435 | -4.90239 | -2.02516 |
| H | -1.11474 | -5.32348 | -5.40438 |
| C | 5.30462 | -1.38064 | -1.75816 |
| C | 1.94968 | -0.22310 | 2.10475 |
| C | 6.10916 | 2.47794 | 1.39522 |
| C | -3.66884 | -5.79699 | -4.64021 |
| C | 1.05036 | -4.24375 | -4.53598 |
| C | -1.99787 | -3.73601 | -0.39481 |
| C | 4.65319 | -0.96949 | -3.08178 |
| H | 3.57421 | -1.10330 | -3.06992 |
| H | 4.85538 | 0.08275 | -3.29418 |
| H | 5.06035 | -1.56767 | -3.90230 |
| C | 6.81753 | -1.19709 | -1.93913 |
| H | 7.08114 | -0.19937 | -2.29568 |
| H | 7.36978 | -1.39628 | -1.01752 |
| H | 7.16379 | -1.90491 | -2.69579 |
| C | 5.11089 | -2.87658 | -1.49213 |
| H | 5.58692 | -3.16826 | -0.55264 |
| H | 4.06292 | -3.18079 | -1.44039 |
| C | 0.66675 | 0.33077 | 1.47621 |
| H | 0.76389 | 1.40354 | 1.29504 |
| H | 0.41229 | -0.14024 | 0.52941 |
| H | -0.17454 | 0.17800 | 2.15840 |
| C | 2.09341 | 0.46926 | 3.46681 |
| H | 3.01533 | 0.18521 | 3.98023 |
| H | 2.05546 | 1.55802 | 3.39016 |
| H | 1.25384 | 0.16728 | 4.09697 |
| C | 1.80761 | -1.71451 | 2.42567 |

| | | | |
|----|----------|----------|----------|
| H | 1.60974 | -2.33351 | 1.54782 |
| H | 2.71388 | -2.09540 | 2.90346 |
| H | 0.96834 | -1.86631 | 3.10954 |
| C | 7.35624 | 2.64944 | 0.53201 |
| H | 7.93832 | 3.49889 | 0.89757 |
| H | 8.00231 | 1.76860 | 0.56847 |
| H | 7.10255 | 2.84756 | -0.51244 |
| C | 5.30206 | 3.78031 | 1.33509 |
| H | 4.97492 | 3.99012 | 0.31386 |
| H | 4.41341 | 3.73547 | 1.96776 |
| H | 5.91430 | 4.61961 | 1.67690 |
| C | 6.55599 | 2.22546 | 2.84009 |
| H | 7.18206 | 3.05079 | 3.19089 |
| H | 5.70484 | 2.14103 | 3.51868 |
| H | 7.13661 | 1.30254 | 2.91362 |
| C | -3.33573 | -3.09045 | -0.02493 |
| H | -4.18161 | -3.60530 | -0.48487 |
| H | -3.47239 | -3.13724 | 1.05920 |
| H | -3.36177 | -2.04605 | -0.33310 |
| C | -2.00593 | -5.19678 | 0.10865 |
| H | -2.10168 | -5.19659 | 1.19787 |
| H | -2.83223 | -5.77974 | -0.29855 |
| H | -1.07354 | -5.70498 | -0.14997 |
| C | -0.87923 | -3.05715 | 0.37996 |
| H | 0.08900 | -3.49998 | 0.13720 |
| H | -0.83765 | -1.98501 | 0.20429 |
| H | -1.05066 | -3.20644 | 1.44928 |
| C | 1.06299 | -3.90588 | -6.02978 |
| H | 2.04983 | -4.13365 | -6.44214 |
| H | 0.33284 | -4.48960 | -6.59294 |
| H | 0.85910 | -2.85015 | -6.20354 |
| C | 1.38490 | -5.74284 | -4.37740 |
| H | 2.38418 | -5.93299 | -4.77912 |
| H | 1.38051 | -6.03352 | -3.32405 |
| H | 0.68103 | -6.38583 | -4.90660 |
| C | 2.18447 | -3.50313 | -3.84943 |
| H | 2.20786 | -3.72666 | -2.78169 |
| H | 3.13456 | -3.83250 | -4.27779 |
| H | 2.12881 | -2.42670 | -3.98236 |
| C | -3.96434 | -5.04572 | -5.94400 |
| H | -3.07768 | -4.97169 | -6.57681 |
| H | -4.74003 | -5.56770 | -6.51119 |
| H | -4.31424 | -4.03118 | -5.73949 |
| C | -3.19261 | -7.21688 | -4.96907 |
| H | -2.29623 | -7.21092 | -5.59247 |
| H | -2.96496 | -7.77459 | -4.05730 |
| H | -3.97230 | -7.75725 | -5.51311 |
| C | -4.96399 | -5.89643 | -3.83883 |
| H | -4.83540 | -6.48229 | -2.92510 |
| H | -5.34627 | -4.91004 | -3.56507 |
| H | -5.72797 | -6.39411 | -4.44090 |
| S | -1.71338 | -0.52286 | -1.80963 |
| Cl | 0.06026 | -1.01216 | -4.45148 |
| H | 5.56332 | -3.45657 | -2.30098 |

R-P=C(Cl)-P(S)MeR

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.87571 | -1.32772 | -0.15207 |
| C | 0.59633 | -0.54944 | -1.60738 |
| P | -1.02898 | -0.75259 | -2.40692 |
| Cl | 1.69880 | 0.41073 | -2.49963 |
| S | -1.01799 | -1.61877 | -4.12601 |
| H | 2.22574 | -0.90207 | 0.01264 |
| H | -1.68637 | -1.44085 | -1.35989 |
| C | -1.77057 | 0.89445 | -2.34944 |

| | | | |
|---|----------|---------|----------|
| H | -2.79361 | 0.81644 | -2.72026 |
| H | -1.76586 | 1.28886 | -1.33165 |
| H | -1.20547 | 1.55231 | -3.01082 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 1.79954 | -0.04881 | -2.25999 |
| C | 0.32837 | -0.02642 | -1.46268 |
| P | -1.16270 | -0.55293 | -2.35997 |
| Cl | 0.07225 | 0.46239 | 0.18104 |
| S | -0.80053 | -1.08398 | -4.18484 |
| C | -1.87315 | -1.85777 | -1.32423 |
| H | -1.20168 | -2.71636 | -1.34562 |
| H | -2.01845 | -1.52175 | -0.29644 |
| H | -2.82998 | -2.14905 | -1.76059 |
| C | 2.95519 | 0.55348 | -0.96253 |
| H | 2.94527 | -0.10660 | -0.09178 |
| H | 3.96257 | 0.57944 | -1.37957 |
| H | 2.68042 | 1.55680 | -0.62806 |
| C | -2.30277 | 0.84470 | -2.19580 |
| H | -1.90130 | 1.68350 | -2.76479 |
| H | -3.25924 | 0.55059 | -2.63103 |
| H | -2.44004 | 1.13184 | -1.15220 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.64394 | 0.11191 | -2.04027 |
| C | 0.23583 | -0.16025 | -1.17522 |
| P | -1.23578 | -0.64574 | -2.15690 |
| Cl | -0.01888 | -0.07247 | 0.54108 |
| S | -0.75930 | -1.35704 | -3.90088 |
| C | -2.08683 | -1.86172 | -1.11412 |
| H | -1.38658 | -2.67392 | -0.91568 |
| H | -2.44111 | -1.44666 | -0.17112 |
| H | -2.92133 | -2.25918 | -1.69182 |
| C | 3.01177 | 0.62982 | -0.85701 |
| C | -2.35359 | 0.84996 | -2.26482 |
| C | 4.20737 | 0.87028 | -1.78528 |
| H | 4.00209 | 1.65975 | -2.51340 |
| H | 5.07619 | 1.17477 | -1.19342 |
| H | 4.47661 | -0.03247 | -2.34014 |
| C | 3.36225 | -0.49220 | 0.11749 |
| H | 4.25465 | -0.20924 | 0.68710 |
| H | 2.55997 | -0.69138 | 0.82676 |
| H | 3.59132 | -1.42170 | -0.41051 |
| C | 2.68242 | 1.93060 | -0.12977 |
| H | 2.42823 | 2.72759 | -0.83385 |
| H | 1.85656 | 1.81649 | 0.57119 |
| H | 3.56133 | 2.26089 | 0.43541 |
| C | -1.68491 | 1.87267 | -3.17876 |
| H | -2.35343 | 2.73022 | -3.30102 |
| H | -0.74446 | 2.23625 | -2.75850 |
| H | -1.47793 | 1.44720 | -4.16162 |
| C | -2.64081 | 1.48098 | -0.90536 |
| H | -3.08393 | 0.77597 | -0.19892 |
| H | -1.74470 | 1.90400 | -0.45040 |
| H | -3.35782 | 2.29614 | -1.04542 |
| C | -3.66148 | 0.37537 | -2.90145 |
| H | -4.29622 | 1.24574 | -3.09313 |
| H | -3.47906 | -0.13348 | -3.84969 |
| H | -4.21701 | -0.29744 | -2.24390 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 1.70938 | -0.11496 | -1.98689 |
| C | 0.20792 | -0.05643 | -1.24135 |
| P | -1.23229 | -0.56660 | -2.24145 |
| Cl | -0.15977 | 0.39921 | 0.38394 |

| | | | |
|---|----------|----------|----------|
| S | -0.72973 | -1.15194 | -4.01797 |
| C | -2.03658 | -1.84616 | -1.24591 |
| H | -1.38587 | -2.72106 | -1.25924 |
| H | -2.20478 | -1.53100 | -0.21614 |
| H | -2.98417 | -2.09853 | -1.72339 |
| C | 2.87885 | 0.50385 | -0.73860 |
| C | 2.75187 | 1.73080 | -0.08499 |
| C | 4.03655 | -0.25048 | -0.53890 |
| C | 3.74925 | 2.17616 | 0.76644 |
| H | 1.87316 | 2.34330 | -0.24822 |
| C | 5.02257 | 0.18571 | 0.33235 |
| H | 4.16451 | -1.18976 | -1.06837 |
| C | 4.88050 | 1.40110 | 0.98494 |
| H | 3.64289 | 3.13343 | 1.26426 |
| H | 5.90835 | -0.41861 | 0.49133 |
| H | 5.65632 | 1.75092 | 1.65647 |
| C | -2.34599 | 0.87022 | -2.21683 |
| C | -3.18405 | 1.15006 | -1.13896 |
| C | -2.34930 | 1.71415 | -3.32429 |
| C | -4.01225 | 2.26146 | -1.17118 |
| H | -3.19813 | 0.50545 | -0.26904 |
| C | -3.17268 | 2.82816 | -3.34944 |
| H | -1.71333 | 1.47269 | -4.16900 |
| C | -4.00508 | 3.10287 | -2.27390 |
| H | -4.66595 | 2.46905 | -0.33174 |
| H | -3.17032 | 3.47884 | -4.21640 |
| H | -4.65431 | 3.97087 | -2.29718 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.78406 | -0.02386 | -2.22482 |
| C | 0.33483 | 0.24235 | -1.42852 |
| P | -1.19456 | -0.45367 | -2.16205 |
| Cl | 0.12291 | 0.96375 | 0.12661 |
| S | -0.93779 | -1.10473 | -3.97276 |
| C | -1.43977 | -1.80027 | -0.96178 |
| H | -0.48422 | -2.32641 | -0.93591 |
| H | -1.67741 | -1.42593 | 0.03457 |
| H | -2.20401 | -2.48868 | -1.31017 |
| C | 3.03932 | 0.60348 | -1.05527 |
| C | 3.65470 | 1.83458 | -1.31651 |
| C | 3.49111 | -0.19824 | 0.00426 |
| C | 4.69283 | 2.25839 | -0.49482 |
| C | 4.53269 | 0.26318 | 0.79738 |
| C | 5.14337 | 1.49150 | 0.57057 |
| H | 5.16661 | 3.21408 | -0.70044 |
| H | 4.88383 | -0.36127 | 1.61414 |
| C | -2.49724 | 0.81797 | -1.98384 |
| C | -3.80847 | 0.49370 | -1.58290 |
| C | -2.20729 | 2.14479 | -2.36207 |
| C | -4.74697 | 1.51160 | -1.45646 |
| C | -3.18516 | 3.12073 | -2.21607 |
| C | -4.45371 | 2.83675 | -1.73654 |
| H | -5.75373 | 1.24718 | -1.14709 |
| H | -2.94397 | 4.13815 | -2.50932 |
| C | 3.20077 | 2.70636 | -2.44920 |
| H | 3.03826 | 2.12997 | -3.36566 |
| H | 2.25395 | 3.20100 | -2.21339 |
| H | 3.93617 | 3.48274 | -2.66514 |
| C | 2.87560 | -1.53503 | 0.29147 |
| H | 1.85011 | -1.42606 | 0.65606 |
| H | 2.83536 | -2.16214 | -0.60436 |
| H | 3.44652 | -2.07076 | 1.05099 |
| C | 6.24736 | 1.97552 | 1.46036 |
| H | 5.84269 | 2.42720 | 2.37160 |
| H | 6.89976 | 1.15550 | 1.76759 |
| H | 6.85794 | 2.73078 | 0.96284 |

| | | | |
|---|----------|----------|----------|
| C | -4.30423 | -0.90509 | -1.34666 |
| H | -5.39438 | -0.90481 | -1.32808 |
| H | -3.99088 | -1.58259 | -2.14328 |
| H | -3.96474 | -1.31772 | -0.39470 |
| C | -5.47383 | 3.91578 | -1.54767 |
| H | -5.39838 | 4.34654 | -0.54417 |
| H | -5.33140 | 4.72834 | -2.26245 |
| H | -6.48850 | 3.53022 | -1.66205 |
| C | -0.90223 | 2.57326 | -2.96549 |
| H | -0.14139 | 2.74190 | -2.19997 |
| H | -0.51604 | 1.83207 | -3.66698 |
| H | -1.04048 | 3.51166 | -3.50451 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 2.23839 | -1.88922 | -0.63350 |
| C | 1.30880 | -0.99707 | -1.70518 |
| P | -0.27719 | -1.55167 | -2.48423 |
| Cl | 1.59565 | 0.66834 | -2.08110 |
| C | -0.16301 | -0.96072 | -4.20032 |
| H | 0.74349 | -1.24108 | -4.72854 |
| H | -1.03945 | -1.34780 | -4.72047 |
| H | -0.23690 | 0.12372 | -4.14411 |
| C | 3.48182 | -0.70364 | 0.04580 |
| C | 4.75450 | -0.55371 | -0.55853 |
| C | 3.15951 | 0.07019 | 1.19699 |
| C | 5.58212 | 0.47546 | -0.11071 |
| C | 4.04123 | 1.07557 | 1.57128 |
| C | 5.23600 | 1.33199 | 0.91621 |
| H | 6.53818 | 0.61069 | -0.58903 |
| H | 3.79087 | 1.68923 | 2.42335 |
| C | -0.67029 | -3.36666 | -2.66922 |
| C | -1.75956 | -3.87979 | -1.90824 |
| C | -0.37769 | -4.02125 | -3.90684 |
| C | -2.70179 | -4.67193 | -2.56267 |
| C | -1.36816 | -4.79990 | -4.48829 |
| C | -2.58986 | -5.06004 | -3.88383 |
| H | -3.56450 | -4.99106 | -1.99577 |
| H | -1.16432 | -5.24179 | -5.45571 |
| C | 5.31379 | -1.44690 | -1.68640 |
| C | 1.92209 | -0.14380 | 2.09728 |
| C | 6.12256 | 2.48792 | 1.36940 |
| C | -3.68147 | -5.81410 | -4.63226 |
| C | 0.99878 | -4.13684 | -4.60152 |
| C | -1.95629 | -3.81997 | -0.37687 |
| C | 4.69202 | -1.05457 | -3.02943 |
| H | 3.61016 | -1.16342 | -3.02446 |
| H | 4.92104 | -0.01257 | -3.26431 |
| H | 5.09592 | -1.68230 | -3.82946 |
| C | 6.83274 | -1.29462 | -1.84469 |
| H | 7.12119 | -0.31085 | -2.22031 |
| H | 7.36444 | -1.48050 | -0.90840 |
| H | 7.17985 | -2.02719 | -2.57715 |
| C | 5.08773 | -2.93298 | -1.39169 |
| H | 5.54055 | -3.21186 | -0.43698 |
| H | 4.03346 | -3.21605 | -1.35241 |
| C | 0.64672 | 0.39847 | 1.44398 |
| H | 0.75616 | 1.46175 | 1.21853 |
| H | 0.38171 | -0.10902 | 0.51918 |
| H | -0.19605 | 0.28495 | 2.13199 |
| C | 2.05986 | 0.58762 | 3.43961 |
| H | 2.97540 | 0.31294 | 3.96947 |
| H | 2.02955 | 1.67396 | 3.33065 |
| H | 1.21289 | 0.30970 | 4.07086 |
| C | 1.76646 | -1.62424 | 2.46149 |
| H | 1.57015 | -2.26680 | 1.60067 |
| H | 2.66582 | -1.99747 | 2.95824 |

| | | | |
|---|----------|----------|----------|
| H | 0.92056 | -1.74836 | 3.14281 |
| C | 7.38430 | 2.61989 | 0.52065 |
| H | 7.97163 | 3.47224 | 0.87087 |
| H | 8.01859 | 1.73261 | 0.59153 |
| H | 7.14834 | 2.79121 | -0.53269 |
| C | 5.33362 | 3.79832 | 1.26173 |
| H | 5.02469 | 3.98430 | 0.23023 |
| H | 4.43491 | 3.78165 | 1.88137 |
| H | 5.95138 | 4.63895 | 1.59025 |
| C | 6.54496 | 2.27000 | 2.82720 |
| H | 7.17657 | 3.09669 | 3.16478 |
| H | 5.68279 | 2.21490 | 3.49477 |
| H | 7.11221 | 1.34211 | 2.93468 |
| C | -3.29958 | -3.20490 | 0.02568 |
| H | -4.14339 | -3.73078 | -0.42613 |
| H | -3.41559 | -3.26920 | 1.11143 |
| H | -3.34789 | -2.15723 | -0.26818 |
| C | -1.93003 | -5.28892 | 0.09981 |
| H | -2.00344 | -5.30891 | 1.19063 |
| H | -2.75491 | -5.87953 | -0.29985 |
| H | -0.99461 | -5.77686 | -0.18596 |
| C | -0.83647 | -3.13320 | 0.38840 |
| H | 0.13292 | -3.56777 | 0.13605 |
| H | -0.80963 | -2.06043 | 0.20975 |
| H | -0.99689 | -3.28445 | 1.45934 |
| C | 0.97105 | -3.71230 | -6.07368 |
| H | 1.95404 | -3.88320 | -6.52112 |
| H | 0.24592 | -4.28879 | -6.65066 |
| H | 0.72638 | -2.65748 | -6.19909 |
| C | 1.36520 | -5.63575 | -4.54903 |
| H | 2.36054 | -5.78087 | -4.97863 |
| H | 1.38389 | -5.99376 | -3.51709 |
| H | 0.66415 | -6.25639 | -5.10740 |
| C | 2.13809 | -3.43094 | -3.88539 |
| H | 2.19098 | -3.73691 | -2.83944 |
| H | 3.08300 | -3.70319 | -4.36214 |
| H | 2.07359 | -2.34730 | -3.91186 |
| C | -4.04629 | -5.02734 | -5.89687 |
| H | -3.18410 | -4.89949 | -6.55474 |
| H | -4.82235 | -5.55478 | -6.45861 |
| H | -4.42432 | -4.03415 | -5.64288 |
| C | -3.17367 | -7.20516 | -5.02957 |
| H | -2.30092 | -7.14809 | -5.68327 |
| H | -2.89561 | -7.78671 | -4.14720 |
| H | -3.95493 | -7.75152 | -5.56541 |
| C | -4.94443 | -5.98490 | -3.79237 |
| H | -4.76468 | -6.59633 | -2.90449 |
| H | -5.34937 | -5.02220 | -3.47103 |
| H | -5.71196 | -6.48771 | -4.38573 |
| S | -1.73993 | -0.54169 | -1.67052 |
| H | 5.54610 | -3.53857 | -2.17830 |

PCPX-E(II) model systems

E = Si(II)

R-P=C(Si(II)Cl)-P(O)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.78783 | 0.09855 | 1.08065 |
| C | 0.44291 | -0.29030 | -0.49355 |
| P | -1.05815 | -0.29005 | -1.34871 |
| Cl | 1.12156 | -2.66830 | -2.35917 |
| Si | 1.30782 | -0.53452 | -2.28854 |

| | | | |
|----|----------|----------|----------|
| O | -0.50531 | -0.12690 | -2.76929 |
| H | 2.19863 | -0.13316 | 1.01997 |
| H | -1.77588 | -1.48710 | -1.19906 |
| Cl | -2.46836 | 1.07178 | -0.92807 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.84161 | 0.22802 | 1.00849 |
| C | 0.43296 | -0.21088 | -0.53535 |
| P | -1.10101 | -0.29269 | -1.32158 |
| Cl | 1.28893 | -2.60619 | -2.35371 |
| Si | 1.23951 | -0.45169 | -2.34237 |
| O | -0.58989 | -0.23174 | -2.77471 |
| C | 2.65918 | -0.02706 | 1.02877 |
| H | 3.10761 | 0.21259 | 0.06173 |
| H | 3.11018 | 0.58194 | 1.81364 |
| H | 2.86536 | -1.07820 | 1.25175 |
| C | -2.03599 | -1.77900 | -1.00372 |
| H | -2.37954 | -1.78431 | 0.03145 |
| H | -2.88908 | -1.81816 | -1.68294 |
| H | -1.36665 | -2.62175 | -1.18972 |
| Cl | -2.41578 | 1.20370 | -0.98560 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.65866 | 0.19207 | 0.61811 |
| C | 0.47677 | -0.29956 | -0.95859 |
| P | -1.04320 | -0.56188 | -1.76551 |
| Cl | 1.94838 | -2.58920 | -2.57951 |
| Si | 1.34042 | -0.53514 | -2.74561 |
| O | -0.48171 | -0.80713 | -3.18094 |
| C | -2.13384 | -1.92414 | -1.20940 |
| C | -2.71573 | -1.58655 | 0.16051 |
| H | -3.37569 | -0.71882 | 0.12239 |
| H | -3.30028 | -2.44260 | 0.50848 |
| H | -1.93371 | -1.39522 | 0.89975 |
| C | -3.23673 | -2.10543 | -2.25280 |
| H | -2.82269 | -2.30575 | -3.24274 |
| H | -3.84855 | -2.96361 | -1.96121 |
| H | -3.88810 | -1.23241 | -2.31564 |
| C | -1.27337 | -3.18685 | -1.12834 |
| H | -0.82330 | -3.43800 | -2.08918 |
| H | -0.47053 | -3.08852 | -0.39618 |
| H | -1.91713 | -4.01588 | -0.82144 |
| C | 2.49338 | 0.16202 | 0.98166 |
| C | 2.92710 | -1.30084 | 1.08784 |
| H | 2.33903 | -1.84540 | 1.83278 |
| H | 2.83178 | -1.81856 | 0.13194 |
| H | 3.97583 | -1.34571 | 1.40218 |
| C | 3.30178 | 0.89170 | -0.08226 |
| H | 4.36046 | 0.89067 | 0.19934 |
| H | 3.22383 | 0.41638 | -1.06286 |
| H | 2.98640 | 1.93266 | -0.18917 |
| C | 2.66378 | 0.85480 | 2.33431 |
| H | 3.71565 | 0.82740 | 2.63447 |
| H | 2.35439 | 1.90277 | 2.29424 |
| H | 2.07923 | 0.36310 | 3.11686 |
| Cl | -2.24052 | 1.07366 | -1.80758 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.97589 | -0.65819 | 1.28578 |
| C | 0.32104 | -0.36603 | -0.21523 |
| P | -1.35280 | -0.29961 | -0.63551 |
| Cl | 0.96406 | -1.14946 | -3.23488 |
| Si | 0.67927 | 0.55101 | -1.94245 |
| O | -1.21782 | 0.53227 | -1.92467 |
| Cl | -2.55539 | 0.64120 | 0.69061 |

| | | | |
|---|----------|----------|----------|
| C | -2.16668 | -1.85843 | -0.94652 |
| C | -2.38816 | -2.24611 | -2.26454 |
| C | -2.53407 | -2.69005 | 0.10990 |
| C | -2.98819 | -3.46969 | -2.52092 |
| H | -2.08582 | -1.59635 | -3.07603 |
| C | -3.12743 | -3.91023 | -0.15735 |
| H | -2.36036 | -2.38421 | 1.13582 |
| C | -3.35560 | -4.29823 | -1.47218 |
| H | -3.16452 | -3.77546 | -3.54533 |
| H | -3.41524 | -4.56027 | 0.66039 |
| H | -3.82271 | -5.25464 | -1.67776 |
| C | 2.75904 | -0.63489 | 1.03086 |
| C | 3.39458 | -0.80391 | -0.20342 |
| C | 3.53857 | -0.43639 | 2.17581 |
| C | 4.77472 | -0.74652 | -0.28809 |
| H | 2.80958 | -1.01498 | -1.09131 |
| C | 4.91864 | -0.37330 | 2.08619 |
| H | 3.05191 | -0.32059 | 3.13959 |
| C | 5.53656 | -0.52557 | 0.85262 |
| H | 5.25977 | -0.88040 | -1.24811 |
| H | 5.51344 | -0.20909 | 2.97730 |
| H | 6.61747 | -0.48222 | 0.78023 |

R = Mes

| | | | |
|---|----------|----------|----------|
| P | 0.84879 | 0.09481 | 1.01712 |
| C | 0.42254 | -0.50327 | -0.47320 |
| P | -1.10997 | -0.48680 | -1.30743 |
| C | 2.68895 | 0.07342 | 0.92447 |
| C | 3.42579 | -1.11295 | 1.16878 |
| C | 3.35896 | 1.24737 | 0.50338 |
| C | 4.75567 | -1.14200 | 0.77071 |
| C | 4.69578 | 1.13166 | 0.12537 |
| C | 5.40022 | -0.05731 | 0.19328 |
| H | 5.32010 | -2.05121 | 0.91950 |
| H | 5.20507 | 2.00839 | -0.24017 |
| C | 2.72915 | 2.65928 | 0.50145 |
| C | 2.87109 | -2.34448 | 1.91518 |
| C | 6.84125 | -0.19527 | -0.28830 |
| C | 2.05294 | -3.25734 | 0.99648 |
| H | 1.16740 | -2.76707 | 0.59696 |
| H | 2.64976 | -3.58675 | 0.14402 |
| H | 1.73279 | -4.14473 | 1.55140 |
| C | 2.02815 | -1.90801 | 3.11647 |
| H | 2.60541 | -1.27244 | 3.79264 |
| H | 1.12599 | -1.35536 | 2.83467 |
| H | 1.69021 | -2.78724 | 3.67183 |
| C | 4.00499 | -3.20074 | 2.49456 |
| H | 4.57814 | -3.71386 | 1.71977 |
| H | 4.69330 | -2.61146 | 3.10533 |
| H | 3.56875 | -3.97515 | 3.12990 |
| C | 1.69321 | 2.85172 | -0.61296 |
| H | 0.77836 | 2.28522 | -0.44081 |
| H | 1.41218 | 3.90726 | -0.67062 |
| H | 2.09687 | 2.55076 | -1.58205 |
| C | 2.09029 | 2.94563 | 1.86660 |
| H | 1.26216 | 2.27164 | 2.09925 |
| H | 2.82880 | 2.85840 | 2.66729 |
| H | 1.68803 | 3.96245 | 1.88036 |
| C | 3.78830 | 3.74834 | 0.29473 |
| H | 4.59548 | 3.68394 | 1.02806 |
| H | 4.22284 | 3.72107 | -0.70712 |
| H | 3.30998 | 4.72346 | 0.41115 |
| C | 7.37345 | 1.09543 | -0.90543 |
| H | 7.39953 | 1.91425 | -0.18176 |
| H | 8.39564 | 0.93596 | -1.25724 |
| H | 6.77386 | 1.41170 | -1.76259 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| C | 6.90711 | -1.29743 | -1.35249 | C | 3.60928 | -0.48247 | 1.40161 |
| H | 6.57914 | -2.26100 | -0.95755 | C | 3.63562 | 1.37999 | -0.18734 |
| H | 6.27085 | -1.05392 | -2.20655 | C | 4.77666 | -0.95184 | 0.81009 |
| H | 7.93364 | -1.41405 | -1.71152 | C | 4.79475 | 0.83710 | -0.73365 |
| C | 7.74612 | -0.57294 | 0.89033 | C | 5.35392 | -0.35269 | -0.30040 |
| H | 7.44458 | -1.51784 | 1.34683 | H | 5.24784 | -1.82970 | 1.22160 |
| H | 8.78047 | -0.68139 | 0.55178 | H | 5.28413 | 1.37846 | -1.53395 |
| H | 7.72056 | 0.19748 | 1.66511 | C | 3.11624 | -1.16431 | 2.69441 |
| C | -2.24049 | -1.88538 | -1.15475 | C | 3.30084 | 2.81301 | -0.65373 |
| C | -2.62836 | -2.68155 | -2.26574 | C | 6.57604 | -0.92757 | -1.00975 |
| C | -2.73444 | -2.17455 | 0.13289 | C | -3.29747 | 2.23329 | 1.40380 |
| C | -3.46314 | -3.76187 | -2.01947 | C | -2.69363 | -2.67224 | -0.02668 |
| C | -3.57270 | -3.26950 | 0.29963 | C | -7.10052 | -0.37333 | -0.60118 |
| C | -3.94294 | -4.08174 | -0.75598 | C | 4.51937 | 3.69103 | -0.31305 |
| H | -3.75513 | -4.38211 | -2.85686 | H | 4.33273 | 4.71958 | -0.63435 |
| H | -3.95137 | -3.49448 | 1.29109 | H | 4.70494 | 3.69848 | 0.76425 |
| C | -2.25392 | -2.38892 | -3.70724 | H | 5.42967 | 3.34817 | -0.80545 |
| C | -3.16826 | -1.29896 | -4.27062 | C | 2.10962 | 3.47350 | 0.03633 |
| C | -2.26982 | -3.61180 | -4.61648 | H | 1.15276 | 3.07575 | -0.30097 |
| H | -1.23656 | -2.00939 | -3.72238 | H | 2.16850 | 3.39734 | 1.12745 |
| H | -3.11458 | -0.37790 | -3.68745 | H | 2.11060 | 4.54085 | -0.20385 |
| H | -2.87976 | -1.05890 | -5.29691 | C | 3.05779 | 2.85994 | -2.16561 |
| H | -4.20976 | -1.63403 | -4.27869 | H | 3.92849 | 2.52015 | -2.72942 |
| H | -1.67890 | -4.43115 | -4.20160 | H | 2.21386 | 2.22759 | -2.45030 |
| H | -3.28071 | -3.97736 | -4.81790 | H | 2.84300 | 3.88699 | -2.47507 |
| H | -1.83261 | -3.34158 | -5.58018 | C | 7.73692 | 0.07101 | -0.93712 |
| C | -2.43828 | -1.34332 | 1.36412 | H | 8.61420 | -0.33311 | -1.45028 |
| C | -1.80843 | -2.17775 | 2.47622 | H | 7.48447 | 1.02204 | -1.41047 |
| C | -3.69683 | -0.63333 | 1.86090 | H | 8.01334 | 0.27509 | 0.10042 |
| H | -1.71621 | -0.56248 | 1.11240 | C | 7.03903 | -2.24474 | -0.39259 |
| H | -0.91907 | -2.70410 | 2.12588 | H | 7.89727 | -2.62617 | -0.95123 |
| H | -1.51953 | -1.53367 | 3.31013 | H | 7.35273 | -2.12114 | 0.64727 |
| H | -2.50902 | -2.92236 | 2.86143 | H | 6.25545 | -3.00548 | -0.42891 |
| H | -4.13724 | -0.00937 | 1.08159 | C | 6.21783 | -1.18589 | -2.47836 |
| H | -4.45224 | -1.35435 | 2.18319 | H | 5.38864 | -1.89248 | -2.55914 |
| H | -3.45607 | 0.00469 | 2.71482 | H | 5.92144 | -0.26740 | -2.98891 |
| C | -4.84369 | -5.27294 | -0.53835 | H | 7.07901 | -1.60227 | -3.00889 |
| C | -4.13077 | -6.58015 | -0.87764 | C | 4.12082 | -2.19805 | 3.21215 |
| C | -6.15115 | -5.14276 | -1.31599 | H | 5.10947 | -1.76449 | 3.37965 |
| H | -5.09076 | -5.29404 | 0.52904 | H | 3.76191 | -2.58358 | 4.16926 |
| H | -3.20876 | -6.69132 | -0.30324 | H | 4.22266 | -3.05036 | 2.53641 |
| H | -4.77586 | -7.43479 | -0.65866 | C | 2.96961 | -0.11039 | 3.80082 |
| H | -3.87010 | -6.62307 | -1.93835 | H | 3.92178 | 0.39411 | 3.98245 |
| H | -6.67729 | -4.22085 | -1.05925 | H | 2.22546 | 0.65117 | 3.55918 |
| H | -5.97089 | -5.13613 | -2.39409 | H | 2.65455 | -0.59058 | 4.73175 |
| H | -6.81114 | -5.98559 | -1.09588 | C | 1.79162 | -1.90925 | 2.50180 |
| Cl | 1.30069 | -2.72813 | -2.55678 | H | 0.95285 | -1.23358 | 2.32033 |
| Si | 1.30520 | -0.58633 | -2.25681 | H | 1.84389 | -2.59801 | 1.65679 |
| O | -0.50559 | -0.28834 | -2.71353 | H | 1.55518 | -2.47733 | 3.40663 |
| Cl | -2.26164 | 1.16582 | -0.96374 | C | -1.81789 | 2.29390 | 1.75525 |
| R = Mes* | | | | H | -1.46152 | 1.34638 | 2.16614 |
| P | 1.20466 | 0.95553 | 1.22664 | H | -1.18785 | 2.57632 | 0.91342 |
| C | 0.44039 | 0.39573 | -0.13846 | H | -1.66129 | 3.05314 | 2.52538 |
| P | -1.23677 | 0.31302 | -0.63610 | C | -4.03812 | 2.05767 | 2.74585 |
| Cl | 1.53608 | -2.36702 | -1.31070 | H | -3.76432 | 2.87532 | 3.41810 |
| O | -0.98909 | -0.66880 | -1.79873 | H | -5.12196 | 2.06874 | 2.62670 |
| C | -2.85166 | -0.03796 | 0.13267 | H | -3.76041 | 1.11572 | 3.22497 |
| C | -3.42209 | -1.31793 | -0.13185 | C | -3.72718 | 3.56609 | 0.78485 |
| C | -3.70296 | 1.01698 | 0.54920 | H | -4.80242 | 3.60461 | 0.60108 |
| C | -4.78913 | -1.36531 | -0.35992 | H | -3.48231 | 4.38119 | 1.47118 |
| C | -5.06748 | 0.87594 | 0.32077 | H | -3.21525 | 3.75261 | -0.15885 |
| C | -5.62657 | -0.26458 | -0.23175 | C | -1.38052 | -2.55833 | 0.74326 |
| H | -5.22241 | -2.31837 | -0.63323 | H | -0.96505 | -3.55712 | 0.89708 |
| H | -5.71392 | 1.69795 | 0.59444 | H | -0.60682 | -2.00011 | 0.22304 |
| C | 2.96664 | 0.63423 | 0.80916 | H | -1.54544 | -2.10929 | 1.72653 |
| | | | | C | -2.48472 | -3.33989 | -1.38882 |

| | | | |
|----|----------|----------|----------|
| H | -1.81709 | -2.76380 | -2.02402 |
| H | -2.05298 | -4.33408 | -1.24537 |
| H | -3.43912 | -3.46156 | -1.90821 |
| C | -3.57490 | -3.61088 | 0.82260 |
| H | -3.84238 | -3.15402 | 1.77848 |
| H | -4.49356 | -3.90973 | 0.31660 |
| H | -3.01103 | -4.52389 | 1.02881 |
| C | -7.84565 | 0.94382 | -0.40231 |
| H | -7.86228 | 1.25023 | 0.64676 |
| H | -7.40451 | 1.75173 | -0.99135 |
| H | -8.88311 | 0.82709 | -0.72414 |
| C | -7.77342 | -1.44517 | 0.26468 |
| H | -7.31818 | -2.42730 | 0.12369 |
| H | -7.70493 | -1.19194 | 1.32550 |
| H | -8.83167 | -1.52778 | 0.00225 |
| C | -7.20880 | -0.77113 | -2.07826 |
| H | -6.74635 | -0.01853 | -2.72124 |
| H | -6.71917 | -1.72646 | -2.27677 |
| H | -8.25964 | -0.86625 | -2.36497 |
| Si | 0.90058 | -0.40351 | -1.91658 |
| Cl | -1.61664 | 2.08730 | -1.59641 |

R-P=C(Si(II)Cl)-P(O)MeR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.84178 | 0.04401 | 1.07484 |
| C | 0.47022 | -0.29468 | -0.50374 |
| P | -1.05794 | -0.24430 | -1.34110 |
| Cl | 1.12088 | -2.69170 | -2.30979 |
| Si | 1.31530 | -0.54912 | -2.30172 |
| O | -0.48505 | -0.16242 | -2.77297 |
| C | -2.23308 | 1.05998 | -0.99714 |
| H | -3.07111 | 0.99102 | -1.69396 |
| H | -2.60021 | 0.95215 | 0.02632 |
| H | -1.73997 | 2.02612 | -1.10992 |
| H | 2.25720 | -0.15447 | 0.99148 |
| H | -1.77725 | -1.44043 | -1.14831 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.76849 | 0.09811 | 1.00485 |
| C | 0.39150 | -0.23545 | -0.57125 |
| P | -1.15284 | -0.27826 | -1.37554 |
| Cl | 1.34418 | -2.55140 | -2.41711 |
| Si | 1.21847 | -0.39302 | -2.37490 |
| O | -0.59466 | -0.23135 | -2.82467 |
| C | -2.28772 | 1.08140 | -1.08779 |
| H | -3.14616 | 0.99617 | -1.75767 |
| H | -2.63054 | 1.06352 | -0.05111 |
| H | -1.76814 | 2.02032 | -1.28083 |
| C | 2.59601 | -0.08972 | 1.04706 |
| H | 3.04935 | 0.18944 | 0.09354 |
| H | 3.01382 | 0.51462 | 1.85402 |
| H | 2.83604 | -1.13780 | 1.24943 |
| C | -2.05120 | -1.79944 | -1.07988 |
| H | -2.39670 | -1.83264 | -0.04460 |
| H | -2.90503 | -1.86169 | -1.75799 |
| H | -1.36953 | -2.62980 | -1.26961 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.66552 | 0.11636 | 0.72656 |
| C | 0.44086 | -0.27808 | -0.86995 |
| P | -1.11618 | -0.46662 | -1.65676 |
| Cl | 1.90574 | -2.45851 | -2.65051 |
| Si | 1.24712 | -0.40849 | -2.69270 |
| O | -0.55592 | -0.68175 | -3.09423 |
| C | -2.13327 | 1.01691 | -1.61701 |

| | | | |
|---|----------|----------|----------|
| H | -3.02279 | 0.89764 | -2.23746 |
| H | -2.42276 | 1.25204 | -0.59189 |
| H | -1.52814 | 1.83423 | -2.01183 |
| C | -2.14658 | -1.89011 | -1.13243 |
| C | -2.74377 | -1.59617 | 0.24291 |
| H | -3.45512 | -0.76777 | 0.21746 |
| H | -3.28251 | -2.48231 | 0.59001 |
| H | -1.97100 | -1.36837 | 0.98233 |
| C | -3.24718 | -2.08448 | -2.17781 |
| H | -2.82879 | -2.23536 | -3.17482 |
| H | -3.82647 | -2.97453 | -1.91611 |
| H | -3.94115 | -1.24170 | -2.21367 |
| C | -1.26624 | -3.13710 | -1.07097 |
| H | -0.79702 | -3.35115 | -2.03185 |
| H | -0.47327 | -3.03649 | -0.32846 |
| H | -1.89115 | -3.99080 | -0.79292 |
| C | 2.51185 | 0.10497 | 1.04121 |
| C | 2.98180 | -1.34995 | 1.03727 |
| H | 2.43042 | -1.95528 | 1.76315 |
| H | 2.86446 | -1.80676 | 0.05316 |
| H | 4.04157 | -1.39097 | 1.31341 |
| C | 3.27194 | 0.92149 | 0.00510 |
| H | 4.34029 | 0.91915 | 0.24839 |
| H | 3.16338 | 0.51613 | -1.00354 |
| H | 2.93731 | 1.96194 | -0.01516 |
| C | 2.70796 | 0.71117 | 2.43092 |
| H | 3.76882 | 0.69053 | 2.69893 |
| H | 2.37333 | 1.75158 | 2.46941 |
| H | 2.15844 | 0.15485 | 3.19548 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.91565 | -0.53044 | 1.06071 |
| C | 0.35667 | -0.33559 | -0.49162 |
| P | -1.31374 | -0.23503 | -0.98296 |
| Cl | 1.13886 | -1.46917 | -3.34916 |
| Si | 0.81908 | 0.38235 | -2.28434 |
| O | -1.05582 | 0.40260 | -2.37485 |
| C | -2.13426 | -1.82013 | -1.16117 |
| C | -2.37344 | -2.32460 | -2.43548 |
| C | -2.51700 | -2.54802 | -0.03552 |
| C | -3.00719 | -3.54979 | -2.57962 |
| H | -2.05225 | -1.76093 | -3.30276 |
| C | -3.14678 | -3.77101 | -0.18735 |
| H | -2.31034 | -2.17237 | 0.96164 |
| C | -3.39432 | -4.26986 | -1.45997 |
| H | -3.19199 | -3.94456 | -3.57176 |
| H | -3.44145 | -4.33887 | 0.68739 |
| H | -3.88624 | -5.22879 | -1.57680 |
| C | 2.71542 | -0.56181 | 0.92895 |
| C | 3.42133 | -0.83436 | -0.24636 |
| C | 3.42705 | -0.29830 | 2.10363 |
| C | 4.80544 | -0.81507 | -0.24633 |
| H | 2.88626 | -1.09333 | -1.15292 |
| C | 4.81164 | -0.27433 | 2.09903 |
| H | 2.88466 | -0.10184 | 3.02371 |
| C | 5.50121 | -0.53005 | 0.92195 |
| H | 5.34501 | -1.02889 | -1.16183 |
| H | 5.35388 | -0.06003 | 3.01289 |
| H | 6.58536 | -0.51724 | 0.91614 |
| C | -2.39017 | 0.80313 | 0.00936 |
| H | -3.36018 | 0.89865 | -0.48231 |
| H | -2.52673 | 0.36241 | 0.99877 |
| H | -1.92600 | 1.78468 | 0.11307 |

R = Mes

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| P | 1.08691 | -1.10708 | 1.43205 | C | 3.54833 | -0.43122 | 1.34711 |
| C | 0.33606 | -0.58878 | 0.04827 | C | 3.67915 | 1.42477 | -0.24401 |
| P | -1.34330 | -0.40256 | -0.43626 | C | 4.72723 | -0.93144 | 0.79916 |
| Cl | 1.12925 | -0.91280 | -2.95583 | C | 4.84770 | 0.85975 | -0.73896 |
| Si | 0.82555 | 0.61729 | -1.44799 | C | 5.35747 | -0.34935 | -0.28748 |
| O | -1.04275 | 0.67026 | -1.52110 | H | 5.16350 | -1.81665 | 1.23301 |
| C | -2.16792 | -1.86652 | -1.10140 | H | 5.39158 | 1.38721 | -1.50982 |
| C | -2.73910 | -1.86779 | -2.39332 | C | 3.01943 | -1.06802 | 2.64991 |
| C | -2.27195 | -3.00909 | -0.28687 | C | 3.32388 | 2.85576 | -0.70852 |
| C | -3.38007 | -3.02228 | -2.82474 | C | 6.59125 | -0.95246 | -0.95148 |
| C | -2.93009 | -4.13138 | -0.77385 | C | -3.31217 | 2.40257 | 1.17590 |
| C | -3.48318 | -4.16477 | -2.04332 | C | -2.75734 | -2.59332 | 0.11069 |
| H | -3.82232 | -3.02094 | -3.81619 | C | -7.14935 | -0.31066 | -0.61477 |
| H | -3.00887 | -5.00505 | -0.13379 | C | 4.58026 | 3.59786 | -1.18738 |
| C | 2.84985 | -0.74714 | 1.10634 | H | 4.32732 | 4.64825 | -1.35089 |
| C | 3.64293 | -1.67764 | 0.42020 | H | 5.38587 | 3.55346 | -0.45073 |
| C | 3.42380 | 0.41345 | 1.64202 | H | 4.95737 | 3.21267 | -2.13669 |
| C | 4.99929 | -1.41698 | 0.27127 | C | 2.77079 | 3.68549 | 0.45336 |
| C | 4.78373 | 0.63406 | 1.46702 | H | 1.80509 | 3.32084 | 0.82022 |
| C | 5.58838 | -0.26654 | 0.78096 | H | 3.46275 | 3.69520 | 1.29894 |
| H | 5.61447 | -2.13839 | -0.25902 | H | 2.61022 | 4.71678 | 0.12683 |
| H | 5.22594 | 1.53676 | 1.87903 | C | 2.32763 | 2.87227 | -1.87132 |
| C | -2.46588 | 0.34798 | 0.75644 | H | 2.67862 | 2.25495 | -2.70039 |
| H | -3.35890 | 0.67379 | 0.21794 | H | 1.35278 | 2.49367 | -1.57005 |
| H | -2.75868 | -0.35057 | 1.53936 | H | 2.20148 | 3.89775 | -2.23297 |
| H | -1.97191 | 1.21449 | 1.19829 | C | 7.77429 | 0.01488 | -0.82962 |
| C | 2.58715 | 1.42732 | 2.36283 | H | 8.65948 | -0.40914 | -1.31246 |
| H | 1.94415 | 1.96771 | 1.66090 | H | 7.56421 | 0.97521 | -1.30488 |
| H | 1.93317 | 0.95914 | 3.10637 | H | 8.01688 | 0.20520 | 0.21899 |
| H | 3.21217 | 2.15846 | 2.87750 | C | 6.99545 | -2.28368 | -0.32341 |
| C | 3.05574 | -2.92973 | -0.15927 | H | 7.86243 | -2.68734 | -0.85229 |
| H | 2.43951 | -3.46239 | 0.57276 | H | 7.27478 | -2.17158 | 0.72749 |
| H | 2.41618 | -2.70173 | -1.01686 | H | 6.19263 | -3.02194 | -0.39024 |
| H | 3.84145 | -3.60924 | -0.49247 | C | 6.28418 | -1.19650 | -2.43411 |
| C | 7.04699 | 0.00647 | 0.57430 | H | 5.44137 | -1.88191 | -2.54963 |
| H | 7.62308 | -0.91956 | 0.52603 | H | 6.03084 | -0.26883 | -2.95128 |
| H | 7.21077 | 0.54223 | -0.36608 | H | 7.15445 | -1.63267 | -2.93313 |
| H | 7.45504 | 0.62338 | 1.37708 | C | 3.99282 | -2.10974 | 3.20997 |
| C | -1.67651 | -3.11136 | 1.08623 | H | 4.98878 | -1.69480 | 3.38148 |
| H | -0.64189 | -3.46091 | 1.03298 | H | 3.61078 | -2.46150 | 4.17119 |
| H | -1.65396 | -2.17134 | 1.63744 | H | 4.08472 | -2.98180 | 2.55830 |
| H | -2.23711 | -3.82950 | 1.68670 | C | 2.88783 | 0.02351 | 3.72156 |
| C | -2.70791 | -0.70802 | -3.34644 | H | 3.84919 | 0.51290 | 3.89657 |
| H | -3.07576 | 0.21538 | -2.89870 | H | 2.16326 | 0.79289 | 3.44658 |
| H | -1.69106 | -0.50621 | -3.68655 | H | 2.55328 | -0.41979 | 4.66405 |
| C | -3.32525 | -0.93744 | -4.21551 | C | 1.67793 | -1.78347 | 2.47149 |
| C | -4.15686 | -5.39510 | -2.56548 | H | 0.86026 | -1.09270 | 2.25983 |
| H | -3.47072 | -5.96984 | -3.19523 | H | 1.71793 | -2.50263 | 1.65191 |
| H | -4.48353 | -6.04694 | -1.75387 | H | 1.42155 | -2.31345 | 3.39397 |
| H | -5.02492 | -5.14375 | -3.17800 | C | -1.83203 | 2.46701 | 1.52731 |
| | | | | H | -1.49672 | 1.55164 | 2.01916 |
| | | | | H | -1.17746 | 2.65610 | 0.67773 |
| | | | | H | -1.66249 | 3.28826 | 2.22785 |
| | | | | C | -4.05005 | 2.33555 | 2.52908 |
| | | | | H | -3.76729 | 3.19715 | 3.14017 |
| | | | | H | -5.13387 | 2.34736 | 2.41038 |
| | | | | H | -3.77975 | 1.42818 | 3.07403 |
| | | | | C | -3.73641 | 3.69380 | 0.46941 |
| | | | | H | -4.81598 | 3.73669 | 0.31496 |
| | | | | H | -3.45850 | 4.55551 | 1.08207 |
| | | | | H | -3.26162 | 3.81101 | -0.50559 |
| | | | | C | -1.43431 | -2.43396 | 0.85290 |
| | | | | H | -1.02144 | -3.42158 | 1.07174 |
| | | | | H | -0.66952 | -1.91487 | 0.28288 |
| | | | | H | -1.58449 | -1.91552 | 1.80386 |
| | | | | C | -2.57090 | -3.36044 | -1.20138 |
| R = Mes* | | | | | | | |
| P | 1.18182 | 1.07424 | 1.07833 | | | | |
| C | 0.40715 | 0.42425 | -0.24018 | | | | |
| P | -1.28667 | 0.36830 | -0.76095 | | | | |
| Cl | 1.46512 | -2.45970 | -1.23156 | | | | |
| O | -1.02849 | -0.75377 | -1.81663 | | | | |
| C | -2.88467 | 0.04234 | 0.07908 | | | | |
| C | -3.47323 | -1.24367 | -0.08685 | | | | |
| C | -3.73171 | 1.13137 | 0.41070 | | | | |
| C | -4.84268 | -1.29742 | -0.30875 | | | | |
| C | -5.09930 | 0.98998 | 0.19592 | | | | |
| C | -5.67175 | -0.18483 | -0.26397 | | | | |
| H | -5.28331 | -2.26515 | -0.50996 | | | | |
| H | -5.73794 | 1.83581 | 0.41017 | | | | |
| C | 2.94959 | 0.68681 | 0.72173 | | | | |

| | | | |
|----|----------|----------|----------|
| H | -1.90927 | -2.83404 | -1.88429 |
| H | -2.14070 | -4.34355 | -0.99180 |
| H | -3.53308 | -3.51566 | -1.69741 |
| C | -3.63704 | -3.45712 | 1.03729 |
| H | -3.88715 | -2.92799 | 1.96014 |
| H | -4.56559 | -3.78254 | 0.56662 |
| H | -3.07953 | -4.35839 | 1.30383 |
| C | -7.88140 | 1.02561 | -0.52399 |
| H | -7.88973 | 1.41923 | 0.49566 |
| H | -7.43578 | 1.77718 | -1.18060 |
| H | -8.92165 | 0.89272 | -0.83030 |
| C | -7.82568 | -1.29823 | 0.34364 |
| H | -7.37869 | -2.29239 | 0.28458 |
| H | -7.74725 | -0.95572 | 1.37836 |
| H | -8.88650 | -1.39418 | 0.09622 |
| C | -7.27374 | -0.83210 | -2.05138 |
| H | -6.81351 | -0.13977 | -2.76053 |
| H | -6.79104 | -1.80379 | -2.17213 |
| H | -8.32752 | -0.94495 | -2.32045 |
| Si | 0.83141 | -0.53326 | -1.94811 |
| C | -1.62980 | 1.81924 | -1.78742 |
| H | -2.55746 | 1.63272 | -2.33172 |
| H | -1.70360 | 2.75563 | -1.24415 |
| H | -0.80363 | 1.87618 | -2.50044 |

R-P=C(Si(III)Cl)-P(S)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.99152 | 0.22682 | 0.98007 |
| C | 0.49617 | -0.11461 | -0.56518 |
| P | -1.10124 | -0.04251 | -1.23519 |
| S | -0.69541 | 0.57755 | -3.07184 |
| Cl | 0.97149 | -2.44742 | -2.53073 |
| Si | 1.42024 | -0.36218 | -2.29969 |
| Cl | -2.50871 | 1.01145 | -0.22884 |
| H | -1.67936 | -1.32215 | -1.20443 |
| H | 2.39015 | 0.01140 | 0.75994 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.99559 | 0.05330 | 0.92101 |
| C | 0.48717 | -0.17723 | -0.64198 |
| P | -1.13172 | -0.10293 | -1.25429 |
| S | -0.77139 | 0.41055 | -3.14649 |
| Cl | 1.23084 | -2.43084 | -2.66621 |
| Si | 1.38975 | -0.30114 | -2.38892 |
| C | 2.79794 | -0.27392 | 0.82146 |
| H | 3.20800 | -0.01883 | -0.15937 |
| H | 3.31445 | 0.28810 | 1.60133 |
| H | 2.97181 | -1.33904 | 1.00196 |
| C | -1.97855 | -1.67824 | -1.09593 |
| H | -1.34208 | -2.43401 | -1.56095 |
| H | -2.12973 | -1.90201 | -0.03874 |
| H | -2.93755 | -1.62008 | -1.61225 |
| Cl | -2.38761 | 1.18338 | -0.28961 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.92547 | -0.11459 | 1.01122 |
| C | 0.51219 | -0.04298 | -0.60267 |
| P | -1.15865 | -0.14499 | -1.11294 |
| S | -1.01959 | 0.53455 | -2.98568 |
| Cl | 1.89748 | -1.38633 | -3.13567 |
| Si | 1.28702 | 0.51038 | -2.33461 |
| C | -1.94543 | -1.82072 | -0.99031 |
| C | -1.05042 | -2.80386 | -1.74198 |
| H | -1.52102 | -3.79036 | -1.70146 |
| H | -0.92759 | -2.52596 | -2.78938 |

| | | | |
|----|----------|----------|----------|
| H | -0.05785 | -2.87951 | -1.29605 |
| C | -3.31870 | -1.74496 | -1.65396 |
| H | -3.76317 | -2.74394 | -1.63886 |
| H | -3.99219 | -1.06767 | -1.12647 |
| H | -3.24453 | -1.42662 | -2.69590 |
| C | -2.07002 | -2.22856 | 0.47411 |
| H | -2.73842 | -1.56962 | 1.02923 |
| H | -2.48161 | -3.24114 | 0.51297 |
| H | -1.10136 | -2.24408 | 0.97852 |
| C | 2.79153 | -0.04764 | 1.13437 |
| C | 3.42265 | -1.23492 | 0.41285 |
| H | 3.04389 | -2.18702 | 0.79535 |
| H | 3.23903 | -1.20995 | -0.66175 |
| H | 4.50626 | -1.22283 | 0.57483 |
| C | 3.09959 | -0.12888 | 2.63084 |
| H | 4.18191 | -0.08869 | 2.78660 |
| H | 2.65010 | 0.70076 | 3.18329 |
| H | 2.73256 | -1.06086 | 3.06960 |
| C | 3.30820 | 1.27600 | 0.57640 |
| H | 3.11844 | 1.37629 | -0.49523 |
| H | 2.85377 | 2.13283 | 1.08105 |
| H | 4.39114 | 1.33641 | 0.73093 |
| Cl | -2.39603 | 1.03535 | 0.00834 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.96493 | 0.36943 | 0.26073 |
| C | 0.45431 | -0.22840 | -1.20826 |
| P | -1.18729 | -0.22059 | -1.76732 |
| C | 2.73102 | 0.01378 | 0.31850 |
| C | 3.35657 | -1.03639 | -0.36107 |
| C | 3.50365 | 0.86068 | 1.12061 |
| C | 4.72715 | -1.20960 | -0.26343 |
| C | 4.87432 | 0.68907 | 1.20895 |
| C | 5.48661 | -0.34497 | 0.51337 |
| H | 5.20362 | -2.02694 | -0.79228 |
| H | 5.46596 | 1.35760 | 1.82364 |
| C | -2.09635 | -1.68543 | -1.24699 |
| C | -2.49161 | -2.63275 | -2.18271 |
| C | -2.36929 | -1.87186 | 0.10712 |
| C | -3.16997 | -3.76706 | -1.76187 |
| C | -3.04467 | -3.00654 | 0.51792 |
| C | -3.44609 | -3.95332 | -0.41685 |
| H | -3.47777 | -4.50810 | -2.49001 |
| H | -3.25855 | -3.15428 | 1.56993 |
| S | -0.91963 | -0.09283 | -3.73493 |
| Cl | 1.15581 | -2.78716 | -2.94222 |
| Si | 1.29589 | -0.63822 | -2.93866 |
| H | -2.05642 | -1.13314 | 0.83710 |
| H | -2.25979 | -2.48346 | -3.23027 |
| H | -3.97467 | -4.84196 | -0.09118 |
| H | 3.02212 | 1.66554 | 1.66776 |
| H | 6.55919 | -0.48503 | 0.58653 |
| H | 2.76642 | -1.74429 | -0.93233 |
| Cl | -2.31068 | 1.31051 | -1.01440 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.12946 | 0.69069 | 1.22483 |
| C | 0.43737 | 0.29826 | -0.24228 |
| P | -1.25661 | 0.31043 | -0.70903 |
| Cl | 1.88974 | -2.23060 | -1.48792 |
| C | -2.83915 | -0.00696 | 0.17148 |
| C | -3.42549 | -1.29020 | -0.03979 |
| C | -3.68103 | 1.06038 | 0.58082 |
| C | -4.79362 | -1.33479 | -0.26206 |
| C | -5.04582 | 0.92972 | 0.34232 |

| | | | |
|---|----------|----------|----------|
| C | -5.61667 | -0.21845 | -0.18278 |
| H | -5.23808 | -2.29654 | -0.48633 |
| H | -5.68396 | 1.76558 | 0.59339 |
| C | 2.92278 | 0.51055 | 0.86181 |
| C | 3.61485 | -0.61346 | 1.38233 |
| C | 3.58650 | 1.38292 | -0.03320 |
| C | 4.82474 | -0.96475 | 0.79551 |
| C | 4.79057 | 0.95319 | -0.58314 |
| C | 5.39892 | -0.24198 | -0.24067 |
| H | 5.33295 | -1.84727 | 1.14887 |
| H | 5.27895 | 1.59482 | -1.30611 |
| C | 3.12707 | -1.42545 | 2.59859 |
| C | 3.21860 | 2.85168 | -0.33839 |
| C | 6.66647 | -0.69073 | -0.96041 |
| C | -3.27455 | 2.25995 | 1.46189 |
| C | -2.73730 | -2.65358 | 0.18308 |
| C | -7.08800 | -0.31724 | -0.56424 |
| C | 4.36501 | 3.71100 | 0.22766 |
| H | 4.16512 | 4.76806 | 0.03046 |
| H | 4.45523 | 3.57634 | 1.30879 |
| H | 5.32731 | 3.46173 | -0.22064 |
| C | 1.94326 | 3.37093 | 0.31943 |
| H | 1.04042 | 2.98350 | -0.15039 |
| H | 1.91249 | 3.15499 | 1.39327 |
| H | 1.91442 | 4.45999 | 0.21926 |
| C | 3.10459 | 3.10499 | -1.84503 |
| H | 4.03676 | 2.89035 | -2.37042 |
| H | 2.32375 | 2.48549 | -2.29107 |
| H | 2.86058 | 4.15602 | -2.02437 |
| C | 7.77078 | 0.35627 | -0.77563 |
| H | 8.67934 | 0.04067 | -1.29633 |
| H | 7.47993 | 1.32914 | -1.17700 |
| H | 8.01285 | 0.48764 | 0.28207 |
| C | 7.18502 | -2.02935 | -0.44171 |
| H | 8.07491 | -2.31807 | -1.00640 |
| H | 7.46788 | -1.97738 | 0.61297 |
| H | 6.44416 | -2.82348 | -0.56201 |
| C | 6.35294 | -0.84339 | -2.45393 |
| H | 5.56370 | -1.58186 | -2.61246 |
| H | 6.01835 | 0.09832 | -2.89377 |
| H | 7.24572 | -1.16955 | -2.99526 |
| C | 4.17436 | -2.44019 | 3.06617 |
| H | 5.12976 | -1.96694 | 3.30441 |
| H | 3.80892 | -2.92400 | 3.97500 |
| H | 4.34797 | -3.22596 | 2.32736 |
| C | 2.88601 | -0.47366 | 3.77884 |
| H | 3.79979 | 0.07109 | 4.02870 |
| H | 2.10229 | 0.25800 | 3.57338 |
| H | 2.57771 | -1.04469 | 4.65936 |
| C | 1.85468 | -2.22112 | 2.30062 |
| H | 0.99402 | -1.57362 | 2.11916 |
| H | 1.97823 | -2.85234 | 1.41911 |
| H | 1.60481 | -2.85354 | 3.15801 |
| C | -1.80300 | 2.29103 | 1.85185 |
| H | -1.47792 | 1.33257 | 2.26183 |
| H | -1.14374 | 2.56411 | 1.03092 |
| H | -1.65591 | 3.04081 | 2.63340 |
| C | -4.04431 | 2.05944 | 2.78564 |
| H | -3.76624 | 2.85198 | 3.48566 |
| H | -5.12531 | 2.09599 | 2.64763 |
| H | -3.79364 | 1.09890 | 3.24218 |
| C | -3.68381 | 3.61266 | 0.87408 |
| H | -4.75407 | 3.66003 | 0.66436 |
| H | -3.45599 | 4.40387 | 1.59343 |
| H | -3.14808 | 3.83035 | -0.04886 |
| C | -1.28885 | -2.56023 | 0.64708 |

| | | | |
|----|----------|----------|----------|
| H | -0.96319 | -3.54610 | 0.98852 |
| H | -0.59508 | -2.26223 | -0.13592 |
| H | -1.19205 | -1.87467 | 1.49266 |
| C | -2.83681 | -3.58653 | -1.02519 |
| H | -2.26780 | -3.20283 | -1.87083 |
| H | -2.43314 | -4.56738 | -0.76023 |
| H | -3.87150 | -3.73099 | -1.34382 |
| C | -3.50285 | -3.30144 | 1.35766 |
| H | -3.47532 | -2.66270 | 2.24400 |
| H | -4.54766 | -3.50188 | 1.11821 |
| H | -3.02775 | -4.25316 | 1.60975 |
| C | -7.81325 | 1.01815 | -0.42148 |
| H | -7.83970 | 1.36068 | 0.61615 |
| H | -7.34935 | 1.79768 | -1.03087 |
| H | -8.84785 | 0.90792 | -0.75467 |
| C | -7.78857 | -1.34635 | 0.33095 |
| H | -7.35048 | -2.34096 | 0.22766 |
| H | -7.72574 | -1.05819 | 1.38317 |
| H | -8.84556 | -1.41922 | 0.06064 |
| C | -7.18575 | -0.76633 | -2.02732 |
| H | -6.70385 | -0.04475 | -2.69119 |
| H | -6.70833 | -1.73540 | -2.18495 |
| H | -8.23453 | -0.85579 | -2.32332 |
| Si | 1.19699 | -0.25169 | -1.98890 |
| S | -1.11410 | -0.80737 | -2.35954 |
| Cl | -1.56241 | 2.21532 | -1.44969 |

R-P=C(Si(II)Cl)-P(S)MeR

R = H

| | | | |
|----|----------|----------|----------|
| P | 1.05530 | -0.00794 | 1.07853 |
| C | 0.59421 | -0.32648 | -0.48245 |
| P | -1.00307 | -0.14272 | -1.17651 |
| S | -0.48629 | 0.34663 | -3.04205 |
| Cl | 1.02407 | -2.71260 | -2.33466 |
| Si | 1.57823 | -0.64039 | -2.16206 |
| H | -1.64786 | -1.39437 | -1.11868 |
| H | 2.45618 | -0.25909 | 0.91202 |
| C | -2.15501 | 0.97779 | -0.36609 |
| H | -3.09072 | 0.99945 | -0.92839 |
| H | -2.34578 | 0.62869 | 0.65156 |
| H | -1.72137 | 1.97775 | -0.34003 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 1.00029 | -0.01430 | 0.87539 |
| C | 0.50963 | -0.19084 | -0.69937 |
| P | -1.14277 | -0.11970 | -1.27356 |
| S | -0.79353 | 0.29313 | -3.20902 |
| Cl | 1.37316 | -2.40412 | -2.67357 |
| Si | 1.41769 | -0.25766 | -2.43803 |
| C | -2.20641 | 1.09376 | -0.46692 |
| H | -1.75607 | 2.08105 | -0.56779 |
| H | -3.18765 | 1.09155 | -0.94619 |
| H | -2.31349 | 0.84473 | 0.59131 |
| C | 2.81854 | -0.25457 | 0.78875 |
| H | 3.22290 | 0.03635 | -0.18411 |
| H | 3.30322 | 0.31738 | 1.58194 |
| H | 3.04000 | -1.31329 | 0.95322 |
| C | -1.94721 | -1.71726 | -1.05788 |
| H | -1.30453 | -2.47679 | -1.50491 |
| H | -2.08067 | -1.92235 | 0.00668 |
| H | -2.91459 | -1.70918 | -1.56383 |

R = t-Bu

| | | | |
|---|---------|----------|----------|
| P | 0.63919 | 0.14610 | 0.54238 |
| C | 0.47687 | -0.28087 | -1.05998 |

| | | | |
|----|----------|----------|----------|
| P | -1.13328 | -0.43848 | -1.77469 |
| Cl | 2.12696 | -2.50805 | -2.56288 |
| Si | 1.53822 | -0.44095 | -2.70840 |
| C | -2.14198 | 1.04234 | -1.53006 |
| H | -3.09766 | 0.94202 | -2.04655 |
| H | -2.30564 | 1.21539 | -0.46526 |
| H | -1.59409 | 1.88428 | -1.95345 |
| C | -2.11307 | -1.88483 | -1.14723 |
| C | -2.57674 | -1.61356 | 0.28193 |
| H | -3.29162 | -0.78983 | 0.33594 |
| H | -3.07712 | -2.50893 | 0.66214 |
| H | -1.74086 | -1.39191 | 0.94987 |
| C | -3.31597 | -2.07367 | -2.07121 |
| H | -3.00567 | -2.24080 | -3.10455 |
| H | -3.87500 | -2.95355 | -1.74023 |
| H | -4.00034 | -1.22244 | -2.04449 |
| C | -1.22587 | -3.12547 | -1.19126 |
| H | -0.84798 | -3.31664 | -2.19676 |
| H | -0.36756 | -3.03471 | -0.52413 |
| H | -1.81749 | -3.98956 | -0.87512 |
| C | 2.45406 | 0.10105 | 1.00007 |
| C | 2.88397 | -1.36295 | 1.09871 |
| H | 2.25370 | -1.92314 | 1.79599 |
| H | 2.84634 | -1.86066 | 0.12856 |
| H | 3.91262 | -1.41402 | 1.47328 |
| C | 3.32842 | 0.86067 | 0.01202 |
| H | 4.36531 | 0.85936 | 0.36649 |
| H | 3.32298 | 0.41068 | -0.98395 |
| H | 3.01299 | 1.90193 | -0.09199 |
| C | 2.54172 | 0.75808 | 2.37882 |
| H | 3.57406 | 0.72125 | 2.74006 |
| H | 2.23483 | 1.80723 | 2.34793 |
| H | 1.91142 | 0.24658 | 3.11157 |
| S | -0.62023 | -0.66947 | -3.71038 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.96901 | 0.21906 | 0.32572 |
| C | 0.46498 | -0.27089 | -1.18373 |
| P | -1.21720 | -0.21652 | -1.67790 |
| C | 2.75204 | -0.05620 | 0.35979 |
| C | 3.42096 | -1.00987 | -0.41308 |
| C | 3.48834 | 0.74641 | 1.23700 |
| C | 4.79831 | -1.13034 | -0.32982 |
| C | 4.86563 | 0.62757 | 1.31240 |
| C | 5.52137 | -0.30950 | 0.52528 |
| H | 5.30879 | -1.87272 | -0.93243 |
| H | 5.42859 | 1.26162 | 1.98774 |
| C | -2.09778 | -1.71032 | -1.16341 |
| C | -2.57878 | -2.61160 | -2.10444 |
| C | -2.28796 | -1.95216 | 0.19639 |
| C | -3.26159 | -3.74474 | -1.68680 |
| C | -2.96978 | -3.08436 | 0.60715 |
| C | -3.45923 | -3.97976 | -0.33537 |
| H | -3.63261 | -4.44883 | -2.42233 |
| H | -3.11395 | -3.27280 | 1.66466 |
| S | -0.98924 | -0.09298 | -3.66730 |
| Cl | 1.22819 | -2.70092 | -3.02659 |
| Si | 1.27633 | -0.54442 | -2.94771 |
| C | -2.16737 | 1.16089 | -0.99996 |
| H | -1.66967 | 2.09290 | -1.26853 |
| H | -3.17216 | 1.14043 | -1.42605 |
| H | -2.22992 | 1.07666 | 0.08670 |
| H | -1.88786 | -1.26895 | 0.93903 |
| H | -2.40481 | -2.42634 | -3.15801 |
| H | -3.98953 | -4.86810 | -0.01162 |
| H | 2.97311 | 1.47551 | 1.85519 |

| | | | |
|---|---------|----------|----------|
| H | 6.59929 | -0.40840 | 0.58681 |
| H | 2.86084 | -1.68515 | -1.05029 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.12944 | 0.09831 | 0.71639 |
| C | 0.62537 | -0.57564 | -0.71821 |
| P | -1.02936 | -0.48446 | -1.33583 |
| C | 2.95374 | 0.05521 | 0.61006 |
| C | 3.66889 | -1.10343 | 0.94232 |
| C | 3.63570 | 1.24294 | 0.30658 |
| C | 5.05746 | -1.05333 | 0.95060 |
| C | 5.02342 | 1.24589 | 0.32381 |
| C | 5.75409 | 0.10702 | 0.63949 |
| H | 5.61074 | -1.95107 | 1.21124 |
| H | 5.54867 | 2.16569 | 0.08267 |
| C | -2.13802 | -1.92307 | -1.17875 |
| C | -3.27727 | -1.95767 | -2.01080 |
| C | -1.92894 | -2.95378 | -0.24113 |
| C | -4.16907 | -3.01612 | -1.88379 |
| C | -2.85389 | -3.98782 | -0.16774 |
| C | -3.97705 | -4.04638 | -0.97809 |
| H | -5.04422 | -3.03060 | -2.52630 |
| H | -2.68332 | -4.77699 | 0.55788 |
| S | -0.47303 | -0.10286 | -3.24380 |
| Cl | 1.32253 | -3.00580 | -2.49312 |
| Si | 1.63338 | -0.85908 | -2.37714 |
| C | -1.93112 | 0.87524 | -0.54780 |
| H | -1.39053 | 1.80516 | -0.72517 |
| H | -2.94815 | 0.95217 | -0.92965 |
| H | -1.97026 | 0.67518 | 0.52612 |
| C | 2.89019 | 2.48701 | -0.07209 |
| H | 2.44042 | 2.38309 | -1.06461 |
| H | 2.07711 | 2.70274 | 0.62952 |
| H | 3.55453 | 3.35198 | -0.09299 |
| C | 2.97259 | -2.38981 | 1.27079 |
| H | 2.12437 | -2.23312 | 1.94438 |
| H | 2.58316 | -2.86580 | 0.36569 |
| H | 3.65736 | -3.09119 | 1.74967 |
| C | 7.25190 | 0.12492 | 0.62113 |
| H | 7.66808 | -0.61824 | 1.30360 |
| H | 7.62853 | -0.10327 | -0.38096 |
| H | 7.64261 | 1.10527 | 0.90055 |
| C | -0.75917 | -3.01841 | 0.69202 |
| H | 0.18090 | -3.05711 | 0.14037 |
| H | -0.71216 | -2.15506 | 1.35896 |
| H | -0.83001 | -3.91413 | 1.30977 |
| C | -3.59508 | -0.94405 | -3.07328 |
| H | -3.38248 | 0.08585 | -2.78805 |
| H | -3.01182 | -1.13798 | -3.97659 |
| H | -4.65317 | -1.00367 | -3.33197 |
| C | -4.93366 | -5.19426 | -0.89285 |
| H | -4.59401 | -6.02387 | -1.52070 |
| H | -5.01379 | -5.57103 | 0.12848 |
| H | -5.92983 | -4.91002 | -1.23567 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.10170 | 0.73783 | 1.12028 |
| C | 0.41127 | 0.28526 | -0.32971 |
| P | -1.30168 | 0.33782 | -0.80787 |
| Cl | 1.85265 | -2.33518 | -1.45518 |
| C | -2.87571 | 0.07743 | 0.12307 |
| C | -3.48791 | -1.20584 | 0.03765 |
| C | -3.70357 | 1.19162 | 0.42289 |
| C | -4.85971 | -1.25110 | -0.16936 |
| C | -5.07258 | 1.06502 | 0.20351 |

| | | | |
|---|----------|----------|----------|
| C | -5.66659 | -0.12144 | -0.19636 |
| H | -5.31878 | -2.22342 | -0.29894 |
| H | -5.69574 | 1.93267 | 0.37184 |
| C | 2.90718 | 0.53563 | 0.80039 |
| C | 3.58645 | -0.59353 | 1.31491 |
| C | 3.60348 | 1.44537 | -0.03679 |
| C | 4.81380 | -0.93128 | 0.75092 |
| C | 4.82216 | 1.03389 | -0.56156 |
| C | 5.41454 | -0.18053 | -0.24554 |
| H | 5.31232 | -1.82290 | 1.09550 |
| H | 5.34104 | 1.69362 | -1.24272 |
| C | 3.08740 | -1.40973 | 2.52469 |
| C | 3.16928 | 2.90591 | -0.30422 |
| C | 6.70050 | -0.60815 | -0.94514 |
| C | -3.26938 | 2.46995 | 1.17169 |
| C | -2.81741 | -2.55465 | 0.36816 |
| C | -7.14380 | -0.23629 | -0.55122 |
| C | 4.39594 | 3.78597 | -0.58962 |
| H | 4.08214 | 4.83262 | -0.60345 |
| H | 5.16621 | 3.67205 | 0.17665 |
| H | 4.84317 | 3.57814 | -1.56344 |
| C | 2.50613 | 3.51425 | 0.93461 |
| H | 1.55124 | 3.04078 | 1.18714 |
| H | 3.15477 | 3.43653 | 1.81045 |
| H | 2.29271 | 4.57193 | 0.75648 |
| C | 2.23409 | 3.04472 | -1.50779 |
| H | 2.66752 | 2.58652 | -2.39877 |
| H | 1.27367 | 2.56674 | -1.32611 |
| H | 2.05666 | 4.10475 | -1.71574 |
| C | 7.80564 | 0.42140 | -0.68295 |
| H | 8.72723 | 0.12250 | -1.19067 |
| H | 7.53180 | 1.41333 | -1.04806 |
| H | 8.01746 | 0.50374 | 0.38617 |
| C | 7.19348 | -1.97168 | -0.46818 |
| H | 8.09560 | -2.24632 | -1.02050 |
| H | 7.44855 | -1.96516 | 0.59479 |
| H | 6.44849 | -2.75244 | -0.63956 |
| C | 6.43355 | -0.69579 | -2.45288 |
| H | 5.64558 | -1.42148 | -2.66710 |
| H | 6.11909 | 0.26610 | -2.86293 |
| H | 7.34093 | -1.00555 | -2.97948 |
| C | 4.12965 | -2.42708 | 2.99755 |
| H | 5.08361 | -1.95640 | 3.24666 |
| H | 3.75527 | -2.91456 | 3.90085 |
| H | 4.30879 | -3.20973 | 2.25667 |
| C | 2.84535 | -0.45341 | 3.70152 |
| H | 3.75810 | 0.09365 | 3.95053 |
| H | 2.06154 | 0.27663 | 3.48960 |
| H | 2.53582 | -1.02106 | 4.58391 |
| C | 1.81186 | -2.19879 | 2.23030 |
| H | 0.96102 | -1.54722 | 2.02638 |
| H | 1.93726 | -2.85000 | 1.36421 |
| H | 1.54924 | -2.81021 | 3.09918 |
| C | -1.80665 | 2.48180 | 1.59949 |
| H | -1.54909 | 1.57752 | 2.15389 |
| H | -1.09471 | 2.58435 | 0.78343 |
| H | -1.63435 | 3.33166 | 2.26471 |
| C | -4.06720 | 2.46362 | 2.49353 |
| H | -3.76161 | 3.31822 | 3.10338 |
| H | -5.14274 | 2.53498 | 2.33059 |
| H | -3.87061 | 1.55197 | 3.06224 |
| C | -3.62115 | 3.75939 | 0.42347 |
| H | -4.69004 | 3.82090 | 0.21020 |
| H | -3.35980 | 4.62375 | 1.03979 |
| H | -3.09231 | 3.85403 | -0.52483 |
| C | -1.36020 | -2.44124 | 0.79559 |

| | | | |
|----|----------|----------|----------|
| H | -1.03828 | -3.39800 | 1.21434 |
| H | -0.68224 | -2.21764 | -0.02543 |
| H | -1.24022 | -1.68589 | 1.57605 |
| C | -2.95156 | -3.58657 | -0.75361 |
| H | -2.39846 | -3.28051 | -1.64044 |
| H | -2.54907 | -4.54479 | -0.41424 |
| H | -3.99439 | -3.74886 | -1.03542 |
| C | -3.57070 | -3.08615 | 1.60686 |
| H | -3.51439 | -2.37544 | 2.43528 |
| H | -4.62355 | -3.28663 | 1.40465 |
| H | -3.10715 | -4.02189 | 1.93024 |
| C | -7.84861 | 1.11749 | -0.53832 |
| H | -7.85707 | 1.56511 | 0.45885 |
| H | -7.38199 | 1.82357 | -1.22984 |
| H | -8.88887 | 0.98974 | -0.84675 |
| C | -7.84817 | -1.15721 | 0.45223 |
| H | -7.42453 | -2.16331 | 0.44744 |
| H | -7.76854 | -0.76339 | 1.46845 |
| H | -8.90927 | -1.24211 | 0.20210 |
| C | -7.26719 | -0.83143 | -1.95908 |
| H | -6.78574 | -0.18831 | -2.69967 |
| H | -6.80383 | -1.81787 | -2.02266 |
| H | -8.32083 | -0.93648 | -2.23190 |
| Si | 1.12649 | -0.39801 | -2.04988 |
| S | -1.16725 | -0.98171 | -2.34218 |
| C | -1.53890 | 1.90868 | -1.69529 |
| H | -1.45654 | 2.79575 | -1.07529 |
| H | -0.75904 | 1.92633 | -2.45878 |
| H | -2.51194 | 1.87714 | -2.18736 |

E = Ge(II)

R-P=C(Ge(II)Cl)-P(O)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.29435 | 0.56617 | 0.60842 |
| C | 0.22926 | 0.36855 | -1.03311 |
| P | -1.12731 | -0.01182 | -2.04410 |
| Ge | 1.31552 | 0.82146 | -2.78519 |
| Cl | 1.83806 | -1.31483 | -3.21569 |
| O | -0.70661 | 0.61857 | -3.36114 |
| H | 1.67818 | 0.92075 | 0.70701 |
| H | -1.34825 | -1.39419 | -2.14827 |
| Cl | -2.93656 | 0.61830 | -1.44062 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.55866 | 0.25480 | 0.66466 |
| C | 0.21676 | 0.15235 | -0.94849 |
| P | -1.31956 | -0.01921 | -1.73437 |
| Ge | 1.06971 | 0.52876 | -2.83525 |
| Cl | 1.40028 | -1.63920 | -3.35883 |
| O | -0.98299 | 0.50475 | -3.12946 |
| C | -1.95133 | -1.68883 | -1.76625 |
| H | -2.20074 | -2.01365 | -0.75559 |
| H | -2.83784 | -1.72212 | -2.40166 |
| H | -1.16423 | -2.31821 | -2.18758 |
| C | 2.38914 | 0.39865 | 0.71760 |
| H | 2.80502 | -0.59767 | 0.89858 |
| H | 2.80907 | 0.79010 | -0.20974 |
| H | 2.68031 | 1.03306 | 1.55732 |
| Cl | -2.83087 | 1.05683 | -0.92521 |

R = t-Bu

| | | | |
|---|---------|----------|----------|
| P | 0.76669 | -0.23326 | 0.59292 |
| C | 0.15162 | 0.09962 | -0.90733 |

| | | | |
|----|----------|----------|----------|
| P | -1.51485 | -0.12009 | -1.38818 |
| Ge | 0.53203 | 0.98241 | -2.79196 |
| Cl | 1.31611 | -0.87798 | -3.79327 |
| O | -1.47478 | 0.44185 | -2.80824 |
| C | -2.24873 | -1.79783 | -1.33161 |
| C | 2.60300 | 0.11753 | 0.56529 |
| Cl | -2.76130 | 1.02082 | -0.25510 |
| C | 3.10727 | 0.82901 | -0.67617 |
| H | 2.61391 | 1.79383 | -0.81922 |
| H | 4.18159 | 1.02209 | -0.58192 |
| H | 2.96546 | 0.22179 | -1.57356 |
| C | 2.87968 | 0.95689 | 1.81564 |
| H | 2.50027 | 0.47470 | 2.72084 |
| H | 3.95943 | 1.09152 | 1.93594 |
| H | 2.42417 | 1.94804 | 1.74489 |
| C | 3.27642 | -1.25137 | 0.70850 |
| H | 4.35578 | -1.11488 | 0.83440 |
| H | 2.90849 | -1.79811 | 1.58164 |
| H | 3.11583 | -1.87040 | -0.17731 |
| C | -2.36263 | -2.27996 | 0.11121 |
| H | -2.74374 | -3.30503 | 0.10553 |
| H | -1.39402 | -2.28811 | 0.61701 |
| H | -3.05100 | -1.66626 | 0.69397 |
| C | -1.32003 | -2.71533 | -2.13080 |
| H | -1.20225 | -2.37978 | -3.16164 |
| H | -0.32655 | -2.78163 | -1.68469 |
| H | -1.75791 | -3.71746 | -2.14124 |
| C | -3.62203 | -1.73182 | -2.00121 |
| H | -4.03486 | -2.74369 | -2.04308 |
| H | -4.31891 | -1.10559 | -1.44180 |
| H | -3.55141 | -1.35089 | -3.02157 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.96480 | -0.20178 | 1.05995 |
| C | 0.24416 | -0.02245 | -0.42218 |
| P | -1.44902 | -0.03100 | -0.79238 |
| C | 2.73767 | -0.10470 | 0.72188 |
| C | 3.55351 | 0.29590 | 1.78384 |
| C | 3.32673 | -0.42806 | -0.50417 |
| C | 4.92316 | 0.41430 | 1.61347 |
| C | 4.69694 | -0.31946 | -0.66776 |
| C | 5.49454 | 0.10894 | 0.38636 |
| H | 5.54615 | 0.73907 | 2.43888 |
| H | 5.14644 | -0.57701 | -1.61992 |
| Ge | 0.60894 | 0.85576 | -2.29204 |
| Cl | 0.82720 | -1.03784 | -3.49713 |
| O | -1.46513 | 0.74764 | -2.10474 |
| H | 2.71454 | -0.80090 | -1.31867 |
| H | 6.56718 | 0.19293 | 0.25304 |
| H | 3.10537 | 0.52576 | 2.74583 |
| Cl | -2.59073 | 0.89447 | 0.60369 |
| C | -2.19443 | -1.64606 | -0.96669 |
| C | -2.47437 | -2.11028 | -2.24838 |
| C | -2.44976 | -2.44403 | 0.14705 |
| C | -3.01966 | -3.37504 | -2.41054 |
| H | -2.25854 | -1.48528 | -3.10575 |
| C | -2.98955 | -3.70550 | -0.02552 |
| H | -2.23143 | -2.07911 | 1.14472 |
| C | -3.27558 | -4.16948 | -1.30401 |
| H | -3.24033 | -3.73970 | -3.40675 |
| H | -3.19037 | -4.32887 | 0.83779 |
| H | -3.70000 | -5.15835 | -1.43545 |

R = Mes

| | | | |
|---|---------|---------|---------|
| P | 0.84382 | 0.10389 | 1.05317 |
|---|---------|---------|---------|

| | | | |
|---|----------|----------|----------|
| C | 0.41343 | -0.51604 | -0.42272 |
| P | -1.10285 | -0.47514 | -1.29025 |
| C | 2.68673 | 0.08341 | 0.93951 |
| C | 3.42585 | -1.10253 | 1.17981 |
| C | 3.35259 | 1.25258 | 0.49715 |
| C | 4.74922 | -1.13760 | 0.75935 |
| C | 4.68382 | 1.13176 | 0.09981 |
| C | 5.38772 | -0.05797 | 0.16604 |
| H | 5.31332 | -2.04762 | 0.90484 |
| H | 5.18959 | 2.00533 | -0.27813 |
| C | 2.72498 | 2.66591 | 0.48672 |
| C | 2.88140 | -2.33045 | 1.93939 |
| C | 6.82260 | -0.20096 | -0.33244 |
| C | 2.07444 | -3.25972 | 1.02693 |
| H | 1.18616 | -2.78090 | 0.61941 |
| H | 2.67677 | -3.59380 | 0.18004 |
| H | 1.75982 | -4.14417 | 1.58952 |
| C | 2.03187 | -1.89195 | 3.13489 |
| H | 2.59909 | -1.24064 | 3.80458 |
| H | 1.12088 | -1.35686 | 2.84751 |
| H | 1.70622 | -2.76976 | 3.69955 |
| C | 4.02411 | -3.16821 | 2.52921 |
| H | 4.60030 | -3.68842 | 1.76151 |
| H | 4.70842 | -2.56377 | 3.12966 |
| H | 3.59599 | -3.93689 | 3.17680 |
| C | 1.70095 | 2.85526 | -0.63937 |
| H | 0.79515 | 2.26811 | -0.49245 |
| H | 1.40090 | 3.90602 | -0.68635 |
| H | 2.12827 | 2.58243 | -1.60730 |
| C | 2.07336 | 2.96183 | 1.84356 |
| H | 1.23567 | 2.29787 | 2.06994 |
| H | 2.80218 | 2.87007 | 2.65256 |
| H | 1.68130 | 3.98258 | 1.84956 |
| C | 3.78851 | 3.75225 | 0.28614 |
| H | 4.59118 | 3.68452 | 1.02410 |
| H | 4.22925 | 3.72554 | -0.71298 |
| H | 3.31247 | 4.72872 | 0.40025 |
| C | 7.34974 | 1.08561 | -0.96236 |
| H | 7.38538 | 1.90819 | -0.24341 |
| H | 8.36757 | 0.92267 | -1.32492 |
| H | 6.74130 | 1.39864 | -1.81454 |
| C | 6.87480 | -1.30906 | -1.39114 |
| H | 6.54684 | -2.26940 | -0.98848 |
| H | 6.23259 | -1.06768 | -2.24148 |
| H | 7.89751 | -1.43147 | -1.75883 |
| C | 7.74047 | -0.57382 | 0.83772 |
| H | 7.44344 | -1.51622 | 1.30220 |
| H | 8.77075 | -0.68480 | 0.48791 |
| H | 7.72441 | 0.20034 | 1.60897 |
| C | -2.23563 | -1.87453 | -1.13708 |
| C | -2.62662 | -2.65782 | -2.25634 |
| C | -2.72725 | -2.18330 | 0.14767 |
| C | -3.46443 | -3.73935 | -2.02429 |
| C | -3.56750 | -3.27887 | 0.30028 |
| C | -3.94347 | -4.07520 | -0.76531 |
| H | -3.75852 | -4.34717 | -2.87009 |
| H | -3.94401 | -3.51735 | 1.28944 |
| C | -2.25256 | -2.35347 | -3.69570 |
| C | -3.18654 | -1.28013 | -4.25840 |
| C | -2.23947 | -3.57455 | -4.60766 |
| H | -1.24395 | -1.95174 | -3.70545 |
| H | -3.14879 | -0.36029 | -3.67211 |
| H | -2.90124 | -1.03244 | -5.28391 |
| H | -4.22180 | -1.63426 | -4.26888 |
| H | -1.63508 | -4.38258 | -4.19012 |
| H | -3.24155 | -3.95956 | -4.81691 |

| | | | |
|----|----------|----------|----------|
| H | -1.80132 | -3.29398 | -5.56810 |
| C | -2.42733 | -1.37685 | 1.39494 |
| C | -1.79191 | -2.23404 | 2.48660 |
| C | -3.68491 | -0.68008 | 1.91253 |
| H | -1.70905 | -0.59005 | 1.15615 |
| H | -0.90185 | -2.74956 | 2.12202 |
| H | -1.50306 | -1.60797 | 3.33433 |
| H | -2.48847 | -2.98981 | 2.85712 |
| H | -4.12955 | -0.04099 | 1.14808 |
| H | -4.43785 | -1.40861 | 2.22358 |
| H | -3.44136 | -0.05908 | 2.77825 |
| C | -4.84905 | -5.26538 | -0.56215 |
| C | -4.14666 | -6.57082 | -0.92864 |
| C | -6.16085 | -5.11399 | -1.32867 |
| H | -5.08932 | -5.30347 | 0.50637 |
| H | -3.22123 | -6.69702 | -0.36291 |
| H | -4.79528 | -7.42536 | -0.71964 |
| H | -3.89363 | -6.59721 | -1.99172 |
| H | -6.68002 | -4.19400 | -1.05160 |
| H | -5.98701 | -5.08799 | -2.40755 |
| H | -6.82431 | -5.95712 | -1.12014 |
| Ge | 1.44748 | -0.62105 | -2.23705 |
| Cl | 1.29913 | -2.85315 | -2.56725 |
| O | -0.54350 | -0.23626 | -2.69338 |
| Cl | -2.24388 | 1.16925 | -0.85645 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.11140 | 0.90602 | 1.34322 |
| C | 0.39006 | 0.41172 | -0.06686 |
| P | -1.27207 | 0.27398 | -0.60259 |
| Cl | 1.60635 | -2.51048 | -1.13673 |
| O | -1.06922 | -0.76619 | -1.70456 |
| C | -2.88804 | -0.00358 | 0.19870 |
| C | -3.46312 | -1.29578 | 0.01482 |
| C | -3.73935 | 1.07787 | 0.54177 |
| C | -4.82968 | -1.35621 | -0.21287 |
| C | -5.10379 | 0.92471 | 0.31734 |
| C | -5.66475 | -0.24798 | -0.15996 |
| H | -5.26362 | -2.32396 | -0.42766 |
| H | -5.74889 | 1.76515 | 0.53163 |
| C | 2.89031 | 0.64466 | 0.94596 |
| C | 3.55413 | -0.47636 | 1.49778 |
| C | 3.55106 | 1.45145 | -0.01140 |
| C | 4.72962 | -0.90260 | 0.88600 |
| C | 4.71415 | 0.95007 | -0.58429 |
| C | 5.28930 | -0.25345 | -0.20316 |
| H | 5.21730 | -1.78660 | 1.26400 |
| H | 5.20077 | 1.53061 | -1.35659 |
| C | 3.08276 | -1.19940 | 2.77586 |
| C | 3.14277 | 2.89173 | -0.39330 |
| C | 6.51525 | -0.78169 | -0.94147 |
| C | -3.34103 | 2.35156 | 1.31371 |
| C | -2.74104 | -2.64525 | 0.20011 |
| C | -7.13774 | -0.37707 | -0.52710 |
| C | 4.40636 | 3.74745 | -0.58883 |
| H | 4.11353 | 4.79391 | -0.70437 |
| H | 5.07833 | 3.67353 | 0.26939 |
| H | 4.96526 | 3.47588 | -1.48526 |
| C | 2.34837 | 3.58521 | 0.71381 |
| H | 1.34425 | 3.16978 | 0.84817 |
| H | 2.86789 | 3.53661 | 1.67387 |
| H | 2.20514 | 4.63812 | 0.45599 |
| C | 2.34346 | 2.93900 | -1.69831 |
| H | 2.87731 | 2.43163 | -2.50503 |
| H | 1.36609 | 2.46885 | -1.59093 |
| H | 2.18346 | 3.97888 | -1.99945 |

| | | | |
|----|----------|----------|----------|
| C | 7.66466 | 0.22660 | -0.83025 |
| H | 8.54386 | -0.14388 | -1.36505 |
| H | 7.39872 | 1.19513 | -1.25859 |
| H | 7.94423 | 0.38694 | 0.21410 |
| C | 6.99574 | -2.11910 | -0.38432 |
| H | 7.85425 | -2.46722 | -0.96390 |
| H | 7.31510 | -2.03660 | 0.65784 |
| H | 6.21948 | -2.88546 | -0.44816 |
| C | 6.15337 | -0.98079 | -2.41844 |
| H | 5.33399 | -1.69548 | -2.52558 |
| H | 5.84334 | -0.04473 | -2.88760 |
| H | 7.01718 | -1.36229 | -2.97039 |
| C | 4.10690 | -2.23172 | 3.25573 |
| H | 5.09068 | -1.78844 | 3.42690 |
| H | 3.76257 | -2.64929 | 4.20470 |
| H | 4.21468 | -3.06290 | 2.55502 |
| C | 2.93389 | -0.17180 | 3.90671 |
| H | 3.87956 | 0.34525 | 4.08742 |
| H | 2.17388 | 0.58117 | 3.68871 |
| H | 2.63894 | -0.67698 | 4.83094 |
| C | 1.76490 | -1.95441 | 2.58248 |
| H | 0.91807 | -1.28367 | 2.41950 |
| H | 1.81584 | -2.62985 | 1.72732 |
| H | 1.54130 | -2.53668 | 3.48155 |
| C | -1.86575 | 2.43750 | 1.67728 |
| H | -1.51805 | 1.52380 | 2.16435 |
| H | -1.22657 | 2.64990 | 0.82227 |
| H | -1.71826 | 3.25413 | 2.38851 |
| C | -4.09549 | 2.27280 | 2.65725 |
| H | -3.82648 | 3.13557 | 3.27273 |
| H | -5.17811 | 2.27695 | 2.52746 |
| H | -3.82434 | 1.36675 | 3.20451 |
| C | -3.76292 | 3.63748 | 0.59737 |
| H | -4.83613 | 3.66305 | 0.39999 |
| H | -3.52448 | 4.49920 | 1.22680 |
| H | -3.24108 | 3.75639 | -0.35176 |
| C | -1.40201 | -2.49996 | 0.91763 |
| H | -1.01941 | -3.49239 | 1.16785 |
| H | -0.62772 | -2.03308 | 0.31515 |
| H | -1.51801 | -1.94308 | 1.85147 |
| C | -2.57558 | -3.40811 | -1.11700 |
| H | -1.92694 | -2.87476 | -1.80774 |
| H | -2.13832 | -4.39041 | -0.91848 |
| H | -3.54422 | -3.56451 | -1.59932 |
| C | -3.60883 | -3.50599 | 1.14112 |
| H | -3.82560 | -2.98178 | 2.07516 |
| H | -4.55524 | -3.81026 | 0.69312 |
| H | -3.05932 | -4.41879 | 1.38394 |
| C | -7.87875 | 0.95328 | -0.42369 |
| H | -7.89884 | 1.33186 | 0.60149 |
| H | -7.43151 | 1.71674 | -1.06511 |
| H | -8.91523 | 0.81831 | -0.74168 |
| C | -7.81786 | -1.38353 | 0.40870 |
| H | -7.36478 | -2.37426 | 0.33875 |
| H | -7.75261 | -1.05683 | 1.44946 |
| H | -8.87538 | -1.48150 | 0.14834 |
| C | -7.24247 | -0.87667 | -1.97315 |
| H | -6.77494 | -0.17230 | -2.66525 |
| H | -6.75539 | -1.84506 | -2.10271 |
| H | -8.29262 | -0.98826 | -2.25660 |
| Ge | 0.99697 | -0.47808 | -1.89424 |
| Cl | -1.61783 | 2.01492 | -1.64698 |

R-P=C(Ge(II)Cl)-P(O)MeR**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.42553 | 0.80794 | 0.52687 |
| C | 0.27561 | 0.49788 | -1.09096 |
| P | -1.16129 | 0.18374 | -2.03701 |
| Ge | 1.35703 | 0.63861 | -2.89398 |
| Cl | 1.65054 | -1.58609 | -3.04703 |
| O | -0.65133 | 0.57819 | -3.42832 |
| C | -2.67034 | 1.03509 | -1.58428 |
| H | -2.49104 | 2.11083 | -1.58887 |
| H | -3.45664 | 0.79212 | -2.30183 |
| H | -2.97833 | 0.71902 | -0.58472 |
| H | 1.83500 | 1.06083 | 0.56413 |
| H | -1.49154 | -1.18469 | -1.96574 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.50824 | 0.33422 | 0.55788 |
| C | 0.21045 | 0.19946 | -1.06025 |
| P | -1.32547 | 0.03277 | -1.88083 |
| Ge | 1.12626 | 0.44209 | -2.93744 |
| Cl | 1.46983 | -1.76914 | -3.27026 |
| O | -0.88610 | 0.40847 | -3.31029 |
| C | -2.64057 | 1.11271 | -1.30574 |
| H | -2.29502 | 2.14581 | -1.35222 |
| H | -3.51944 | 0.99613 | -1.94347 |
| H | -2.90167 | 0.86488 | -0.27476 |
| C | -1.95287 | -1.64512 | -1.80514 |
| H | -2.23670 | -1.89575 | -0.78116 |
| H | -2.81836 | -1.74211 | -2.46426 |
| H | -1.15879 | -2.31251 | -2.14363 |
| C | 2.33665 | 0.49092 | 0.67556 |
| H | 2.74774 | -0.48402 | 0.95542 |
| H | 2.79091 | 0.80790 | -0.26379 |
| H | 2.59287 | 1.19424 | 1.47104 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.69725 | -0.19789 | 0.50722 |
| C | 0.16785 | 0.10469 | -1.02985 |
| P | -1.49740 | -0.04862 | -1.58118 |
| Ge | 0.66012 | 0.91305 | -2.92316 |
| Cl | 1.47173 | -0.99240 | -3.82575 |
| O | -1.32622 | 0.44019 | -3.03630 |
| C | -2.22935 | -1.73207 | -1.53304 |
| C | 2.54264 | 0.11116 | 0.58081 |
| C | 3.13205 | 0.76262 | -0.65614 |
| H | 2.67234 | 1.73261 | -0.86180 |
| H | 4.20487 | 0.93191 | -0.51065 |
| H | 3.01989 | 0.12700 | -1.53774 |
| C | 2.76830 | 0.99228 | 1.81174 |
| H | 2.32497 | 0.55487 | 2.71080 |
| H | 3.84221 | 1.10798 | 1.99104 |
| H | 2.34207 | 1.98985 | 1.67631 |
| C | 3.17680 | -1.26361 | 0.81313 |
| H | 4.25058 | -1.14578 | 0.99461 |
| H | 2.74737 | -1.76873 | 1.68329 |
| H | 3.05104 | -1.91272 | -0.05665 |
| C | -2.49683 | -2.14143 | -0.08618 |
| H | -2.85679 | -3.17424 | -0.07183 |
| H | -1.59096 | -2.09862 | 0.52445 |
| H | -3.26188 | -1.52056 | 0.38524 |
| C | -1.25128 | -2.70737 | -2.18586 |
| H | -1.01525 | -2.42036 | -3.21117 |
| H | -0.31182 | -2.76909 | -1.63458 |
| H | -1.70665 | -3.70204 | -2.20052 |

| | | | |
|---|----------|----------|----------|
| C | -3.53129 | -1.69476 | -2.33704 |
| H | -3.94361 | -2.70675 | -2.38667 |
| H | -4.28738 | -1.05586 | -1.87476 |
| H | -3.35915 | -1.34839 | -3.35779 |
| C | -2.59737 | 1.06130 | -0.68364 |
| H | -2.18933 | 2.06902 | -0.77358 |
| H | -3.59915 | 1.04436 | -1.11566 |
| H | -2.64107 | 0.78952 | 0.37175 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.85677 | -0.02478 | 0.77304 |
| C | 0.24094 | 0.01495 | -0.76362 |
| P | -1.44603 | 0.00864 | -1.22452 |
| C | 2.65477 | 0.02984 | 0.56724 |
| C | 3.39738 | 0.53772 | 1.63608 |
| C | 3.32567 | -0.42930 | -0.56938 |
| C | 4.77777 | 0.62633 | 1.55582 |
| C | 4.70596 | -0.34937 | -0.64248 |
| C | 5.43223 | 0.18485 | 0.41468 |
| H | 5.34414 | 1.03431 | 2.38524 |
| H | 5.21873 | -0.71198 | -1.52607 |
| Ge | 0.72951 | 0.61912 | -2.71241 |
| Cl | 0.99670 | -1.44284 | -3.59928 |
| O | -1.32683 | 0.56913 | -2.65393 |
| H | 2.76733 | -0.88151 | -1.38243 |
| H | 6.51292 | 0.24569 | 0.35250 |
| H | 2.88444 | 0.87417 | 2.53218 |
| C | -2.17241 | -1.63412 | -1.23901 |
| C | -2.48592 | -2.22283 | -2.45973 |
| C | -2.41425 | -2.31920 | -0.04950 |
| C | -3.05269 | -3.48849 | -2.48651 |
| H | -2.27287 | -1.69002 | -3.37840 |
| C | -2.97842 | -3.58260 | -0.08321 |
| H | -2.14772 | -1.87704 | 0.90538 |
| C | -3.30025 | -4.16559 | -1.30242 |
| H | -3.29404 | -3.94854 | -3.43759 |
| H | -3.16316 | -4.11662 | 0.84161 |
| H | -3.73987 | -5.15626 | -1.32705 |
| C | -2.51795 | 1.03392 | -0.21026 |
| H | -2.11230 | 2.04614 | -0.18629 |
| H | -3.52087 | 1.04662 | -0.64109 |
| H | -2.56470 | 0.64005 | 0.80680 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.06709 | -0.48152 | 1.16641 |
| C | 0.27967 | -0.21897 | -0.26477 |
| P | -1.41603 | -0.11249 | -0.72644 |
| C | 2.81144 | -0.11343 | 0.75178 |
| C | 3.36803 | 1.10499 | 1.16451 |
| C | 3.61058 | -1.07771 | 0.11912 |
| C | 4.71173 | 1.35225 | 0.91397 |
| C | 4.95031 | -0.78786 | -0.10831 |
| C | 5.51895 | 0.42117 | 0.27327 |
| H | 5.13927 | 2.29926 | 1.23113 |
| H | 5.56999 | -1.53522 | -0.59561 |
| Ge | 0.81069 | 0.81601 | -1.99622 |
| Cl | 0.96005 | -1.01004 | -3.33603 |
| O | -1.23573 | 0.85355 | -1.91588 |
| C | -2.20493 | -1.67504 | -1.18876 |
| C | -2.83492 | -1.83126 | -2.44367 |
| C | -2.22667 | -2.73286 | -0.26034 |
| C | -3.45134 | -3.04474 | -2.72356 |
| C | -2.86296 | -3.92093 | -0.59796 |
| C | -3.47446 | -4.10348 | -1.82714 |
| H | -3.93817 | -3.16005 | -3.68707 |

| | | | |
|---|----------|----------|----------|
| H | -2.87687 | -4.72675 | 0.12985 |
| C | -2.50341 | 0.69251 | 0.46599 |
| H | -2.03160 | 1.62096 | 0.79095 |
| H | -3.44339 | 0.92250 | -0.04079 |
| H | -2.71082 | 0.06250 | 1.33009 |
| C | 2.53072 | 2.14954 | 1.84120 |
| H | 1.84856 | 2.62799 | 1.13154 |
| H | 1.91417 | 1.72109 | 2.63836 |
| H | 3.15543 | 2.92846 | 2.28068 |
| C | 3.05370 | -2.40225 | -0.31070 |
| H | 2.48459 | -2.87872 | 0.49417 |
| H | 2.37706 | -2.29100 | -1.16271 |
| H | 3.85558 | -3.08216 | -0.60170 |
| C | 6.95837 | 0.71873 | -0.01679 |
| H | 7.56689 | -0.18707 | 0.01526 |
| H | 7.07051 | 1.15134 | -1.01600 |
| H | 7.36963 | 1.43429 | 0.69750 |
| C | -2.89038 | -0.77982 | -3.51441 |
| H | -3.27106 | 0.17408 | -3.14975 |
| H | -1.89723 | -0.58395 | -3.92137 |
| H | -3.53571 | -1.12252 | -4.32402 |
| C | -1.56352 | -2.67999 | 1.08444 |
| H | -0.51256 | -2.97159 | 1.00763 |
| H | -1.57610 | -1.69625 | 1.55260 |
| H | -2.04964 | -3.37565 | 1.77013 |
| C | -4.12440 | -5.40293 | -2.18709 |
| H | -3.44552 | -6.01892 | -2.78494 |
| H | -4.39203 | -5.97574 | -1.29784 |
| H | -5.02666 | -5.24529 | -2.78126 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.09169 | 1.08510 | 1.19825 |
| C | 0.34967 | 0.46462 | -0.14751 |
| P | -1.32367 | 0.34806 | -0.71278 |
| Cl | 1.53612 | -2.56875 | -1.00209 |
| O | -1.09906 | -0.80982 | -1.71793 |
| C | -2.92453 | 0.07361 | 0.14749 |
| C | -3.50850 | -1.22123 | 0.04219 |
| C | -3.77999 | 1.17208 | 0.42238 |
| C | -4.87666 | -1.29410 | -0.18188 |
| C | -5.14608 | 1.01335 | 0.20663 |
| C | -5.71131 | -0.18510 | -0.19672 |
| H | -5.31089 | -2.27299 | -0.33860 |
| H | -5.78958 | 1.86607 | 0.37375 |
| C | 2.87082 | 0.74349 | 0.84486 |
| C | 3.49758 | -0.34750 | 1.49036 |
| C | 3.57616 | 1.46991 | -0.14704 |
| C | 4.67828 | -0.84060 | 0.93995 |
| C | 4.74700 | 0.91169 | -0.64577 |
| C | 5.28345 | -0.27685 | -0.17061 |
| H | 5.13428 | -1.70801 | 1.38912 |
| H | 5.27261 | 1.43004 | -1.43568 |
| C | 2.99032 | -0.96424 | 2.81079 |
| C | 3.19786 | 2.88702 | -0.63609 |
| C | 6.51741 | -0.87732 | -0.83666 |
| C | -3.37694 | 2.48399 | 1.12690 |
| C | -2.78862 | -2.55828 | 0.30336 |
| C | -7.18638 | -0.33498 | -0.54906 |
| C | 4.45430 | 3.65564 | -1.07382 |
| H | 4.18549 | 4.69981 | -1.25141 |
| H | 5.23285 | 3.63036 | -0.30793 |
| H | 4.87528 | 3.27564 | -2.00644 |
| C | 2.57865 | 3.71644 | 0.49151 |
| H | 1.60581 | 3.33686 | 0.82155 |
| H | 3.23415 | 3.75123 | 1.36491 |
| H | 2.41057 | 4.74029 | 0.14595 |

| | | | |
|----|----------|----------|----------|
| C | 2.24621 | 2.86461 | -1.83590 |
| H | 2.64870 | 2.25210 | -2.64578 |
| H | 1.27142 | 2.46414 | -1.56263 |
| H | 2.10445 | 3.88147 | -2.21529 |
| C | 7.68605 | 0.11173 | -0.75782 |
| H | 8.57121 | -0.31111 | -1.24167 |
| H | 7.45402 | 1.05547 | -1.25568 |
| H | 7.94007 | 0.33415 | 0.28169 |
| C | 6.95186 | -2.18506 | -0.18017 |
| H | 7.81765 | -2.58870 | -0.71097 |
| H | 7.24428 | -2.04091 | 0.86319 |
| H | 6.16005 | -2.93718 | -0.21606 |
| C | 6.19296 | -1.16536 | -2.30770 |
| H | 5.35999 | -1.86722 | -2.39238 |
| H | 5.91833 | -0.25541 | -2.84537 |
| H | 7.06271 | -1.60105 | -2.80794 |
| C | 3.98461 | -1.97896 | 3.38313 |
| H | 4.97552 | -1.54525 | 3.53702 |
| H | 3.61672 | -2.31643 | 4.35489 |
| H | 4.08385 | -2.86278 | 2.74864 |
| C | 2.85055 | 0.14831 | 3.85963 |
| H | 3.80550 | 0.65648 | 4.01552 |
| H | 2.11120 | 0.89936 | 3.57415 |
| H | 2.53171 | -0.27989 | 4.81440 |
| C | 1.65874 | -1.70396 | 2.65745 |
| H | 0.82820 | -1.03027 | 2.43831 |
| H | 1.70356 | -2.43921 | 1.85275 |
| H | 1.41667 | -2.21727 | 3.59309 |
| C | -1.90401 | 2.57188 | 1.50267 |
| H | -1.57893 | 1.68605 | 2.05179 |
| H | -1.23364 | 2.71033 | 0.65631 |
| H | -1.74981 | 3.43230 | 2.15852 |
| C | -4.13802 | 2.48863 | 2.46896 |
| H | -3.86399 | 3.38081 | 3.03884 |
| H | -5.21970 | 2.49538 | 2.33242 |
| H | -3.87836 | 1.61079 | 3.06506 |
| C | -3.79143 | 3.73443 | 0.34503 |
| H | -4.86780 | 3.76303 | 0.16645 |
| H | -3.53003 | 4.62869 | 0.91717 |
| H | -3.29720 | 3.80258 | -0.62490 |
| C | -1.45345 | -2.36656 | 1.01513 |
| H | -1.05381 | -3.34241 | 1.30116 |
| H | -0.69027 | -1.90513 | 0.39569 |
| H | -1.58096 | -1.77709 | 1.92723 |
| C | -2.61906 | -3.39248 | -0.96929 |
| H | -1.97068 | -2.89527 | -1.68647 |
| H | -2.17939 | -4.36115 | -0.71630 |
| H | -3.58727 | -3.57823 | -1.44261 |
| C | -3.65738 | -3.36799 | 1.28745 |
| H | -3.88377 | -2.79183 | 2.18810 |
| H | -4.59880 | -3.70520 | 0.85213 |
| H | -3.10331 | -4.26109 | 1.58682 |
| C | -7.92576 | 1.00009 | -0.52450 |
| H | -7.94027 | 1.44135 | 0.47541 |
| H | -7.48104 | 1.72225 | -1.21392 |
| H | -8.96407 | 0.84753 | -0.82839 |
| C | -7.86354 | -1.28030 | 0.45041 |
| H | -7.41129 | -2.27376 | 0.44013 |
| H | -7.79239 | -0.88965 | 1.46849 |
| H | -8.92252 | -1.39321 | 0.20207 |
| C | -7.30052 | -0.92323 | -1.96048 |
| H | -6.83938 | -0.26228 | -2.69841 |
| H | -6.81232 | -1.89695 | -2.03330 |
| H | -8.35225 | -1.05373 | -2.22986 |
| Ge | 0.93510 | -0.58619 | -1.89034 |
| C | -1.64986 | 1.77733 | -1.77831 |

| | | | |
|---|----------|---------|----------|
| H | -2.58594 | 1.59086 | -2.30778 |
| H | -1.70044 | 2.73244 | -1.26583 |
| H | -0.83454 | 1.80223 | -2.50506 |

| | | | |
|---|----------|----------|----------|
| H | -0.25797 | -2.56793 | -2.05008 |
| H | -1.66457 | -3.57156 | -2.43800 |

R-P=C(Ge(II)Cl)-P(S)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.18249 | 0.84541 | 0.54154 |
| C | 0.17159 | 0.39415 | -1.05207 |
| P | -1.17688 | -0.12328 | -2.01041 |
| Ge | 1.47816 | 0.64897 | -2.66504 |
| S | -0.82260 | 0.74149 | -3.75590 |
| Cl | 1.85163 | -1.55080 | -2.95280 |
| H | 1.56470 | 1.21442 | 0.61550 |
| Cl | -3.02618 | 0.19711 | -1.24832 |
| H | -1.17824 | -1.52544 | -2.08391 |

R= Me

| | | | |
|----|----------|----------|----------|
| P | 0.51829 | 0.36678 | 0.61726 |
| C | 0.18402 | 0.16405 | -0.99175 |
| P | -1.38282 | -0.00282 | -1.71547 |
| Ge | 1.25233 | 0.41866 | -2.76702 |
| S | -1.10738 | 0.81841 | -3.50957 |
| Cl | 1.43021 | -1.77866 | -3.26651 |
| C | -1.89567 | -1.72109 | -1.79709 |
| H | -1.10135 | -2.26898 | -2.30896 |
| H | -2.03689 | -2.10544 | -0.78582 |
| H | -2.82642 | -1.78647 | -2.36201 |
| C | 2.35229 | 0.43538 | 0.68237 |
| H | 2.72165 | -0.55644 | 0.96147 |
| H | 2.80523 | 0.72313 | -0.26788 |
| H | 2.65892 | 1.13210 | 1.46528 |
| Cl | -2.90605 | 0.86941 | -0.67534 |

R= t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.66956 | -0.10529 | 0.57230 |
| C | 0.11335 | 0.18396 | -0.96630 |
| P | -1.58255 | -0.02290 | -1.36046 |
| Ge | 0.72381 | 1.10415 | -2.74855 |
| S | -1.75448 | 0.90799 | -3.11457 |
| Cl | 1.43754 | -0.75248 | -3.82169 |
| C | -2.19181 | -1.77497 | -1.40708 |
| C | 2.52747 | 0.09277 | 0.61783 |
| Cl | -2.79295 | 0.85018 | 0.04185 |
| C | 2.81742 | 0.92611 | 1.86935 |
| H | 3.89782 | 0.96475 | 2.04140 |
| H | 2.45809 | 1.95281 | 1.76218 |
| H | 2.35194 | 0.49670 | 2.76077 |
| C | 3.06520 | -1.32900 | 0.81614 |
| H | 4.14411 | -1.28556 | 0.99967 |
| H | 2.60419 | -1.82530 | 1.67519 |
| H | 2.89802 | -1.94681 | -0.06922 |
| C | 3.16270 | 0.73085 | -0.60330 |
| H | 2.77980 | 1.73864 | -0.78157 |
| H | 4.24489 | 0.81607 | -0.45339 |
| H | 3.00977 | 0.12756 | -1.50158 |
| C | -2.11892 | -2.39564 | -0.01601 |
| H | -2.44229 | -3.43793 | -0.08968 |
| H | -1.10203 | -2.39078 | 0.38191 |
| H | -2.77095 | -1.88830 | 0.69584 |
| C | -3.63121 | -1.75900 | -1.91768 |
| H | -3.97511 | -2.79320 | -2.00735 |
| H | -4.30275 | -1.23767 | -1.23361 |
| H | -3.70315 | -1.29434 | -2.90302 |
| C | -1.29760 | -2.54282 | -2.37908 |
| H | -1.31963 | -2.11282 | -3.38104 |

R= Ph

| | | | |
|----|----------|----------|----------|
| P | 0.85068 | 0.02553 | 1.03352 |
| C | 0.18133 | 0.06215 | -0.48649 |
| P | -1.51466 | 0.06577 | -0.84678 |
| C | 2.63404 | -0.02257 | 0.73944 |
| C | 3.44737 | 0.54573 | 1.72394 |
| C | 3.23076 | -0.61573 | -0.37742 |
| C | 4.82430 | 0.56278 | 1.57506 |
| C | 4.60858 | -0.60641 | -0.51735 |
| C | 5.40479 | -0.01105 | 0.45245 |
| H | 5.44604 | 1.01818 | 2.33725 |
| H | 5.06299 | -1.07149 | -1.38458 |
| C | -2.16575 | -1.60266 | -1.03593 |
| C | -2.57424 | -2.05427 | -2.28435 |
| C | -2.21966 | -2.44565 | 0.07300 |
| C | -3.04790 | -3.35078 | -2.42086 |
| C | -2.69156 | -3.73726 | -0.07254 |
| C | -3.10705 | -4.18920 | -1.31939 |
| H | -3.36540 | -3.70510 | -3.39435 |
| H | -2.73544 | -4.39445 | 0.78798 |
| Ge | 0.86082 | 0.68615 | -2.35472 |
| S | -1.61839 | 1.16217 | -2.50212 |
| Cl | 0.88704 | -1.32564 | -3.38360 |
| H | -3.47561 | -5.20266 | -1.43007 |
| H | -2.51076 | -1.39529 | -3.14154 |
| H | -1.89659 | -2.09334 | 1.04652 |
| H | 2.99285 | 0.98613 | 2.60624 |
| H | 2.61879 | -1.11937 | -1.11870 |
| H | 6.48288 | -0.00568 | 0.33831 |
| Cl | -2.65577 | 0.83149 | 0.66556 |

R= Mes

| | | | |
|----|----------|----------|----------|
| P | 0.93354 | -0.14691 | 1.19103 |
| C | 0.19540 | -0.11595 | -0.29451 |
| P | -1.49080 | -0.02520 | -0.73209 |
| C | 2.70094 | 0.03572 | 0.75876 |
| C | 3.33117 | 1.26029 | 1.02497 |
| C | 3.44273 | -1.05108 | 0.26937 |
| C | 4.69053 | 1.38748 | 0.77209 |
| C | 4.80100 | -0.87722 | 0.03465 |
| C | 5.44252 | 0.33259 | 0.27104 |
| H | 5.17505 | 2.33842 | 0.97420 |
| H | 5.37708 | -1.71833 | -0.34006 |
| C | -2.20474 | -1.62129 | -1.21769 |
| C | -2.86075 | -1.82256 | -2.45359 |
| C | -2.08495 | -2.69451 | -0.30625 |
| C | -3.32815 | -3.09702 | -2.74935 |
| C | -2.57718 | -3.94167 | -0.66748 |
| C | -3.18751 | -4.17367 | -1.88820 |
| H | -3.83220 | -3.24536 | -3.69896 |
| H | -2.48239 | -4.75636 | 0.04378 |
| Ge | 1.01754 | 0.64863 | -2.04513 |
| S | -1.35878 | 1.43984 | -2.08469 |
| Cl | 0.80354 | -1.22313 | -3.30916 |
| C | 2.81178 | -2.38643 | 0.00517 |
| H | 2.22180 | -2.72718 | 0.86197 |
| H | 2.14007 | -2.35096 | -0.85720 |
| H | 3.57517 | -3.13942 | -0.19459 |
| C | 2.55311 | 2.43339 | 1.54202 |
| H | 1.90885 | 2.85390 | 0.76353 |
| H | 1.90181 | 2.15301 | 2.37653 |
| H | 3.21974 | 3.22487 | 1.88697 |

| | | | |
|----|----------|----------|----------|
| C | 6.90136 | 0.49904 | -0.02523 |
| H | 7.05152 | 0.80729 | -1.06472 |
| H | 7.35294 | 1.26255 | 0.61064 |
| H | 7.44665 | -0.43550 | 0.11898 |
| C | -1.45280 | -2.60055 | 1.05041 |
| H | -0.36790 | -2.71291 | 0.98294 |
| H | -1.65210 | -1.65995 | 1.56114 |
| H | -1.82840 | -3.40488 | 1.68411 |
| C | -3.11422 | -0.77199 | -3.49362 |
| H | -3.60105 | 0.11406 | -3.08653 |
| H | -2.18496 | -0.44387 | -3.96171 |
| H | -3.75919 | -1.18614 | -4.26927 |
| C | -3.67315 | -5.53647 | -2.26873 |
| H | -3.89611 | -6.14147 | -1.38850 |
| H | -4.57021 | -5.48125 | -2.88804 |
| H | -2.90952 | -6.06550 | -2.84746 |
| Cl | -2.73151 | 0.61792 | 0.78131 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.04478 | 0.72566 | 1.35970 |
| C | 0.38535 | 0.30895 | -0.11085 |
| P | -1.28886 | 0.28486 | -0.62922 |
| Cl | 1.89127 | -2.42350 | -1.22625 |
| C | -2.88835 | 0.01936 | 0.24012 |
| C | -3.46869 | -1.27577 | 0.09276 |
| C | -3.74115 | 1.10451 | 0.57303 |
| C | -4.83235 | -1.33870 | -0.15031 |
| C | -5.10064 | 0.95631 | 0.31367 |
| C | -5.65899 | -0.22212 | -0.15406 |
| H | -5.27038 | -2.31364 | -0.32476 |
| H | -5.74513 | 1.80366 | 0.50240 |
| C | 2.84283 | 0.57559 | 1.00175 |
| C | 3.55718 | -0.52800 | 1.53159 |
| C | 3.47681 | 1.43522 | 0.07397 |
| C | 4.75496 | -0.88267 | 0.92134 |
| C | 4.66421 | 0.99879 | -0.50626 |
| C | 5.29071 | -0.18470 | -0.15180 |
| H | 5.27967 | -1.75262 | 1.28188 |
| H | 5.12536 | 1.62444 | -1.26092 |
| C | 3.10304 | -1.31171 | 2.77834 |
| C | 3.08156 | 2.89483 | -0.24229 |
| C | 6.53610 | -0.64696 | -0.90109 |
| C | -3.35824 | 2.35179 | 1.39702 |
| C | -2.78055 | -2.62175 | 0.40516 |
| C | -7.12224 | -0.34753 | -0.55804 |
| C | 4.27941 | 3.77405 | 0.16541 |
| H | 4.04353 | 4.82516 | -0.02250 |
| H | 4.50154 | 3.65893 | 1.22936 |
| H | 5.18414 | 3.53118 | -0.39220 |
| C | 1.88817 | 3.43527 | 0.54173 |
| H | 0.93756 | 3.03992 | 0.18532 |
| H | 1.97902 | 3.24216 | 1.61538 |
| H | 1.84466 | 4.52109 | 0.41622 |
| C | 2.80518 | 3.09904 | -1.73422 |
| H | 3.64989 | 2.79044 | -2.35280 |
| H | 1.93165 | 2.52985 | -2.05809 |
| H | 2.61339 | 4.15716 | -1.93468 |
| C | 7.64028 | 0.40965 | -0.78277 |
| H | 8.53270 | 0.08345 | -1.32438 |
| H | 7.33131 | 1.36968 | -1.20133 |
| H | 7.91669 | 0.57186 | 0.26214 |
| C | 7.07843 | -1.96874 | -0.36392 |
| H | 7.95022 | -2.26914 | -0.95030 |
| H | 7.39650 | -1.88659 | 0.67873 |
| H | 6.33760 | -2.76849 | -0.43757 |
| C | 6.17287 | -0.84271 | -2.37830 |

| | | | |
|----|----------|----------|----------|
| H | 5.38340 | -1.58970 | -2.48888 |
| H | 5.81912 | 0.08523 | -2.83252 |
| H | 7.04859 | -1.17948 | -2.94056 |
| C | 4.17491 | -2.29638 | 3.25367 |
| H | 5.12834 | -1.80229 | 3.45505 |
| H | 3.83709 | -2.75666 | 4.18510 |
| H | 4.34324 | -3.10227 | 2.53565 |
| C | 2.86772 | -0.32846 | 3.93358 |
| H | 3.77647 | 0.23820 | 4.15124 |
| H | 2.06871 | 0.38391 | 3.71890 |
| H | 2.58344 | -0.87714 | 4.83607 |
| C | 1.83647 | -2.13328 | 2.52745 |
| H | 0.96138 | -1.50280 | 2.35314 |
| H | 1.94912 | -2.78221 | 1.65771 |
| H | 1.61663 | -2.74862 | 3.40525 |
| C | -1.89882 | 2.40216 | 1.82860 |
| H | -1.59081 | 1.46870 | 2.30419 |
| H | -1.21591 | 2.62205 | 1.01169 |
| H | -1.77136 | 3.19776 | 2.56713 |
| C | -4.16648 | 2.22847 | 2.70720 |
| H | -3.90352 | 3.05750 | 3.36986 |
| H | -5.24294 | 2.26219 | 2.53711 |
| H | -3.93437 | 1.29375 | 3.22321 |
| C | -3.74676 | 3.66952 | 0.72201 |
| H | -4.80989 | 3.70357 | 0.47620 |
| H | -3.54126 | 4.50000 | 1.40288 |
| H | -3.18230 | 3.83587 | -0.19442 |
| C | -1.33573 | -2.50086 | 0.87405 |
| H | -1.01577 | -3.46301 | 1.28201 |
| H | -0.63454 | -2.25845 | 0.07826 |
| H | -1.24284 | -1.76134 | 1.67344 |
| C | -2.86755 | -3.62729 | -0.74447 |
| H | -2.29180 | -3.29360 | -1.60669 |
| H | -2.46292 | -4.58850 | -0.41656 |
| H | -3.89881 | -3.79493 | -1.06274 |
| C | -3.55699 | -3.19618 | 1.61034 |
| H | -3.53382 | -2.50554 | 2.45706 |
| H | -4.60079 | -3.40683 | 1.37501 |
| H | -3.08721 | -4.13260 | 1.92257 |
| C | -7.85133 | 0.99260 | -0.51274 |
| H | -7.89971 | 1.39827 | 0.50109 |
| H | -7.37523 | 1.73414 | -1.15903 |
| H | -8.87873 | 0.86020 | -0.85991 |
| C | -7.83969 | -1.32077 | 0.38494 |
| H | -7.39814 | -2.31867 | 0.35261 |
| H | -7.79856 | -0.96758 | 1.41825 |
| H | -8.89089 | -1.41308 | 0.09837 |
| C | -7.19060 | -0.88639 | -1.99218 |
| H | -6.69549 | -0.20656 | -2.68956 |
| H | -6.70998 | -1.86269 | -2.08019 |
| H | -8.23325 | -0.99541 | -2.30304 |
| Ge | 1.25622 | -0.35766 | -1.90388 |
| S | -1.17236 | -0.91016 | -2.22535 |
| Cl | -1.54897 | 2.16403 | -1.45732 |

R-P=C(Ge(II)Cl)-P(S)MeR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.32897 | 1.07023 | 0.55315 |
| C | 0.14659 | 0.46782 | -0.97974 |
| P | -1.36391 | 0.07867 | -1.77700 |
| Ge | 1.37533 | 0.33335 | -2.65217 |
| S | -0.95068 | 0.61849 | -3.65510 |
| Cl | 1.38815 | -1.92294 | -2.63541 |
| H | 1.74723 | 1.27230 | 0.51981 |
| C | -2.87284 | 0.78533 | -1.09496 |

| | | | |
|---|----------|----------|----------|
| H | -3.72466 | 0.46137 | -1.69609 |
| H | -3.00034 | 0.44587 | -0.06432 |
| H | -2.80106 | 1.87292 | -1.12051 |
| H | -1.55507 | -1.31216 | -1.66179 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.47572 | 0.49529 | 0.43608 |
| C | 0.21324 | 0.21321 | -1.17370 |
| P | -1.36531 | 0.06059 | -1.92052 |
| C | -2.66800 | 1.06751 | -1.18162 |
| H | -3.59217 | 0.93496 | -1.74789 |
| H | -2.82595 | 0.76507 | -0.14394 |
| H | -2.36901 | 2.11492 | -1.21670 |
| Ge | 1.36548 | 0.26551 | -2.90326 |
| S | -0.94673 | 0.60169 | -3.81029 |
| Cl | 1.50410 | -1.98737 | -3.11929 |
| C | -1.93512 | -1.64543 | -1.82033 |
| H | -1.14775 | -2.28383 | -2.22379 |
| H | -2.13151 | -1.90876 | -0.77867 |
| H | -2.84348 | -1.75903 | -2.41518 |
| C | 2.30484 | 0.55840 | 0.60090 |
| H | 2.64535 | -0.39485 | 1.01661 |
| H | 2.81162 | 0.72908 | -0.35020 |
| H | 2.57759 | 1.34157 | 1.31174 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.64514 | -0.06737 | 0.39256 |
| C | 0.15594 | 0.17902 | -1.17433 |
| P | -1.55582 | 0.02519 | -1.60006 |
| Ge | 0.86855 | 0.94778 | -2.98499 |
| S | -1.57458 | 0.75029 | -3.47899 |
| Cl | 1.60468 | -1.01630 | -3.84405 |
| C | -2.21016 | -1.71150 | -1.53207 |
| C | 2.50253 | 0.11287 | 0.52546 |
| C | 2.74351 | 0.97348 | 1.76821 |
| H | 3.81522 | 1.00794 | 1.98921 |
| H | 2.39899 | 2.00031 | 1.62001 |
| H | 2.23375 | 0.56960 | 2.64742 |
| C | 3.02292 | -1.30602 | 0.77838 |
| H | 4.09393 | -1.26577 | 1.00462 |
| H | 2.52305 | -1.77936 | 1.62860 |
| H | 2.88666 | -1.94250 | -0.09899 |
| C | 3.19393 | 0.71911 | -0.68152 |
| H | 2.81654 | 1.71906 | -0.90824 |
| H | 4.26783 | 0.81164 | -0.48306 |
| H | 3.08440 | 0.08971 | -1.56801 |
| C | -2.30343 | -2.17665 | -0.08083 |
| H | -2.61827 | -3.22428 | -0.07038 |
| H | -1.34178 | -2.11476 | 0.43381 |
| H | -3.03922 | -1.60723 | 0.49092 |
| C | -3.59407 | -1.71887 | -2.18123 |
| H | -3.96625 | -2.74729 | -2.19600 |
| H | -4.31808 | -1.11687 | -1.62711 |
| H | -3.55588 | -1.35950 | -3.21135 |
| C | -1.26619 | -2.61649 | -2.31816 |
| H | -1.15752 | -2.28699 | -3.35240 |
| H | -0.26977 | -2.64892 | -1.87551 |
| H | -1.67561 | -3.63100 | -2.32001 |
| C | -2.60057 | 1.02715 | -0.51375 |
| H | -3.64096 | 0.97675 | -0.83783 |
| H | -2.51007 | 0.68813 | 0.51930 |
| H | -2.25509 | 2.05837 | -0.58749 |

R = Ph

| | | | |
|---|---------|---------|---------|
| P | 0.75275 | 0.15675 | 0.68606 |
|---|---------|---------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.20134 | 0.08260 | -0.87836 |
| P | -1.50015 | 0.07398 | -1.30251 |
| C | 2.55745 | 0.11649 | 0.55345 |
| C | 3.28287 | 0.76657 | 1.55499 |
| C | 3.24728 | -0.55070 | -0.46272 |
| C | 4.66751 | 0.78874 | 1.51919 |
| C | 4.63208 | -0.53471 | -0.48980 |
| C | 5.34241 | 0.14016 | 0.49438 |
| H | 5.22140 | 1.30698 | 2.29363 |
| H | 5.15898 | -1.05685 | -1.28021 |
| C | -2.56353 | 0.97801 | -0.15609 |
| H | -3.58686 | 0.95978 | -0.53532 |
| H | -2.53234 | 0.51602 | 0.83252 |
| H | -2.21128 | 2.00771 | -0.09191 |
| C | -2.14195 | -1.61730 | -1.31898 |
| C | -2.57403 | -2.20133 | -2.50266 |
| C | -2.19587 | -2.33587 | -0.12556 |
| C | -3.07390 | -3.49534 | -2.48996 |
| C | -2.69544 | -3.62653 | -0.11876 |
| C | -3.13728 | -4.20553 | -1.30161 |
| H | -3.40610 | -3.95088 | -3.41544 |
| H | -2.73357 | -4.18508 | 0.80927 |
| Ge | 0.99648 | 0.50325 | -2.74996 |
| S | -1.46877 | 0.91006 | -3.12525 |
| Cl | 1.09799 | -1.63142 | -3.50057 |
| H | -3.52404 | -5.21825 | -1.29537 |
| H | -2.50337 | -1.64337 | -3.42898 |
| H | -1.83047 | -1.89838 | 0.79822 |
| H | 2.75445 | 1.26612 | 2.36145 |
| H | 2.70082 | -1.11378 | -1.21247 |
| H | 6.42622 | 0.15012 | 0.46877 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.96591 | -0.20870 | 1.15034 |
| C | 0.24053 | -0.15585 | -0.34171 |
| P | -1.47882 | -0.05452 | -0.73114 |
| C | 2.73679 | 0.03070 | 0.75499 |
| C | 3.33259 | 1.26923 | 1.03409 |
| C | 3.51429 | -1.03510 | 0.27582 |
| C | 4.69295 | 1.43029 | 0.80738 |
| C | 4.87223 | -0.82804 | 0.06588 |
| C | 5.47987 | 0.39567 | 0.31766 |
| H | 5.15021 | 2.39250 | 1.01988 |
| H | 5.47471 | -1.65329 | -0.30271 |
| C | -2.56893 | 0.56460 | 0.57936 |
| H | -3.51556 | 0.83802 | 0.10778 |
| H | -2.75980 | -0.17812 | 1.35274 |
| H | -2.11432 | 1.45551 | 1.01374 |
| C | -2.20013 | -1.65504 | -1.24272 |
| C | -2.88631 | -1.84426 | -2.46385 |
| C | -2.09676 | -2.73217 | -0.33689 |
| C | -3.42645 | -3.09573 | -2.73441 |
| C | -2.66302 | -3.95812 | -0.66744 |
| C | -3.32463 | -4.16925 | -1.86359 |
| H | -3.95368 | -3.22927 | -3.67379 |
| H | -2.57692 | -4.77320 | 0.04483 |
| Ge | 1.06620 | 0.61972 | -2.07389 |
| S | -1.31042 | 1.40708 | -2.11259 |
| Cl | 0.82381 | -1.26820 | -3.32351 |
| C | 2.91956 | -2.38269 | -0.00948 |
| H | 2.31759 | -2.74055 | 0.83197 |
| H | 2.26594 | -2.35611 | -0.88612 |
| H | 3.70368 | -3.11759 | -0.19636 |
| C | 2.51780 | 2.42294 | 1.53812 |
| H | 1.86684 | 2.81786 | 0.75178 |
| H | 1.87066 | 2.12881 | 2.37100 |

| | | | |
|---|----------|----------|----------|
| H | 3.15931 | 3.23600 | 1.88074 |
| C | 6.93930 | 0.59928 | 0.04795 |
| H | 7.09955 | 0.92653 | -0.98422 |
| H | 7.36313 | 1.36318 | 0.70238 |
| H | 7.50334 | -0.32477 | 0.18774 |
| C | -1.37402 | -2.68366 | 0.97794 |
| H | -0.31105 | -2.89554 | 0.83754 |
| H | -1.43223 | -1.72807 | 1.49510 |
| H | -1.77727 | -3.44378 | 1.64863 |
| C | -3.08650 | -0.80094 | -3.52375 |
| H | -3.54978 | 0.10882 | -3.14188 |
| H | -2.13683 | -0.50968 | -3.97439 |
| H | -3.72909 | -1.20449 | -4.30715 |
| C | -3.89526 | -5.50717 | -2.21552 |
| H | -4.05427 | -6.12001 | -1.32696 |
| H | -4.84676 | -5.40789 | -2.74171 |
| H | -3.21434 | -6.05262 | -2.87617 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 1.02219 | 0.81062 | 1.23389 |
| C | 0.35356 | 0.33431 | -0.21281 |
| P | -1.34079 | 0.33882 | -0.73559 |
| Cl | 1.83358 | -2.50005 | -1.17776 |
| C | -2.92519 | 0.10433 | 0.19004 |
| C | -3.52651 | -1.18648 | 0.15060 |
| C | -3.76672 | 1.22080 | 0.43954 |
| C | -4.89572 | -1.25299 | -0.06737 |
| C | -5.13239 | 1.07340 | 0.21133 |
| C | -5.71221 | -0.13287 | -0.14751 |
| H | -5.34452 | -2.23405 | -0.16259 |
| H | -5.76466 | 1.94132 | 0.33946 |
| C | 2.83084 | 0.62285 | 0.92105 |
| C | 3.51951 | -0.47562 | 1.48728 |
| C | 3.51393 | 1.48761 | 0.02815 |
| C | 4.74142 | -0.83919 | 0.92771 |
| C | 4.72757 | 1.05196 | -0.48989 |
| C | 5.32779 | -0.14187 | -0.11532 |
| H | 5.24545 | -1.71139 | 1.31151 |
| H | 5.23588 | 1.67594 | -1.21195 |
| C | 3.03239 | -1.23104 | 2.74040 |
| C | 3.07339 | 2.93046 | -0.31324 |
| C | 6.60442 | -0.60611 | -0.80864 |
| C | -3.35425 | 2.53101 | 1.14508 |
| C | -2.84797 | -2.51491 | 0.54180 |
| C | -7.18453 | -0.27450 | -0.51295 |
| C | 4.30451 | 3.80990 | -0.58501 |
| H | 3.98576 | 4.85311 | -0.65078 |
| H | 5.04442 | 3.72955 | 0.21457 |
| H | 4.79218 | 3.56936 | -1.53126 |
| C | 2.35353 | 3.58666 | 0.86732 |
| H | 1.38970 | 3.12085 | 1.09746 |
| H | 2.96315 | 3.55150 | 1.77331 |
| H | 2.14414 | 4.63436 | 0.63400 |
| C | 2.18661 | 3.00399 | -1.55876 |
| H | 2.66521 | 2.51776 | -2.41162 |
| H | 1.22596 | 2.52012 | -1.39164 |
| H | 2.00180 | 4.05046 | -1.82127 |
| C | 7.70983 | 0.44014 | -0.62628 |
| H | 8.62409 | 0.11384 | -1.13029 |
| H | 7.42711 | 1.40806 | -1.04516 |
| H | 7.93868 | 0.58636 | 0.43244 |
| C | 7.10994 | -1.93770 | -0.25988 |
| H | 8.00533 | -2.24090 | -0.80816 |
| H | 7.37999 | -1.86784 | 0.79708 |
| H | 6.36604 | -2.72972 | -0.37470 |
| C | 6.31248 | -0.78430 | -2.30377 |

| | | | |
|----|----------|----------|----------|
| H | 5.52348 | -1.52362 | -2.46018 |
| H | 5.98866 | 0.15107 | -2.76504 |
| H | 7.21170 | -1.12316 | -2.82638 |
| C | 4.08037 | -2.22338 | 3.25188 |
| H | 5.03695 | -1.74092 | 3.46613 |
| H | 3.71657 | -2.66454 | 4.18283 |
| H | 4.25081 | -3.04227 | 2.54911 |
| C | 2.80025 | -0.21738 | 3.87028 |
| H | 3.71537 | 0.34002 | 4.08561 |
| H | 2.01567 | 0.50209 | 3.62762 |
| H | 2.49664 | -0.74043 | 4.78178 |
| C | 1.75476 | -2.03499 | 2.49654 |
| H | 0.89563 | -1.39363 | 2.29207 |
| H | 1.86534 | -2.71168 | 1.64832 |
| H | 1.51276 | -2.61918 | 3.38977 |
| C | -1.89910 | 2.57043 | 1.59655 |
| H | -1.64641 | 1.69172 | 2.19275 |
| H | -1.17474 | 2.64120 | 0.78841 |
| H | -1.74298 | 3.44891 | 2.22780 |
| C | -4.17317 | 2.57089 | 2.45346 |
| H | -3.88077 | 3.44931 | 3.03536 |
| H | -5.24627 | 2.63122 | 2.27138 |
| H | -3.98204 | 1.68219 | 3.05915 |
| C | -3.70258 | 3.78784 | 0.34183 |
| H | -4.76756 | 3.83023 | 0.10544 |
| H | -3.46170 | 4.67751 | 0.92992 |
| H | -3.15570 | 3.85180 | -0.59876 |
| C | -1.39365 | -2.37358 | 0.97003 |
| H | -1.06793 | -3.30857 | 1.43270 |
| H | -0.71274 | -2.18519 | 0.14265 |
| H | -1.28145 | -1.58294 | 1.71587 |
| C | -2.96834 | -3.59541 | -0.53484 |
| H | -2.41216 | -3.32314 | -1.43067 |
| H | -2.56012 | -4.53465 | -0.15210 |
| H | -4.00822 | -3.77819 | -0.81509 |
| C | -3.60440 | -2.99731 | 1.79857 |
| H | -3.55586 | -2.25146 | 2.59609 |
| H | -4.65531 | -3.21169 | 1.60013 |
| H | -3.13746 | -3.91581 | 2.16384 |
| C | -7.90213 | 1.07200 | -0.55422 |
| H | -7.92362 | 1.55454 | 0.42634 |
| H | -7.43582 | 1.75762 | -1.26625 |
| H | -8.93836 | 0.92347 | -0.86698 |
| C | -7.89112 | -1.16681 | 0.51444 |
| H | -7.45826 | -2.16838 | 0.54893 |
| H | -7.82584 | -0.73736 | 1.51716 |
| H | -8.94871 | -1.27047 | 0.25652 |
| C | -7.28756 | -0.91913 | -1.90048 |
| H | -6.80399 | -0.29752 | -2.65788 |
| H | -6.81424 | -1.90257 | -1.92468 |
| H | -8.33724 | -1.04363 | -2.18046 |
| Ge | 1.18461 | -0.47975 | -1.96823 |
| S | -1.22515 | -1.03131 | -2.22715 |
| C | -1.57955 | 1.88299 | -1.67086 |
| H | -1.49170 | 2.78866 | -1.07898 |
| H | -0.80890 | 1.87921 | -2.44286 |
| H | -2.55607 | 1.83759 | -2.15460 |

E = Sn (II)

R-P=C(Sn(II)Cl)-P(O)ClR

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.69394 | 0.17761 | 0.95797 |
| C | 0.43367 | -0.24523 | -0.62073 |
| P | -1.08519 | -0.26900 | -1.46159 |
| Cl | 1.12794 | -2.83210 | -2.73632 |
| Sn | 1.51799 | -0.45893 | -2.65407 |
| O | -0.71546 | 0.00340 | -2.90543 |
| Cl | -2.49120 | 1.01015 | -0.79574 |
| H | -1.74987 | -1.49475 | -1.29647 |
| H | 2.12060 | 0.04682 | 0.97532 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.72181 | 0.13247 | 0.93344 |
| C | 0.43372 | -0.24877 | -0.64741 |
| P | -1.11358 | -0.30536 | -1.43756 |
| Cl | 1.26300 | -2.82658 | -2.78254 |
| Sn | 1.45565 | -0.41400 | -2.71131 |
| O | -0.76960 | -0.09686 | -2.90620 |
| Cl | -2.41790 | 1.12315 | -0.82561 |
| C | 2.54508 | -0.00237 | 1.11754 |
| H | 2.76234 | -0.89088 | 1.71900 |
| H | 3.06826 | -0.08207 | 0.16443 |
| H | 2.91551 | 0.86062 | 1.67671 |
| C | -1.99834 | -1.83290 | -1.16096 |
| H | -2.26663 | -1.92689 | -0.10835 |
| H | -2.89607 | -1.84112 | -1.78113 |
| H | -1.33187 | -2.64585 | -1.45894 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.77775 | 0.26149 | 0.18967 |
| C | 0.68143 | -0.67807 | -1.16759 |
| P | -0.79635 | -1.01124 | -2.04391 |
| Cl | 1.86171 | -3.93198 | -1.50801 |
| Sn | 1.88495 | -1.85709 | -2.75632 |
| O | -0.32695 | -1.85354 | -3.22266 |
| C | 2.55218 | 0.25173 | 0.78867 |
| C | 2.94326 | 1.72393 | 0.94238 |
| H | 3.00026 | 2.22938 | -0.02520 |
| H | 2.22961 | 2.26936 | 1.56612 |
| H | 3.92653 | 1.79670 | 1.41852 |
| C | 3.53819 | -0.47031 | -0.10865 |
| H | 3.29150 | -1.53137 | -0.20491 |
| H | 3.58256 | -0.01799 | -1.10370 |
| H | 4.54542 | -0.40958 | 0.31792 |
| C | 2.50455 | -0.41153 | 2.16884 |
| H | 2.24867 | -1.47128 | 2.09522 |
| H | 3.48671 | -0.33360 | 2.64703 |
| H | 1.77652 | 0.07158 | 2.82683 |
| C | -2.17744 | -1.82307 | -1.15138 |
| C | -2.73177 | -0.91109 | -0.06231 |
| H | -3.17359 | -0.00345 | -0.47615 |
| H | -3.51286 | -1.45188 | 0.47970 |
| H | -1.96428 | -0.62278 | 0.65987 |
| C | -3.25746 | -2.16925 | -2.17727 |
| H | -2.86181 | -2.79732 | -2.97704 |
| H | -4.05289 | -2.72213 | -1.66942 |
| H | -3.69828 | -1.27515 | -2.62152 |
| C | -1.60949 | -3.10570 | -0.53748 |
| H | -1.18108 | -3.76606 | -1.29240 |
| H | -0.83561 | -2.89738 | 0.20287 |
| H | -2.42541 | -3.63638 | -0.03852 |

| | | | |
|----|----------|---------|----------|
| Cl | -1.59733 | 0.72375 | -2.75716 |
|----|----------|---------|----------|

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.76869 | 0.40716 | 0.36710 |
| C | 0.32912 | -0.27270 | -1.07706 |
| P | -1.25917 | -0.38268 | -1.76459 |
| C | 2.56010 | 0.14271 | 0.44785 |
| C | 3.21703 | -0.93231 | -0.15842 |
| C | 3.30465 | 1.05937 | 1.19390 |
| C | 4.59118 | -1.06259 | -0.04746 |
| C | 4.68133 | 0.93433 | 1.29198 |
| C | 5.32515 | -0.12531 | 0.66908 |
| H | 5.09098 | -1.90392 | -0.51389 |
| H | 5.25211 | 1.66014 | 1.85982 |
| C | -2.22898 | -1.75818 | -1.15748 |
| C | -2.39833 | -2.86300 | -1.98638 |
| C | -2.76453 | -1.75195 | 0.12912 |
| C | -3.11306 | -3.95871 | -1.52577 |
| C | -3.47382 | -2.84996 | 0.58061 |
| C | -3.64868 | -3.95237 | -0.24755 |
| H | -3.24646 | -4.82042 | -2.16905 |
| H | -3.89339 | -2.84738 | 1.57976 |
| Cl | 1.22683 | -3.09893 | -2.96803 |
| Sn | 1.26292 | -0.68361 | -3.13364 |
| O | -1.00178 | -0.48986 | -3.25919 |
| Cl | -2.40697 | 1.24632 | -1.36611 |
| H | -2.63164 | -0.88961 | 0.77323 |
| H | -4.20557 | -4.81131 | 0.10941 |
| H | -1.96630 | -2.86150 | -2.97919 |
| H | 2.79902 | 1.88222 | 1.69024 |
| H | 6.40090 | -0.23014 | 0.75313 |
| H | 2.64327 | -1.69023 | -0.68310 |

R = Mes

| | | | |
|---|----------|----------|----------|
| P | 0.81483 | 0.14849 | 1.06723 |
| C | 0.40895 | -0.51623 | -0.39429 |
| P | -1.08090 | -0.46356 | -1.30350 |
| C | 2.66191 | 0.10628 | 0.97024 |
| C | 3.38637 | -1.09611 | 1.16780 |
| C | 3.34124 | 1.27726 | 0.55304 |
| C | 4.70096 | -1.14259 | 0.71921 |
| C | 4.66443 | 1.14742 | 0.13074 |
| C | 5.34798 | -0.05662 | 0.14628 |
| H | 5.25123 | -2.06624 | 0.82958 |
| H | 5.17952 | 2.02416 | -0.22711 |
| C | 2.73339 | 2.69829 | 0.59763 |
| C | 2.83977 | -2.32862 | 1.91827 |
| C | 6.77099 | -0.20911 | -0.38269 |
| C | 2.04408 | -3.26144 | 0.99906 |
| H | 1.15112 | -2.78828 | 0.59490 |
| H | 2.64998 | -3.58720 | 0.15124 |
| H | 1.73793 | -4.15184 | 1.55678 |
| C | 1.97837 | -1.89747 | 3.10732 |
| H | 2.53641 | -1.24629 | 3.78480 |
| H | 1.06729 | -1.36578 | 2.81347 |
| H | 1.65091 | -2.77859 | 3.66562 |
| C | 3.98535 | -3.15837 | 2.51514 |
| H | 4.56520 | -3.68102 | 1.75196 |
| H | 4.66613 | -2.54686 | 3.11247 |
| H | 3.55988 | -3.92521 | 3.16662 |
| C | 1.67875 | 2.93158 | -0.49152 |
| H | 0.77237 | 2.34527 | -0.34172 |
| H | 1.38444 | 3.98493 | -0.49466 |
| H | 2.07818 | 2.69269 | -1.48075 |
| C | 2.12519 | 2.96216 | 1.98142 |

| | | | |
|----|----------|----------|----------|
| H | -5.27646 | 2.49317 | 2.37300 |
| H | -3.92947 | 1.64609 | 3.13935 |
| C | -3.84068 | 3.69554 | 0.35579 |
| H | -4.91094 | 3.69779 | 0.14143 |
| H | -3.61613 | 4.60774 | 0.91544 |
| H | -3.30555 | 3.73905 | -0.59239 |
| C | -1.43489 | -2.40693 | 1.12774 |
| H | -1.06914 | -3.37685 | 1.47307 |
| H | -0.66290 | -2.02189 | 0.46729 |
| H | -1.52189 | -1.75552 | 2.00163 |
| C | -2.64970 | -3.46042 | -0.80549 |
| H | -2.02271 | -2.97595 | -1.55061 |
| H | -2.19788 | -4.42059 | -0.54189 |
| H | -3.62746 | -3.66187 | -1.25117 |
| C | -3.64340 | -3.37186 | 1.47376 |
| H | -3.82648 | -2.77641 | 2.37169 |
| H | -4.60672 | -3.69077 | 1.07502 |
| H | -3.10133 | -4.27355 | 1.76929 |
| C | -7.93909 | 0.92099 | -0.45702 |
| H | -7.96354 | 1.37521 | 0.53688 |
| H | -7.49410 | 1.63669 | -1.15278 |
| H | -8.97413 | 0.75722 | -0.76618 |
| C | -7.87028 | -1.34708 | 0.54626 |
| H | -7.41241 | -2.33805 | 0.55148 |
| H | -7.81040 | -0.94397 | 1.56021 |
| H | -8.92635 | -1.46927 | 0.29017 |
| C | -7.28770 | -1.01509 | -1.86426 |
| H | -6.82039 | -0.36161 | -2.60474 |
| H | -6.79568 | -1.98806 | -1.91997 |
| H | -8.33620 | -1.15236 | -2.14272 |
| Sn | 1.11531 | -0.60660 | -1.88096 |
| Cl | -1.63779 | 1.92929 | -1.71858 |

R-P=C(Sn(II)Cl)-P(O)MeR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.72355 | 0.08207 | 1.06498 |
| C | 0.50601 | -0.27368 | -0.53604 |
| P | -0.99701 | -0.21989 | -1.43563 |
| Cl | 1.17390 | -2.93133 | -2.53486 |
| Sn | 1.64945 | -0.56471 | -2.51938 |
| O | -0.51930 | -0.03131 | -2.87599 |
| H | 2.14801 | -0.05751 | 1.13695 |
| H | -1.67650 | -1.44386 | -1.26598 |
| C | -2.19104 | 1.02356 | -0.94288 |
| H | -3.06460 | 0.97197 | -1.59553 |
| H | -2.49551 | 0.84593 | 0.09129 |
| H | -1.73392 | 2.01058 | -1.02340 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.71825 | 0.06447 | 0.93512 |
| C | 0.44651 | -0.23992 | -0.66390 |
| P | -1.11538 | -0.25737 | -1.46330 |
| Cl | 1.30734 | -2.83990 | -2.74302 |
| Sn | 1.47410 | -0.41763 | -2.71947 |
| O | -0.72259 | -0.10740 | -2.94180 |
| C | 2.54378 | -0.03232 | 1.13969 |
| H | 2.77930 | -0.92775 | 1.72309 |
| H | 3.07257 | -0.07795 | 0.18728 |
| H | 2.89039 | 0.82814 | 1.71789 |
| C | -1.97362 | -1.80618 | -1.17140 |
| H | -2.24602 | -1.89647 | -0.11817 |
| H | -2.87096 | -1.84853 | -1.79255 |
| H | -1.30010 | -2.61870 | -1.44976 |
| C | -2.23315 | 1.05979 | -0.96442 |
| H | -3.15316 | 1.00457 | -1.55001 |

| | | | |
|---|----------|---------|----------|
| H | -2.46840 | 0.96763 | 0.09793 |
| H | -1.74953 | 2.02056 | -1.14348 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.72196 | 0.23363 | 0.43195 |
| C | 0.55535 | -0.54342 | -1.01629 |
| P | -0.97651 | -0.77277 | -1.85938 |
| Cl | 1.80772 | -3.70459 | -1.86256 |
| Sn | 1.67091 | -1.47832 | -2.81757 |
| O | -0.53233 | -1.46702 | -3.15976 |
| C | -1.74174 | 0.81497 | -2.24376 |
| H | -2.63930 | 0.67308 | -2.84771 |
| H | -1.98750 | 1.35624 | -1.32931 |
| H | -1.01961 | 1.39881 | -2.81636 |
| C | 2.53229 | 0.21797 | 0.92297 |
| C | 2.90065 | 1.67472 | 1.21247 |
| H | 2.88601 | 2.28202 | 0.30354 |
| H | 2.21500 | 2.12962 | 1.93297 |
| H | 3.90986 | 1.72548 | 1.63446 |
| C | 3.47300 | -0.37482 | -0.10776 |
| H | 3.23759 | -1.42306 | -0.31120 |
| H | 3.44664 | 0.18616 | -1.04637 |
| H | 4.50380 | -0.33854 | 0.26195 |
| C | 2.59084 | -0.59124 | 2.22198 |
| H | 2.35277 | -1.64349 | 2.04843 |
| H | 3.60027 | -0.53846 | 2.64383 |
| H | 1.89653 | -0.20347 | 2.97298 |
| C | -2.22315 | -1.79834 | -0.97848 |
| C | -2.77935 | -1.04139 | 0.22496 |
| H | -3.34695 | -0.15577 | -0.06945 |
| H | -3.45891 | -1.69967 | 0.77419 |
| H | -1.98934 | -0.73230 | 0.91441 |
| C | -3.33933 | -2.12472 | -1.97356 |
| H | -2.94695 | -2.62306 | -2.86164 |
| H | -4.05533 | -2.79761 | -1.49250 |
| H | -3.88821 | -1.23400 | -2.28851 |
| C | -1.55000 | -3.09220 | -0.52277 |
| H | -1.10985 | -3.63838 | -1.35804 |
| H | -0.75780 | -2.90324 | 0.20320 |
| H | -2.30185 | -3.73170 | -0.05064 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77065 | 0.34447 | 0.42772 |
| C | 0.33531 | -0.27034 | -1.04485 |
| P | -1.27787 | -0.33920 | -1.72168 |
| C | 2.56982 | 0.11580 | 0.50511 |
| C | 3.24088 | -0.93150 | -0.13175 |
| C | 3.30171 | 1.02029 | 1.27690 |
| C | 4.61705 | -1.04596 | -0.02490 |
| C | 4.68020 | 0.91149 | 1.37183 |
| C | 5.33876 | -0.12048 | 0.71860 |
| H | 5.12794 | -1.86615 | -0.51643 |
| H | 5.24102 | 1.62840 | 1.96073 |
| C | -2.19987 | -1.75821 | -1.11236 |
| C | -2.51386 | -2.78697 | -1.99410 |
| C | -2.59245 | -1.83913 | 0.22239 |
| C | -3.22981 | -3.88601 | -1.54263 |
| C | -3.30709 | -2.93778 | 0.66725 |
| C | -3.62771 | -3.96038 | -0.21687 |
| H | -3.46990 | -4.68948 | -2.22916 |
| H | -3.60951 | -3.00122 | 1.70611 |
| Cl | 1.19731 | -3.10657 | -2.91185 |
| Sn | 1.23295 | -0.69016 | -3.11513 |
| O | -1.00314 | -0.47317 | -3.22542 |
| H | -2.32649 | -1.05338 | 0.92269 |

| | | | |
|---|----------|----------|----------|
| H | -4.18411 | -4.82216 | 0.13402 |
| H | -2.18503 | -2.72361 | -3.02424 |
| H | 2.78507 | 1.82131 | 1.79723 |
| H | 6.41593 | -0.21285 | 0.79959 |
| H | 2.67686 | -1.67984 | -0.68023 |
| C | -2.28913 | 1.10885 | -1.37979 |
| H | -3.24521 | 1.01314 | -1.89756 |
| H | -2.46419 | 1.20367 | -0.30647 |
| H | -1.76358 | 1.99519 | -1.73781 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.87119 | 0.14466 | 0.97501 |
| C | 0.30879 | -0.28708 | -0.51883 |
| P | -1.28340 | -0.24806 | -1.27078 |
| C | 2.68939 | 0.07091 | 0.75779 |
| C | 3.36260 | -1.16138 | 0.74362 |
| C | 3.41370 | 1.27000 | 0.68944 |
| C | 4.74790 | -1.16294 | 0.62919 |
| C | 4.79708 | 1.21922 | 0.57297 |
| C | 5.48317 | 0.01220 | 0.53361 |
| H | 5.26887 | -2.11612 | 0.62277 |
| H | 5.35377 | 2.15040 | 0.51565 |
| C | -2.24537 | -1.77291 | -1.07095 |
| C | -2.75354 | -2.46716 | -2.19246 |
| C | -2.52655 | -2.24764 | 0.22486 |
| C | -3.51038 | -3.61192 | -1.97286 |
| C | -3.29299 | -3.39652 | 0.37895 |
| C | -3.78844 | -4.10116 | -0.70508 |
| H | -3.90165 | -4.13884 | -2.83769 |
| H | -3.50581 | -3.74636 | 1.38476 |
| Cl | 1.22043 | -2.69121 | -2.86199 |
| Sn | 1.33293 | -0.27873 | -2.55540 |
| O | -0.88113 | 0.02316 | -2.72926 |
| C | -2.34615 | 1.11552 | -0.74971 |
| H | -3.19635 | 1.15782 | -1.43394 |
| H | -2.71383 | 0.99662 | 0.26857 |
| H | -1.77571 | 2.04240 | -0.82753 |
| C | 2.71767 | 2.59930 | 0.71303 |
| H | 2.19519 | 2.79139 | -0.22937 |
| H | 1.96723 | 2.64941 | 1.50846 |
| H | 3.42987 | 3.41069 | 0.86964 |
| C | 2.63043 | -2.46597 | 0.86012 |
| H | 1.90135 | -2.44479 | 1.67598 |
| H | 2.08044 | -2.70308 | -0.05487 |
| H | 3.32850 | -3.28151 | 1.05399 |
| C | 6.97270 | -0.02371 | 0.37695 |
| H | 7.24951 | -0.10658 | -0.67884 |
| H | 7.43675 | 0.88418 | 0.76643 |
| H | 7.40715 | -0.88097 | 0.89471 |
| C | -2.01667 | -1.60990 | 1.48379 |
| H | -1.02090 | -1.98785 | 1.73119 |
| H | -1.93041 | -0.52547 | 1.43505 |
| H | -2.67685 | -1.85005 | 2.31867 |
| C | -2.53815 | -2.06838 | -3.62447 |
| H | -2.79877 | -1.02833 | -3.81696 |
| H | -1.49138 | -2.18734 | -3.90860 |
| H | -3.14453 | -2.70439 | -4.27051 |
| C | -4.58250 | -5.35660 | -0.52048 |
| H | -3.94366 | -6.23664 | -0.64371 |
| H | -5.02429 | -5.40709 | 0.47593 |
| H | -5.38394 | -5.43248 | -1.25804 |

R = Mes*

| | | | |
|---|---------|---------|----------|
| P | 0.98449 | 1.17810 | 1.26456 |
| C | 0.28364 | 0.51089 | -0.07810 |

| | | | |
|----|----------|----------|----------|
| P | -1.36975 | 0.32425 | -0.67518 |
| Cl | 1.58008 | -2.82633 | -0.67886 |
| O | -1.18000 | -0.90053 | -1.59494 |
| C | -2.97933 | 0.12442 | 0.20040 |
| C | -3.55979 | -1.17623 | 0.19970 |
| C | -3.84166 | 1.23703 | 0.38145 |
| C | -4.92657 | -1.27459 | -0.02228 |
| C | -5.20634 | 1.05485 | 0.17117 |
| C | -5.76571 | -0.17455 | -0.13340 |
| H | -5.35548 | -2.26529 | -0.10070 |
| H | -5.85348 | 1.91631 | 0.26161 |
| C | 2.77732 | 0.86049 | 0.94036 |
| C | 3.42123 | -0.18983 | 1.63459 |
| C | 3.47261 | 1.54973 | -0.08516 |
| C | 4.60699 | -0.69345 | 1.10399 |
| C | 4.64972 | 0.98366 | -0.56204 |
| C | 5.20321 | -0.17445 | -0.03317 |
| H | 5.07362 | -1.53402 | 1.59157 |
| H | 5.16842 | 1.47355 | -1.37469 |
| C | 2.92475 | -0.74872 | 2.98428 |
| C | 3.08032 | 2.94135 | -0.63382 |
| C | 6.44616 | -0.78763 | -0.67071 |
| C | -3.45395 | 2.60719 | 0.97673 |
| C | -2.83758 | -2.48670 | 0.56854 |
| C | -7.23836 | -0.35890 | -0.47967 |
| C | 4.33611 | 3.71731 | -1.06182 |
| H | 4.05552 | 4.74976 | -1.28408 |
| H | 5.09086 | 3.73222 | -0.27228 |
| H | 4.79275 | 3.31320 | -1.96700 |
| C | 2.41215 | 3.80010 | 0.44243 |
| H | 1.43432 | 3.41845 | 0.75338 |
| H | 3.03802 | 3.87622 | 1.33466 |
| H | 2.24223 | 4.80840 | 0.05466 |
| C | 2.16466 | 2.85612 | -1.85861 |
| H | 2.61178 | 2.23663 | -2.64013 |
| H | 1.19508 | 2.43352 | -1.59875 |
| H | 2.00241 | 3.85622 | -2.27262 |
| C | 7.60085 | 0.22016 | -0.63409 |
| H | 8.49340 | -0.21212 | -1.09541 |
| H | 7.35776 | 1.13694 | -1.17525 |
| H | 7.84807 | 0.49339 | 0.39484 |
| C | 6.89651 | -2.05891 | 0.04406 |
| H | 7.76775 | -2.47503 | -0.46783 |
| H | 7.18651 | -1.86405 | 1.07978 |
| H | 6.11423 | -2.82174 | 0.04214 |
| C | 6.12993 | -1.14562 | -2.12805 |
| H | 5.31111 | -1.86707 | -2.18263 |
| H | 5.84067 | -0.26531 | -2.70606 |
| H | 7.00820 | -1.58723 | -2.60763 |
| C | 3.93471 | -1.71999 | 3.60248 |
| H | 4.91990 | -1.26547 | 3.73165 |
| H | 3.57414 | -2.01410 | 4.59089 |
| H | 4.04420 | -2.63263 | 3.01199 |
| C | 2.77012 | 0.41268 | 3.97651 |
| H | 3.71739 | 0.94261 | 4.10489 |
| H | 2.01867 | 1.13654 | 3.65494 |
| H | 2.45957 | 0.02772 | 4.95215 |
| C | 1.60358 | -1.51363 | 2.86963 |
| H | 0.76319 | -0.86228 | 2.62201 |
| H | 1.65745 | -2.28626 | 2.10124 |
| H | 1.37081 | -1.98476 | 3.82949 |
| C | -1.98917 | 2.73190 | 1.37280 |
| H | -1.67719 | 1.90066 | 2.00792 |
| H | -1.30170 | 2.78882 | 0.53138 |
| H | -1.84834 | 3.65001 | 1.94874 |
| C | -4.23921 | 2.72900 | 2.29939 |

| | | | |
|----|----------|----------|----------|
| H | -3.97227 | 3.66660 | 2.79494 |
| H | -5.31836 | 2.72635 | 2.14444 |
| H | -3.99295 | 1.90547 | 2.97355 |
| C | -3.85568 | 3.78311 | 0.08071 |
| H | -4.92833 | 3.79031 | -0.12121 |
| H | -3.60899 | 4.72521 | 0.57786 |
| H | -3.34199 | 3.76871 | -0.88126 |
| C | -1.49100 | -2.24400 | 1.24162 |
| H | -1.10131 | -3.19148 | 1.62111 |
| H | -0.73046 | -1.85991 | 0.56859 |
| H | -1.59736 | -1.56226 | 2.08979 |
| C | -2.68750 | -3.42803 | -0.62940 |
| H | -2.05828 | -2.98773 | -1.39928 |
| H | -2.23363 | -4.36791 | -0.30353 |
| H | -3.66289 | -3.66073 | -1.06564 |
| C | -3.69532 | -3.20201 | 1.63236 |
| H | -3.89533 | -2.55040 | 2.48670 |
| H | -4.65036 | -3.55887 | 1.24527 |
| H | -3.14666 | -4.07550 | 1.99337 |
| C | -7.98349 | 0.97053 | -0.56496 |
| H | -8.00348 | 1.49046 | 0.39630 |
| H | -7.53885 | 1.63701 | -1.30840 |
| H | -9.01999 | 0.78953 | -0.85940 |
| C | -7.91699 | -1.22447 | 0.58861 |
| H | -7.46110 | -2.21381 | 0.65925 |
| H | -7.85173 | -0.75393 | 1.57273 |
| H | -8.97448 | -1.36101 | 0.34560 |
| C | -7.34323 | -1.05811 | -1.84023 |
| H | -6.88096 | -0.45589 | -2.62619 |
| H | -6.85025 | -2.03210 | -1.83262 |
| H | -8.39305 | -1.21457 | -2.10341 |
| Sn | 1.04999 | -0.76816 | -1.84906 |
| C | -1.67888 | 1.68714 | -1.83223 |
| H | -2.62307 | 1.48478 | -2.34079 |
| H | -1.70424 | 2.67625 | -1.38659 |
| H | -0.87234 | 1.64947 | -2.56812 |

R-P=C(Sn(II)Cl)-P(S)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.04347 | 0.93418 | 0.51148 |
| C | 0.15358 | 0.42272 | -1.06044 |
| P | -1.15150 | -0.15594 | -2.04328 |
| Cl | 1.98926 | -1.66301 | -3.04141 |
| Sn | 1.63672 | 0.71514 | -2.79121 |
| S | -0.88388 | 0.68025 | -3.82066 |
| H | 1.40813 | 1.33760 | 0.68077 |
| Cl | -3.02228 | 0.08518 | -1.29632 |
| H | -1.08601 | -1.55781 | -2.09220 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.47280 | 0.42786 | 0.60047 |
| C | 0.19222 | 0.15376 | -1.00729 |
| P | -1.37691 | -0.03348 | -1.72371 |
| Cl | 1.42712 | -1.93366 | -3.49360 |
| Sn | 1.36302 | 0.43680 | -2.96333 |
| S | -1.23062 | 0.82849 | -3.51695 |
| Cl | -2.90685 | 0.76724 | -0.63210 |
| C | 2.30197 | 0.52513 | 0.74319 |
| H | 2.64605 | -0.35339 | 1.29800 |
| H | 2.81629 | 0.56142 | -0.21785 |
| H | 2.56725 | 1.40293 | 1.33814 |
| C | -1.83641 | -1.76633 | -1.82376 |
| H | -1.93861 | -2.17242 | -0.81634 |
| H | -2.77882 | -1.85137 | -2.36610 |

| | | | |
|---|----------|----------|----------|
| H | -1.03982 | -2.28151 | -2.36589 |
|---|----------|----------|----------|

R =t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.31834 | 0.07007 | 0.55364 |
| C | 0.06825 | 0.23399 | -1.07896 |
| P | -1.54089 | 0.03444 | -1.74327 |
| Cl | 1.91897 | -0.97641 | -3.83029 |
| Sn | 1.10169 | 1.12776 | -2.93425 |
| S | -1.50441 | 0.90379 | -3.54000 |
| C | 2.14809 | 0.21017 | 0.92293 |
| C | 2.26744 | 1.25131 | 2.03890 |
| H | 3.29788 | 1.27920 | 2.40792 |
| H | 2.01022 | 2.25301 | 1.68511 |
| H | 1.61637 | 1.01484 | 2.88502 |
| C | 2.53218 | -1.16908 | 1.47082 |
| H | 3.55828 | -1.13613 | 1.85210 |
| H | 1.88222 | -1.47615 | 2.29528 |
| H | 2.48595 | -1.93636 | 0.69418 |
| C | 3.04273 | 0.57591 | -0.24522 |
| H | 4.08928 | 0.59322 | 0.07877 |
| H | 2.96825 | -0.15085 | -1.05880 |
| H | 2.81398 | 1.57359 | -0.63078 |
| C | -2.13284 | -1.72407 | -1.82389 |
| C | -1.10395 | -2.51474 | -2.63050 |
| C | -2.26118 | -2.30242 | -0.41877 |
| C | -3.48336 | -1.73962 | -2.53685 |
| H | -0.98343 | -2.11904 | -3.63955 |
| H | -0.12202 | -2.51925 | -2.15569 |
| H | -1.45303 | -3.54863 | -2.70701 |
| H | -3.00651 | -1.77476 | 0.17742 |
| H | -2.57411 | -3.34681 | -0.50676 |
| H | -1.31160 | -2.28523 | 0.11989 |
| H | -3.80573 | -2.77971 | -2.63808 |
| H | -4.24890 | -1.20150 | -1.97548 |
| H | -3.41446 | -1.30930 | -3.53760 |
| Cl | -2.95664 | 0.94086 | -0.56767 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.79669 | 0.50120 | 0.49437 |
| C | 0.27373 | -0.12477 | -0.95053 |
| P | -1.36146 | -0.12752 | -1.52336 |
| C | 2.56713 | 0.11028 | 0.51518 |
| C | 3.11400 | -1.03855 | -0.06525 |
| C | 3.41009 | 0.99748 | 1.18852 |
| C | 4.47832 | -1.27093 | -0.00119 |
| C | 4.77577 | 0.76867 | 1.23979 |
| C | 5.31050 | -0.36429 | 0.64261 |
| H | 4.89189 | -2.16742 | -0.44876 |
| H | 5.42350 | 1.47135 | 1.75135 |
| C | -2.20735 | -1.64461 | -1.04291 |
| C | -2.55129 | -2.58616 | -2.00447 |
| C | -2.47388 | -1.88259 | 0.30464 |
| C | -3.17294 | -3.76415 | -1.61707 |
| C | -3.09360 | -3.05958 | 0.68218 |
| C | -3.44424 | -4.00009 | -0.27917 |
| H | -3.43918 | -4.50019 | -2.36631 |
| H | -3.30365 | -3.24553 | 1.72894 |
| Cl | 1.06515 | -2.92125 | -2.93321 |
| Sn | 1.33096 | -0.50811 | -2.94067 |
| S | -1.24599 | 0.12561 | -3.49360 |
| Cl | -2.51026 | 1.32678 | -0.65510 |
| H | -2.20107 | -1.14908 | 1.05538 |
| H | -2.32368 | -2.39829 | -3.04647 |
| H | -3.92853 | -4.92255 | 0.02038 |
| H | 2.46423 | -1.77266 | -0.53242 |

| | | | |
|---|---------|----------|---------|
| H | 2.99089 | 1.87838 | 1.66524 |
| H | 6.37768 | -0.54890 | 0.69026 |

R = Mes

| | | | |
|---|----------|----------|----------|
| P | -0.93732 | -0.20597 | 1.88111 |
| C | -0.02011 | -0.45939 | 0.51954 |
| P | 1.44833 | -1.39282 | 0.37799 |
| C | -2.55934 | 0.30818 | 1.15171 |
| C | -2.76982 | 1.60905 | 0.62756 |
| C | -3.57029 | -0.67635 | 1.01266 |
| C | -3.86415 | 1.80556 | -0.20666 |
| C | -4.64432 | -0.39358 | 0.16903 |
| C | -4.78698 | 0.81135 | -0.49751 |
| H | -4.01137 | 2.78343 | -0.64253 |
| H | -5.39857 | -1.14987 | 0.02484 |
| C | -3.59316 | -2.01946 | 1.77874 |
| C | -1.91020 | 2.84056 | 0.97870 |
| C | -5.92633 | 1.08979 | -1.47324 |
| C | -0.67090 | 2.94718 | 0.08409 |
| H | 0.00591 | 2.10301 | 0.20280 |
| H | -0.95329 | 2.99324 | -0.97000 |
| H | -0.12055 | 3.86245 | 0.32264 |
| C | -1.50643 | 2.81139 | 2.45428 |
| H | -2.38583 | 2.76196 | 3.10125 |
| H | -0.85864 | 1.96739 | 2.71116 |
| H | -0.94452 | 3.71557 | 2.70285 |
| C | -2.70707 | 4.13992 | 0.79438 |
| H | -2.89483 | 4.37119 | -0.25591 |
| H | -3.66363 | 4.11199 | 1.32192 |
| H | -2.12221 | 4.96918 | 1.19911 |
| C | -2.54750 | -3.01484 | 1.26118 |
| H | -1.52186 | -2.70137 | 1.45400 |
| H | -2.68828 | -3.98121 | 1.75361 |
| H | -2.65423 | -3.16943 | 0.18438 |
| C | -3.39009 | -1.77090 | 3.27938 |
| H | -2.41322 | -1.34312 | 3.51271 |
| H | -4.15587 | -1.09393 | 3.66607 |
| H | -3.46475 | -2.71702 | 3.82244 |
| C | -4.95062 | -2.72055 | 1.64944 |
| H | -5.77698 | -2.08276 | 1.97180 |
| H | -5.14942 | -3.06244 | 0.63108 |
| H | -4.94509 | -3.60563 | 2.28942 |
| C | -6.83223 | -0.12293 | -1.66972 |
| H | -7.32638 | -0.41891 | -0.74079 |
| H | -7.61360 | 0.12024 | -2.39373 |
| H | -6.28010 | -0.98343 | -2.05586 |
| C | -5.33490 | 1.47230 | -2.83529 |
| H | -4.70409 | 2.36086 | -2.76789 |
| H | -4.72523 | 0.66008 | -3.23856 |
| H | -6.13645 | 1.68405 | -3.54849 |
| C | -6.78227 | 2.24871 | -0.94859 |
| H | -6.19915 | 3.16457 | -0.83359 |
| H | -7.59896 | 2.45897 | -1.64489 |
| H | -7.21815 | 2.00388 | 0.02322 |
| C | 2.98458 | -0.40887 | 0.21642 |
| C | 3.83798 | -0.44987 | -0.91934 |
| C | 3.31871 | 0.43026 | 1.30631 |
| C | 4.97018 | 0.35327 | -0.91711 |
| C | 4.47156 | 1.20242 | 1.23077 |
| C | 5.31255 | 1.18646 | 0.13544 |
| H | 5.61438 | 0.32185 | -1.78625 |
| H | 4.72392 | 1.84125 | 2.07032 |
| C | 3.65406 | -1.34946 | -2.12545 |
| C | 4.30732 | -2.70737 | -1.86787 |
| C | 4.16339 | -0.75268 | -3.43341 |
| H | 2.58969 | -1.50847 | -2.26809 |

| | | | |
|----|----------|----------|----------|
| H | 3.90858 | -3.18789 | -0.97215 |
| H | 4.13273 | -3.37866 | -2.71276 |
| H | 5.38808 | -2.59646 | -1.73817 |
| H | 3.76918 | 0.25249 | -3.59326 |
| H | 5.25489 | -0.71708 | -3.48973 |
| H | 3.82488 | -1.37873 | -4.26237 |
| C | 2.53825 | 0.55795 | 2.60170 |
| C | 2.11608 | 2.00168 | 2.86606 |
| C | 3.33912 | 0.01203 | 3.78369 |
| H | 1.62281 | -0.02913 | 2.54124 |
| H | 1.56251 | 2.41791 | 2.02354 |
| H | 1.47887 | 2.04720 | 3.75269 |
| H | 2.97931 | 2.64525 | 3.05026 |
| H | 3.64231 | -1.02243 | 3.61885 |
| H | 4.24068 | 0.60556 | 3.95489 |
| H | 2.73581 | 0.05049 | 4.69432 |
| C | 6.55354 | 2.04367 | 0.09345 |
| C | 6.48822 | 3.06694 | -1.03806 |
| C | 7.82014 | 1.19668 | -0.00507 |
| H | 6.59244 | 2.59383 | 1.04048 |
| H | 5.59735 | 3.69315 | -0.95700 |
| H | 7.36709 | 3.71643 | -1.01732 |
| H | 6.46115 | 2.57446 | -2.01356 |
| H | 7.88493 | 0.48035 | 0.81673 |
| H | 7.84633 | 0.63404 | -0.94194 |
| H | 8.70850 | 1.83271 | 0.02467 |
| Cl | 0.67675 | 0.75464 | -2.72052 |
| Sn | -0.87825 | -0.74190 | -1.57971 |
| S | 0.89542 | -2.68608 | -1.05223 |
| Cl | 1.84440 | -2.59883 | 2.01188 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.92866 | 0.74682 | 1.43933 |
| C | 0.31814 | 0.34860 | -0.05561 |
| P | -1.34254 | 0.24874 | -0.60098 |
| Cl | 1.93487 | -2.68408 | -1.03843 |
| C | -2.94999 | 0.06365 | 0.28455 |
| C | -3.53686 | -1.23679 | 0.25199 |
| C | -3.79874 | 1.17699 | 0.52189 |
| C | -4.90173 | -1.31587 | 0.02096 |
| C | -5.16034 | 1.01055 | 0.28287 |
| C | -5.72544 | -0.20168 | -0.07595 |
| H | -5.34293 | -2.30085 | -0.06777 |
| H | -5.80095 | 1.87376 | 0.39774 |
| C | 2.74326 | 0.63526 | 1.12938 |
| C | 3.46606 | -0.45899 | 1.66182 |
| C | 3.38659 | 1.52546 | 0.23400 |
| C | 4.68114 | -0.78817 | 1.06768 |
| C | 4.59047 | 1.11674 | -0.33007 |
| C | 5.22518 | -0.06800 | 0.01562 |
| H | 5.21159 | -1.65528 | 1.42660 |
| H | 5.06277 | 1.76065 | -1.06042 |
| C | 3.01273 | -1.24993 | 2.90437 |
| C | 2.92841 | 2.97112 | -0.06413 |
| C | 6.49226 | -0.49958 | -0.71544 |
| C | -3.41618 | 2.49777 | 1.22428 |
| C | -2.85592 | -2.55743 | 0.67197 |
| C | -7.19115 | -0.35651 | -0.46050 |
| C | 4.16156 | 3.89182 | -0.09125 |
| H | 3.82955 | 4.93129 | -0.15173 |
| H | 4.76502 | 3.77809 | 0.81227 |
| H | 4.80363 | 3.71361 | -0.95461 |
| C | 2.02424 | 3.53634 | 1.03092 |
| H | 1.03870 | 3.06299 | 1.06194 |
| H | 2.48104 | 3.43920 | 2.01879 |
| H | 1.84397 | 4.59824 | 0.84244 |

| | | | |
|----|----------|----------|----------|
| C | 2.22470 | 3.09269 | -1.41770 |
| H | 2.84362 | 2.68685 | -2.22155 |
| H | 1.26845 | 2.56896 | -1.42216 |
| H | 2.02860 | 4.14536 | -1.64333 |
| C | 7.58034 | 0.56742 | -0.54956 |
| H | 8.48870 | 0.26358 | -1.07749 |
| H | 7.26902 | 1.53300 | -0.95334 |
| H | 7.83106 | 0.70945 | 0.50469 |
| C | 7.03777 | -1.82646 | -0.19427 |
| H | 7.92371 | -2.10639 | -0.76946 |
| H | 7.33524 | -1.76170 | 0.85560 |
| H | 6.30645 | -2.63165 | -0.29762 |
| C | 6.16632 | -0.66840 | -2.20455 |
| H | 5.39613 | -1.42972 | -2.34971 |
| H | 5.80550 | 0.26277 | -2.64674 |
| H | 7.06063 | -0.97589 | -2.75403 |
| C | 4.09252 | -2.22339 | 3.38426 |
| H | 5.03922 | -1.71965 | 3.59361 |
| H | 3.75354 | -2.68948 | 4.31234 |
| H | 4.27370 | -3.02553 | 2.66514 |
| C | 2.76244 | -0.26530 | 4.05558 |
| H | 3.66337 | 0.31323 | 4.27491 |
| H | 1.95584 | 0.43621 | 3.83356 |
| H | 2.48135 | -0.81433 | 4.95883 |
| C | 1.75454 | -2.08238 | 2.65223 |
| H | 0.87514 | -1.45838 | 2.47816 |
| H | 1.87331 | -2.73232 | 1.78425 |
| H | 1.53858 | -2.69704 | 3.53148 |
| C | -1.95567 | 2.59864 | 1.64310 |
| H | -1.64092 | 1.71865 | 2.20773 |
| H | -1.27861 | 2.73971 | 0.80410 |
| H | -1.83252 | 3.46423 | 2.29920 |
| C | -4.21795 | 2.49636 | 2.54408 |
| H | -3.95674 | 3.38613 | 3.12348 |
| H | -5.29530 | 2.50806 | 2.37704 |
| H | -3.97835 | 1.61622 | 3.14555 |
| C | -3.81259 | 3.74425 | 0.42869 |
| H | -4.87745 | 3.75407 | 0.18864 |
| H | -3.60325 | 4.63657 | 1.02498 |
| H | -3.25521 | 3.82203 | -0.50378 |
| C | -1.40559 | -2.41302 | 1.11518 |
| H | -1.09333 | -3.33779 | 1.60668 |
| H | -0.70990 | -2.25222 | 0.29406 |
| H | -1.29762 | -1.60498 | 1.84300 |
| C | -2.96245 | -3.65680 | -0.38659 |
| H | -2.39415 | -3.40158 | -1.28000 |
| H | -2.55980 | -4.58922 | 0.01796 |
| H | -3.99796 | -3.84419 | -0.67876 |
| C | -3.62442 | -3.01949 | 1.92957 |
| H | -3.58350 | -2.26021 | 2.71466 |
| H | -4.67331 | -3.23596 | 1.72412 |
| H | -3.16180 | -3.93204 | 2.31474 |
| C | -7.91821 | 0.98427 | -0.51850 |
| H | -7.95734 | 1.47120 | 0.45932 |
| H | -7.44660 | 1.66981 | -1.22694 |
| H | -8.94866 | 0.82609 | -0.84531 |
| C | -7.90522 | -1.24975 | 0.56091 |
| H | -7.46615 | -2.24827 | 0.60559 |
| H | -7.85722 | -0.81565 | 1.56262 |
| H | -8.95831 | -1.36191 | 0.28858 |
| C | -7.26830 | -1.00813 | -1.84655 |
| H | -6.77598 | -0.38714 | -2.59864 |
| H | -6.78917 | -1.98904 | -1.85844 |
| H | -8.31280 | -1.13989 | -2.14217 |
| Sn | 1.34991 | -0.49570 | -1.93953 |
| S | -1.27089 | -1.08018 | -2.09336 |

| | | | |
|----|----------|---------|----------|
| Cl | -1.60583 | 2.04713 | -1.59608 |
|----|----------|---------|----------|

R-P=C(Sn(II)Cl)-P(S)MeR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.14006 | 1.22038 | 0.52450 |
| C | 0.09232 | 0.53244 | -0.98295 |
| P | -1.38030 | 0.05366 | -1.80612 |
| Cl | 1.46433 | -2.05666 | -2.65996 |
| Sn | 1.49981 | 0.36486 | -2.77288 |
| S | -1.04351 | 0.56808 | -3.70953 |
| H | 1.54755 | 1.48074 | 0.59750 |
| C | -2.93538 | 0.68045 | -1.14607 |
| H | -3.76232 | 0.28726 | -1.74018 |
| H | -3.04507 | 0.36288 | -0.10656 |
| H | -2.93290 | 1.76939 | -1.20107 |
| H | -1.48855 | -1.34373 | -1.66450 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.41911 | 0.55090 | 0.42353 |
| C | 0.22966 | 0.21528 | -1.18559 |
| P | -1.34575 | 0.06851 | -1.94670 |
| Cl | 1.49838 | -2.17341 | -3.31381 |
| Sn | 1.51654 | 0.25158 | -3.07401 |
| S | -1.01458 | 0.67066 | -3.83869 |
| C | 2.23661 | 0.62344 | 0.68954 |
| H | 2.52588 | -0.21980 | 1.32396 |
| H | 2.80823 | 0.58340 | -0.23856 |
| H | 2.48441 | 1.53699 | 1.23630 |
| C | -1.88183 | -1.65089 | -1.88715 |
| H | -2.06262 | -1.94473 | -0.85088 |
| H | -2.79358 | -1.76548 | -2.47638 |
| H | -1.08763 | -2.26543 | -2.31463 |
| C | -2.66387 | 1.02666 | -1.16818 |
| H | -3.59105 | 0.88473 | -1.72684 |
| H | -2.80148 | 0.69779 | -0.13578 |
| H | -2.39119 | 2.08176 | -1.18230 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.56346 | -0.00369 | 0.24580 |
| C | 0.20244 | 0.36965 | -1.32928 |
| P | -1.46089 | 0.15893 | -1.90186 |
| Cl | 1.99211 | -0.47670 | -4.22735 |
| Sn | 1.07723 | 1.49596 | -3.13170 |
| S | -1.51761 | 1.14443 | -3.66103 |
| C | 2.38943 | 0.26495 | 0.56910 |
| C | 2.46646 | 1.17307 | 1.79859 |
| H | 3.50658 | 1.25859 | 2.13008 |
| H | 2.10027 | 2.17947 | 1.57952 |
| H | 1.88246 | 0.77518 | 2.63327 |
| C | 2.93184 | -1.12273 | 0.92676 |
| H | 3.96966 | -1.03368 | 1.26517 |
| H | 2.35838 | -1.58846 | 1.73338 |
| H | 2.91540 | -1.79341 | 0.06427 |
| C | 3.18279 | 0.85521 | -0.58020 |
| H | 4.23822 | 0.94156 | -0.29837 |
| H | 3.13624 | 0.22421 | -1.47196 |
| H | 2.83719 | 1.86118 | -0.83414 |
| C | -1.94578 | -1.62226 | -2.12406 |
| C | -0.88206 | -2.31237 | -2.97279 |
| C | -2.05997 | -2.30479 | -0.76329 |
| C | -3.29122 | -1.66273 | -2.84819 |
| H | -0.75924 | -1.82804 | -3.94249 |
| H | 0.09202 | -2.31834 | -2.48197 |
| H | -1.18821 | -3.34897 | -3.14235 |

| | | | |
|---|----------|----------|----------|
| H | -2.87282 | -1.89496 | -0.16007 |
| H | -2.27187 | -3.36611 | -0.92299 |
| H | -1.13386 | -2.23524 | -0.18824 |
| H | -3.55922 | -2.70825 | -3.02581 |
| H | -4.09527 | -1.21418 | -2.25994 |
| H | -3.24184 | -1.15750 | -3.81433 |
| C | -2.65385 | 0.88669 | -0.74984 |
| H | -3.66676 | 0.78830 | -1.14226 |
| H | -2.57866 | 0.40864 | 0.22795 |
| H | -2.41236 | 1.94529 | -0.65323 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.80164 | 0.37975 | 0.54177 |
| C | 0.30266 | -0.16374 | -0.94387 |
| P | -1.36835 | -0.12300 | -1.47453 |
| C | 2.58705 | 0.05599 | 0.56211 |
| C | 3.17256 | -1.04326 | -0.07255 |
| C | 3.39744 | 0.93346 | 1.28518 |
| C | 4.54351 | -1.23510 | -0.01182 |
| C | 4.76955 | 0.74550 | 1.33430 |
| C | 5.34344 | -0.33756 | 0.68329 |
| H | 4.98754 | -2.09344 | -0.50298 |
| H | 5.39193 | 1.44109 | 1.88568 |
| C | -2.19034 | -1.66598 | -1.00418 |
| C | -2.66930 | -2.54059 | -1.97080 |
| C | -2.33809 | -1.97222 | 0.34781 |
| C | -3.30818 | -3.71043 | -1.58628 |
| C | -2.97760 | -3.13982 | 0.72602 |
| C | -3.46510 | -4.00856 | -0.24210 |
| H | -3.67576 | -4.39393 | -2.34265 |
| H | -3.08895 | -3.37731 | 1.77765 |
| Cl | 1.09664 | -2.91723 | -2.92846 |
| Sn | 1.33242 | -0.49623 | -2.94776 |
| S | -1.25377 | 0.10492 | -3.46572 |
| H | -1.93753 | -1.31029 | 1.10918 |
| H | -2.52734 | -2.30583 | -3.01913 |
| H | -3.96074 | -4.92560 | 0.05559 |
| H | 2.54834 | -1.77109 | -0.58255 |
| H | 2.94805 | 1.77521 | 1.80346 |
| H | 6.41577 | -0.49045 | 0.72830 |
| C | -2.35678 | 1.19026 | -0.72205 |
| H | -3.36725 | 1.15215 | -1.13234 |
| H | -2.39647 | 1.05941 | 0.36103 |
| H | -1.89872 | 2.15084 | -0.95889 |

R = Mes

| | | | |
|---|----------|----------|----------|
| P | 0.93983 | 0.19335 | 1.07394 |
| C | 0.30451 | -0.24543 | -0.39465 |
| P | -1.36033 | -0.07448 | -0.95311 |
| C | 2.74335 | 0.02288 | 0.79747 |
| C | 3.35423 | -1.24122 | 0.75021 |
| C | 3.52497 | 1.18536 | 0.71346 |
| C | 4.73332 | -1.31034 | 0.58964 |
| C | 4.89917 | 1.06674 | 0.55170 |
| C | 5.52271 | -0.17240 | 0.47986 |
| H | 5.20570 | -2.28791 | 0.55681 |
| H | 5.49929 | 1.96956 | 0.48175 |
| C | -2.25582 | -1.67117 | -0.94718 |
| C | -2.89003 | -2.21766 | -2.08679 |
| C | -2.34293 | -2.35906 | 0.28282 |
| C | -3.56950 | -3.42287 | -1.95515 |
| C | -3.04186 | -3.55940 | 0.34630 |
| C | -3.65613 | -4.11802 | -0.75951 |
| H | -4.05419 | -3.83116 | -2.83636 |
| H | -3.10104 | -4.06975 | 1.30296 |

| | | | |
|----|----------|----------|----------|
| Cl | 0.86444 | -2.55201 | -2.92200 |
| Sn | 1.43610 | -0.24384 | -2.36070 |
| S | -1.00358 | 0.81374 | -2.73139 |
| C | -2.41709 | 1.07050 | -0.02102 |
| H | -3.29932 | 1.26601 | -0.63421 |
| H | -2.73451 | 0.66699 | 0.93920 |
| H | -1.86888 | 2.00209 | 0.12359 |
| C | 2.89703 | 2.54709 | 0.76570 |
| H | 2.33017 | 2.75855 | -0.14644 |
| H | 2.19777 | 2.63851 | 1.60281 |
| H | 3.65593 | 3.32325 | 0.87348 |
| C | 2.56573 | -2.51178 | 0.88119 |
| H | 1.88915 | -2.47383 | 1.74045 |
| H | 1.95082 | -2.70352 | -0.00267 |
| H | 3.23301 | -3.36396 | 1.01652 |
| C | 7.00241 | -0.27981 | 0.27250 |
| H | 7.24050 | -0.33514 | -0.79446 |
| H | 7.52612 | 0.58708 | 0.67947 |
| H | 7.40666 | -1.17794 | 0.74304 |
| C | -1.69734 | -1.92183 | 1.56627 |
| H | -0.67029 | -2.29149 | 1.62146 |
| H | -1.64475 | -0.84501 | 1.70873 |
| H | -2.24440 | -2.33843 | 2.41335 |
| C | -2.89606 | -1.61302 | -3.46029 |
| H | -3.26815 | -0.58886 | -3.47103 |
| H | -1.89223 | -1.59373 | -3.88632 |
| H | -3.53271 | -2.21250 | -4.11206 |
| C | -4.37222 | -5.42949 | -0.67724 |
| H | -4.65532 | -5.66647 | 0.34948 |
| H | -5.27379 | -5.42972 | -1.29313 |
| H | -3.73157 | -6.23946 | -1.03939 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.91279 | 0.90362 | 1.31404 |
| C | 0.28475 | 0.37652 | -0.13009 |
| P | -1.39171 | 0.31040 | -0.69050 |
| Cl | 1.84504 | -2.78716 | -0.86494 |
| C | -2.98938 | 0.15191 | 0.23748 |
| C | -3.58904 | -1.13855 | 0.30658 |
| C | -3.83558 | 1.28303 | 0.38556 |
| C | -4.95698 | -1.22724 | 0.08951 |
| C | -5.19969 | 1.11296 | 0.16113 |
| C | -5.77531 | -0.12089 | -0.09399 |
| H | -5.40336 | -2.21390 | 0.07776 |
| H | -5.83418 | 1.98745 | 0.20789 |
| C | 2.73156 | 0.74027 | 1.02711 |
| C | 3.43411 | -0.32083 | 1.64563 |
| C | 3.40639 | 1.57091 | 0.09595 |
| C | 4.66133 | -0.69537 | 1.10404 |
| C | 4.62730 | 1.12761 | -0.40004 |
| C | 5.24236 | -0.03953 | 0.03137 |
| H | 5.17401 | -1.54385 | 1.52730 |
| H | 5.12975 | 1.72514 | -1.14836 |
| C | 2.95624 | -1.01924 | 2.93483 |
| C | 2.94985 | 2.99067 | -0.31410 |
| C | 6.52883 | -0.51763 | -0.63413 |
| C | -3.43507 | 2.65218 | 0.97828 |
| C | -2.91184 | -2.42949 | 0.81039 |
| C | -7.24498 | -0.29816 | -0.45440 |
| C | 4.17469 | 3.88134 | -0.57979 |
| H | 3.84155 | 4.91543 | -0.69771 |
| H | 4.88730 | 3.84524 | 0.24730 |
| H | 4.69979 | 3.61308 | -1.49801 |
| C | 2.17883 | 3.68110 | 0.81295 |
| H | 1.21422 | 3.21071 | 1.02747 |
| H | 2.75669 | 3.69216 | 1.74007 |

| | | | |
|----|----------|----------|----------|
| H | 1.96364 | 4.71537 | 0.53025 |
| C | 2.10405 | 2.99443 | -1.59000 |
| H | 2.62977 | 2.49968 | -2.41034 |
| H | 1.15455 | 2.48386 | -1.43622 |
| H | 1.89399 | 4.02430 | -1.89535 |
| C | 7.61818 | 0.55184 | -0.49465 |
| H | 8.54058 | 0.21481 | -0.97620 |
| H | 7.32535 | 1.49463 | -0.96132 |
| H | 7.83701 | 0.75163 | 0.55736 |
| C | 7.04941 | -1.81542 | -0.02204 |
| H | 7.95129 | -2.13146 | -0.55208 |
| H | 7.31376 | -1.69275 | 1.03150 |
| H | 6.31667 | -2.62187 | -0.10282 |
| C | 6.24893 | -0.76871 | -2.12101 |
| H | 5.47698 | -1.53154 | -2.24765 |
| H | 5.90964 | 0.13829 | -2.62596 |
| H | 7.15746 | -1.11279 | -2.62360 |
| C | 4.01406 | -1.97758 | 3.48899 |
| H | 4.96767 | -1.47820 | 3.67642 |
| H | 3.65708 | -2.37615 | 4.44147 |
| H | 4.18764 | -2.82791 | 2.82544 |
| C | 2.71945 | 0.04780 | 4.01338 |
| H | 3.63054 | 0.62252 | 4.19853 |
| H | 1.92849 | 0.74749 | 3.73608 |
| H | 2.42207 | -0.43163 | 4.95052 |
| C | 1.68369 | -1.84378 | 2.73611 |
| H | 0.81534 | -1.21777 | 2.52276 |
| H | 1.78992 | -2.55013 | 1.91181 |
| H | 1.45927 | -2.39702 | 3.65328 |
| C | -1.98715 | 2.73606 | 1.44667 |
| H | -1.74384 | 1.91615 | 2.12490 |
| H | -1.25082 | 2.73209 | 0.64668 |
| H | -1.84197 | 3.66941 | 1.99665 |
| C | -4.27243 | 2.80764 | 2.26633 |
| H | -3.98679 | 3.73384 | 2.77266 |
| H | -5.34284 | 2.85235 | 2.06518 |
| H | -4.09119 | 1.97568 | 2.95056 |
| C | -3.77335 | 3.83189 | 0.06159 |
| H | -4.83471 | 3.84906 | -0.19357 |
| H | -3.54366 | 4.77114 | 0.57205 |
| H | -3.21223 | 3.81409 | -0.87243 |
| C | -1.45564 | -2.25766 | 1.21952 |
| H | -1.13202 | -3.14940 | 1.76197 |
| H | -0.77790 | -2.14729 | 0.37550 |
| H | -1.33692 | -1.40421 | 1.89132 |
| C | -3.03772 | -3.59950 | -0.16772 |
| H | -2.48840 | -3.40448 | -1.08763 |
| H | -2.62438 | -4.50123 | 0.29196 |
| H | -4.07896 | -3.80808 | -0.42374 |
| C | -3.66535 | -2.79832 | 2.10668 |
| H | -3.60960 | -1.98701 | 2.83701 |
| H | -4.71826 | -3.02247 | 1.93084 |
| H | -3.20207 | -3.68487 | 2.54781 |
| C | -7.96383 | 1.03748 | -0.62460 |
| H | -7.99306 | 1.60798 | 0.30731 |
| H | -7.49265 | 1.65559 | -1.39302 |
| H | -8.99752 | 0.85898 | -0.93007 |
| C | -7.95688 | -1.09289 | 0.64682 |
| H | -7.52190 | -2.08567 | 0.77705 |
| H | -7.89891 | -0.57188 | 1.60566 |
| H | -9.01260 | -1.22290 | 0.39304 |
| C | -7.33857 | -1.06865 | -1.77690 |
| H | -6.85082 | -0.51891 | -2.58546 |
| H | -6.86366 | -2.04914 | -1.70707 |
| H | -8.38630 | -1.22061 | -2.05073 |
| Sn | 1.28719 | -0.66682 | -1.93018 |

| | | | |
|---|----------|----------|----------|
| S | -1.32241 | -1.17446 | -2.07603 |
| C | -1.62008 | 1.77880 | -1.74502 |
| H | -1.52233 | 2.72776 | -1.22712 |
| H | -0.85373 | 1.70941 | -2.51788 |
| H | -2.59821 | 1.70351 | -2.22135 |

E = Pb(II)

R-P=C(Pb(II)Cl)-P(O)ClR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.74445 | 0.05730 | 1.03903 |
| C | 0.55043 | -0.27560 | -0.56974 |
| P | -0.95773 | -0.37109 | -1.42649 |
| O | -0.66733 | 0.07034 | -2.84053 |
| Pb | 1.73236 | -0.22944 | -2.67214 |
| Cl | 1.56902 | -2.69827 | -2.96595 |
| H | 2.17718 | 0.04900 | 1.08979 |
| H | -1.48508 | -1.67128 | -1.35966 |
| Cl | -2.47867 | 0.68126 | -0.61557 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.90353 | 0.29640 | 0.88416 |
| C | 0.59512 | -0.21487 | -0.65421 |
| P | -0.97078 | -0.31466 | -1.40622 |
| O | -0.71293 | -0.16893 | -2.89395 |
| Pb | 1.63496 | -0.56190 | -2.79913 |
| Cl | 1.38963 | -3.05660 | -2.69189 |
| C | 2.72968 | 0.17283 | 1.06806 |
| H | 3.22820 | -0.19998 | 0.17321 |
| H | 3.12791 | 1.15607 | 1.33520 |
| H | 2.94833 | -0.49536 | 1.90646 |
| C | -1.81928 | -1.83808 | -1.01086 |
| H | -2.03960 | -1.88274 | 0.05590 |
| H | -2.74275 | -1.88996 | -1.58971 |
| H | -1.15491 | -2.65752 | -1.29672 |
| Cl | -2.26732 | 1.12589 | -0.78962 |

R = t-Bu

| | | | |
|---|----------|----------|----------|
| P | 0.71803 | 0.32595 | 0.23937 |
| C | 0.61858 | -0.62568 | -1.10658 |
| P | -0.85234 | -0.95388 | -1.99684 |
| O | -0.42158 | -1.77293 | -3.19872 |
| C | 2.49262 | 0.30287 | 0.84799 |
| C | 2.89865 | 1.77139 | 0.99339 |
| H | 2.96476 | 2.26999 | 0.02270 |
| H | 2.18634 | 2.32775 | 1.60888 |
| H | 3.87993 | 1.83917 | 1.47460 |
| C | 3.47680 | -0.43556 | -0.03781 |
| H | 3.22038 | -1.49544 | -0.12470 |
| H | 3.53080 | 0.01341 | -1.03486 |
| H | 4.48294 | -0.38091 | 0.39208 |
| C | 2.43285 | -0.35113 | 2.23179 |
| H | 2.16696 | -1.40878 | 2.16355 |
| H | 3.41257 | -0.27907 | 2.71603 |
| H | 1.70503 | 0.14293 | 2.88173 |
| C | -2.22046 | -1.77469 | -1.08997 |
| C | -2.75790 | -0.88298 | 0.02336 |
| H | -3.20346 | 0.03305 | -0.36749 |
| H | -3.53245 | -1.43205 | 0.56665 |
| H | -1.97992 | -0.60893 | 0.73973 |
| C | -3.31872 | -2.10472 | -2.10157 |
| H | -2.93690 | -2.71972 | -2.91792 |
| H | -4.10633 | -2.66470 | -1.58912 |
| H | -3.76567 | -1.20318 | -2.52442 |
| C | -1.64221 | -3.06758 | -0.50717 |

| | | | |
|----|----------|----------|----------|
| H | -1.22879 | -3.71639 | -1.28043 |
| H | -0.85383 | -2.87216 | 0.22137 |
| H | -2.44828 | -3.60689 | -0.00128 |
| Cl | -1.66157 | 0.80348 | -2.65880 |
| Pb | 1.91623 | -1.86800 | -2.71183 |
| Cl | 1.88286 | -4.00331 | -1.38999 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77895 | 0.43510 | 0.40549 |
| C | 0.32367 | -0.22947 | -1.03787 |
| P | -1.26032 | -0.32183 | -1.73818 |
| C | 2.57399 | 0.15329 | 0.45781 |
| C | 3.20263 | -0.94414 | -0.13848 |
| C | 3.34777 | 1.07367 | 1.16726 |
| C | 4.57748 | -1.09218 | -0.05541 |
| C | 4.72505 | 0.93113 | 1.23710 |
| C | 5.34081 | -0.15020 | 0.62350 |
| H | 5.05405 | -1.95239 | -0.51194 |
| H | 5.31814 | 1.66086 | 1.77647 |
| C | -2.20162 | -1.73058 | -1.15809 |
| C | -2.35347 | -2.81633 | -2.01514 |
| C | -2.72839 | -1.77196 | 0.13137 |
| C | -3.04103 | -3.93979 | -1.58059 |
| C | -3.41189 | -2.89647 | 0.55687 |
| C | -3.56870 | -3.97973 | -0.29973 |
| H | -3.15925 | -4.78664 | -2.24622 |
| H | -3.82524 | -2.92979 | 1.55812 |
| O | -1.04373 | -0.36364 | -3.23593 |
| Pb | 1.35411 | -0.61546 | -3.16056 |
| Cl | 1.32205 | -3.12247 | -3.04755 |
| Cl | -2.41591 | 1.28092 | -1.24343 |
| H | -1.92894 | -2.77856 | -3.01051 |
| H | -4.10477 | -4.85984 | 0.03705 |
| H | -2.60905 | -0.92489 | 0.79792 |
| H | 2.60623 | -1.70529 | -0.63328 |
| H | 2.86526 | 1.91361 | 1.65804 |
| H | 6.41657 | -0.26873 | 0.68660 |

R = Mes

| | | | |
|---|----------|----------|----------|
| P | 0.79515 | 0.20083 | 1.11754 |
| C | 0.38237 | -0.45803 | -0.34086 |
| P | -1.08012 | -0.40723 | -1.28726 |
| C | 2.64565 | 0.13049 | 0.99246 |
| C | 3.35019 | -1.08751 | 1.16665 |
| C | 3.33831 | 1.28674 | 0.55543 |
| C | 4.64852 | -1.16318 | 0.67451 |
| C | 4.64601 | 1.12932 | 0.09281 |
| C | 5.30324 | -0.08999 | 0.08545 |
| H | 5.18016 | -2.09981 | 0.76543 |
| H | 5.17061 | 1.99646 | -0.27515 |
| C | 2.76254 | 2.72066 | 0.61839 |
| C | 2.80102 | -2.30812 | 1.93484 |
| C | 6.70913 | -0.27136 | -0.47968 |
| C | 1.96687 | -3.23106 | 1.03967 |
| H | 1.07002 | -2.74476 | 0.66029 |
| H | 2.54227 | -3.56772 | 0.17503 |
| H | 1.66344 | -4.11506 | 1.60884 |
| C | 1.97692 | -1.85882 | 3.14377 |
| H | 2.56163 | -1.21322 | 3.80397 |
| H | 1.06607 | -1.31622 | 2.87105 |
| H | 1.65291 | -2.73333 | 3.71420 |
| C | 3.94878 | -3.15387 | 2.50492 |
| H | 4.49846 | -3.69074 | 1.72938 |
| H | 4.65577 | -2.55081 | 3.08012 |
| H | 3.52847 | -3.90982 | 3.17216 |

| | | | |
|----|----------|----------|----------|
| C | 1.70961 | 2.98764 | -0.46482 |
| H | 0.80231 | 2.39828 | -0.33506 |
| H | 1.41844 | 4.04153 | -0.43942 |
| H | 2.11248 | 2.78012 | -1.46031 |
| C | 2.16514 | 2.98575 | 2.00647 |
| H | 1.31076 | 2.34471 | 2.23260 |
| H | 2.91587 | 2.83426 | 2.78589 |
| H | 1.81537 | 4.02004 | 2.06526 |
| C | 3.85803 | 3.77536 | 0.42255 |
| H | 4.68059 | 3.65014 | 1.13049 |
| H | 4.26644 | 3.77284 | -0.59071 |
| H | 3.42269 | 4.76314 | 0.58922 |
| C | 7.25868 | 1.01353 | -1.09369 |
| H | 7.35822 | 1.81100 | -0.35291 |
| H | 8.25247 | 0.82361 | -1.50611 |
| H | 6.62725 | 1.37710 | -1.90844 |
| C | 6.67682 | -1.34861 | -1.57028 |
| H | 6.31841 | -2.30554 | -1.18624 |
| H | 6.02154 | -1.05358 | -2.39380 |
| H | 7.68020 | -1.50520 | -1.97584 |
| C | 7.65952 | -0.71280 | 0.63980 |
| H | 7.34810 | -1.65881 | 1.08705 |
| H | 8.67018 | -0.84772 | 0.24444 |
| H | 7.70194 | 0.03646 | 1.43420 |
| C | -2.18635 | -1.83366 | -1.13051 |
| C | -2.51217 | -2.65507 | -2.24327 |
| C | -2.72462 | -2.12904 | 0.14037 |
| C | -3.34489 | -3.74416 | -2.02488 |
| C | -3.55495 | -3.23402 | 0.27978 |
| C | -3.87678 | -4.05783 | -0.78266 |
| H | -3.58896 | -4.37616 | -2.86907 |
| H | -3.96824 | -3.45843 | 1.25758 |
| C | -2.07022 | -2.39512 | -3.67249 |
| C | -3.03040 | -1.40946 | -4.34074 |
| C | -1.92721 | -3.65629 | -4.51706 |
| H | -1.08946 | -1.93099 | -3.64487 |
| H | -3.07750 | -0.46336 | -3.79901 |
| H | -2.70095 | -1.19436 | -5.36061 |
| H | -4.04094 | -1.82638 | -4.39109 |
| H | -1.30344 | -4.40243 | -4.02083 |
| H | -2.88907 | -4.11239 | -4.76802 |
| H | -1.44427 | -3.39638 | -5.46185 |
| C | -2.48512 | -1.30730 | 1.39207 |
| C | -1.87346 | -2.14745 | 2.51094 |
| C | -3.77284 | -0.63287 | 1.86274 |
| H | -1.77456 | -0.50993 | 1.17272 |
| H | -0.96544 | -2.65377 | 2.17920 |
| H | -1.62020 | -1.51082 | 3.36248 |
| H | -2.57041 | -2.91046 | 2.86574 |
| H | -4.20195 | -0.00569 | 1.07993 |
| H | -4.52261 | -1.37370 | 2.15189 |
| H | -3.57116 | -0.00310 | 2.73306 |
| C | -4.77558 | -5.25529 | -0.59174 |
| C | -4.03842 | -6.55955 | -0.88759 |
| C | -6.04974 | -5.14431 | -1.42549 |
| H | -5.06784 | -5.26857 | 0.46442 |
| H | -3.14126 | -6.65733 | -0.27277 |
| H | -4.68516 | -7.41818 | -0.68935 |
| H | -3.73082 | -6.60895 | -1.93538 |
| H | -6.59412 | -4.22488 | -1.19973 |
| H | -5.82282 | -5.14442 | -2.49478 |
| H | -6.71146 | -5.99132 | -1.22696 |
| O | -0.56297 | -0.13075 | -2.68445 |
| Pb | 1.78436 | -0.55147 | -2.25974 |
| Cl | 1.60875 | -3.02126 | -2.72483 |
| Cl | -2.25786 | 1.21548 | -0.81818 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.82808 | 1.22193 | 1.54125 |
| C | 0.19234 | 0.55664 | 0.16708 |
| P | -1.40756 | 0.24983 | -0.45924 |
| Cl | 1.79779 | -2.78639 | -0.37800 |
| O | -1.21159 | -0.93874 | -1.37678 |
| C | -3.05222 | 0.09550 | 0.33062 |
| C | -3.59236 | -1.22399 | 0.36051 |
| C | -3.94102 | 1.19363 | 0.45452 |
| C | -4.94962 | -1.36544 | 0.11439 |
| C | -5.29398 | 0.96284 | 0.21927 |
| C | -5.81252 | -0.29079 | -0.05427 |
| H | -5.35232 | -2.36858 | 0.06071 |
| H | -5.96455 | 1.80972 | 0.25777 |
| C | 2.62788 | 0.96562 | 1.20110 |
| C | 3.31933 | -0.05202 | 1.89776 |
| C | 3.25289 | 1.61114 | 0.10740 |
| C | 4.47634 | -0.56870 | 1.31969 |
| C | 4.38813 | 1.01419 | -0.43540 |
| C | 4.98639 | -0.11176 | 0.11429 |
| H | 4.97947 | -1.38339 | 1.81484 |
| H | 4.83946 | 1.46483 | -1.31103 |
| C | 2.87836 | -0.58378 | 3.27508 |
| C | 2.86757 | 2.99745 | -0.45637 |
| C | 6.17979 | -0.76153 | -0.57923 |
| C | -3.60931 | 2.59796 | 0.99985 |
| C | -2.84616 | -2.50560 | 0.78603 |
| C | -7.26987 | -0.52605 | -0.43178 |
| C | 4.14773 | 3.84952 | -0.53867 |
| H | 3.88750 | 4.86386 | -0.85198 |
| H | 4.64213 | 3.90927 | 0.43378 |
| H | 4.86880 | 3.46352 | -1.25946 |
| C | 1.91091 | 3.78604 | 0.43717 |
| H | 0.89310 | 3.39176 | 0.42605 |
| H | 2.26106 | 3.82185 | 1.47198 |
| H | 1.84624 | 4.81510 | 0.07278 |
| C | 2.26428 | 2.89523 | -1.85961 |
| H | 2.91869 | 2.33990 | -2.53646 |
| H | 1.28745 | 2.40756 | -1.83571 |
| H | 2.12094 | 3.89410 | -2.28219 |
| C | 7.32986 | 0.24581 | -0.69071 |
| H | 8.18619 | -0.21424 | -1.19188 |
| H | 7.04371 | 1.12887 | -1.26593 |
| H | 7.65372 | 0.58000 | 0.29812 |
| C | 6.68735 | -1.98936 | 0.17234 |
| H | 7.51999 | -2.43402 | -0.37819 |
| H | 7.05298 | -1.73448 | 1.17040 |
| H | 5.90998 | -2.75059 | 0.27194 |
| C | 5.75293 | -1.20560 | -1.98379 |
| H | 4.93886 | -1.93282 | -1.92946 |
| H | 5.41558 | -0.36088 | -2.58900 |
| H | 6.59390 | -1.67268 | -2.50413 |
| C | 3.94447 | -1.48840 | 3.89958 |
| H | 4.91424 | -0.99054 | 3.97608 |
| H | 3.62742 | -1.75393 | 4.91069 |
| H | 4.07179 | -2.42065 | 3.34467 |
| C | 2.68512 | 0.59695 | 4.23628 |
| H | 3.60838 | 1.17374 | 4.33385 |
| H | 1.89501 | 1.27560 | 3.90923 |
| H | 2.40869 | 0.22611 | 5.22735 |
| C | 1.59181 | -1.41184 | 3.19845 |
| H | 0.71960 | -0.80366 | 2.94815 |
| H | 1.67160 | -2.19847 | 2.44623 |
| H | 1.39346 | -1.87037 | 4.17198 |
| C | -2.15796 | 2.79155 | 1.41453 |

| | | | |
|----|----------|----------|----------|
| H | -1.82312 | 1.99387 | 2.08107 |
| H | -1.47824 | 2.85349 | 0.56767 |
| H | -2.06471 | 3.73127 | 1.96499 |
| C | -4.43064 | 2.74697 | 2.29750 |
| H | -4.20569 | 3.71332 | 2.75716 |
| H | -5.50537 | 2.70260 | 2.11933 |
| H | -4.17444 | 1.96208 | 3.01322 |
| C | -4.01807 | 3.71860 | 0.03949 |
| H | -5.07979 | 3.67521 | -0.21051 |
| H | -3.83064 | 4.68792 | 0.50981 |
| H | -3.44984 | 3.67638 | -0.88923 |
| C | -1.49612 | -2.23312 | 1.44435 |
| H | -1.13525 | -3.15187 | 1.91276 |
| H | -0.71982 | -1.93625 | 0.74453 |
| H | -1.58635 | -1.47631 | 2.22834 |
| C | -2.68550 | -3.49245 | -0.37307 |
| H | -2.06827 | -3.06971 | -1.16309 |
| H | -2.21110 | -4.40928 | -0.01256 |
| H | -3.65680 | -3.76205 | -0.79619 |
| C | -3.69593 | -3.18129 | 1.88219 |
| H | -3.87891 | -2.50073 | 2.71759 |
| H | -4.65962 | -3.53909 | 1.51908 |
| H | -3.15085 | -4.04813 | 2.26397 |
| C | -8.04429 | 0.77938 | -0.59247 |
| H | -8.10538 | 1.33678 | 0.34576 |
| H | -7.59404 | 1.42636 | -1.34946 |
| H | -9.06684 | 0.55978 | -0.90865 |
| C | -7.95622 | -1.36463 | 0.65301 |
| H | -7.47813 | -2.33822 | 0.77689 |
| H | -7.93049 | -0.85270 | 1.61812 |
| H | -9.00272 | -1.53833 | 0.38726 |
| C | -7.31855 | -1.28229 | -1.76488 |
| H | -6.84561 | -0.70207 | -2.56077 |
| H | -6.80539 | -2.24391 | -1.70310 |
| H | -8.35652 | -1.47311 | -2.05129 |
| Pb | 1.20371 | -0.68090 | -1.63090 |
| Cl | -1.69114 | 1.82846 | -1.77198 |

R-P=C(Pb (II)Cl)-P(O)MeR**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.57719 | 0.06487 | 1.08137 |
| C | 0.43195 | -0.24338 | -0.53713 |
| P | -1.05550 | -0.22315 | -1.46700 |
| O | -0.61193 | 0.07413 | -2.89411 |
| Pb | 1.70355 | -0.42060 | -2.56975 |
| Cl | 1.33322 | -2.88970 | -2.69871 |
| H | 2.00296 | -0.01551 | 1.21088 |
| H | -1.65547 | -1.49544 | -1.35495 |
| C | -2.32447 | 0.91035 | -0.89512 |
| H | -3.19926 | 0.83896 | -1.54409 |
| H | -2.60628 | 0.65713 | 0.12965 |
| H | -1.93352 | 1.92828 | -0.92316 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.81455 | 0.15763 | 0.87749 |
| C | 0.51441 | -0.22188 | -0.69918 |
| P | -1.07241 | -0.25822 | -1.45304 |
| O | -0.77434 | -0.12391 | -2.94909 |
| Pb | 1.54519 | -0.52136 | -2.84917 |
| Cl | 1.32359 | -3.02703 | -2.76717 |
| C | -2.18107 | 1.04924 | -0.90422 |
| H | -3.13210 | 0.97269 | -1.43523 |
| H | -2.35320 | 0.96908 | 0.17108 |
| H | -1.72429 | 2.01489 | -1.12341 |

| | | | |
|---|----------|----------|----------|
| C | -1.89022 | -1.81496 | -1.08704 |
| H | -2.10950 | -1.89008 | -0.02041 |
| H | -2.81544 | -1.88357 | -1.66339 |
| H | -1.21847 | -2.62331 | -1.38288 |
| C | 2.64358 | 0.06240 | 1.06766 |
| H | 3.15189 | -0.17844 | 0.13359 |
| H | 3.01592 | 1.01319 | 1.45940 |
| H | 2.87809 | -0.70388 | 1.81243 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.71160 | 0.32899 | 0.23787 |
| C | 0.59668 | -0.62937 | -1.10041 |
| P | -0.88212 | -0.89788 | -2.02446 |
| O | -0.42580 | -1.72801 | -3.23005 |
| C | 2.48595 | 0.29745 | 0.85597 |
| C | 2.91407 | 1.76100 | 0.97888 |
| H | 2.99021 | 2.24215 | 0.00002 |
| H | 2.20794 | 2.33792 | 1.58270 |
| H | 3.89499 | 1.82355 | 1.46190 |
| C | 3.45871 | -0.46979 | -0.01782 |
| H | 3.17990 | -1.52436 | -0.09785 |
| H | 3.52490 | -0.03327 | -1.01948 |
| H | 4.46415 | -0.43157 | 0.41587 |
| C | 2.41789 | -0.33367 | 2.24943 |
| H | 2.13575 | -1.38803 | 2.19722 |
| H | 3.39843 | -0.26936 | 2.73342 |
| H | 1.69667 | 0.18065 | 2.89103 |
| C | -2.20508 | -1.78521 | -1.10162 |
| C | -2.78357 | -0.89967 | -0.00160 |
| H | -3.30319 | -0.02700 | -0.40383 |
| H | -3.51143 | -1.47876 | 0.57455 |
| H | -2.01321 | -0.55307 | 0.69211 |
| C | -3.29153 | -2.16933 | -2.10873 |
| H | -2.88146 | -2.76311 | -2.92731 |
| H | -4.05167 | -2.76831 | -1.59832 |
| H | -3.79302 | -1.29511 | -2.53107 |
| C | -1.60072 | -3.05134 | -0.49564 |
| H | -1.14888 | -3.69131 | -1.25479 |
| H | -0.83103 | -2.82122 | 0.24257 |
| H | -2.39404 | -3.61722 | 0.00221 |
| Pb | 1.87280 | -1.88272 | -2.71449 |
| Cl | 1.84279 | -4.04461 | -1.42485 |
| C | -1.56846 | 0.67540 | -2.58495 |
| H | -2.44364 | 0.50911 | -3.21493 |
| H | -1.83226 | 1.30715 | -1.73588 |
| H | -0.80101 | 1.17936 | -3.17423 |

R = Ph

| | | | |
|---|----------|----------|----------|
| P | 0.79562 | 0.36193 | 0.48366 |
| C | 0.34127 | -0.22534 | -0.99194 |
| P | -1.27111 | -0.27412 | -1.67372 |
| C | 2.59851 | 0.11740 | 0.52708 |
| C | 3.24014 | -0.95036 | -0.10638 |
| C | 3.36121 | 1.02405 | 1.26457 |
| C | 4.61737 | -1.08212 | -0.03151 |
| C | 4.74063 | 0.89838 | 1.32699 |
| C | 5.36991 | -0.15333 | 0.67661 |
| H | 5.10423 | -1.91980 | -0.51821 |
| H | 5.32502 | 1.61809 | 1.88907 |
| C | -2.16006 | -1.73103 | -1.09925 |
| C | -2.50150 | -2.71500 | -2.02082 |
| C | -2.50119 | -1.88585 | 0.24293 |
| C | -3.19252 | -3.84257 | -1.60171 |
| C | -3.19243 | -3.01163 | 0.65593 |
| C | -3.53984 | -3.98948 | -0.26788 |

| | | | |
|----|----------|----------|----------|
| H | -3.45260 | -4.61134 | -2.32001 |
| H | -3.45487 | -3.13186 | 1.70069 |
| O | -1.04402 | -0.33395 | -3.18361 |
| Pb | 1.32285 | -0.62291 | -3.13483 |
| Cl | 1.29171 | -3.13184 | -2.97939 |
| H | -2.21357 | -2.59367 | -3.05808 |
| H | -4.07680 | -4.87319 | 0.05792 |
| H | -2.21228 | -1.13608 | 0.97299 |
| H | 2.65239 | -1.70107 | -0.62691 |
| H | 2.86864 | 1.84054 | 1.78427 |
| H | 6.44740 | -0.25900 | 0.73334 |
| C | -2.28952 | 1.14378 | -1.23148 |
| H | -3.25653 | 1.06401 | -1.73122 |
| H | -2.43967 | 1.18226 | -0.15093 |
| H | -1.78308 | 2.05385 | -1.55612 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.89816 | 0.15221 | 1.03172 |
| C | 0.32391 | -0.26795 | -0.45866 |
| P | -1.25573 | -0.19972 | -1.23136 |
| C | 2.71612 | 0.05992 | 0.78737 |
| C | 3.37570 | -1.17917 | 0.72813 |
| C | 3.45358 | 1.25208 | 0.72733 |
| C | 4.75751 | -1.19308 | 0.57274 |
| C | 4.83280 | 1.18878 | 0.56916 |
| C | 5.50363 | -0.02442 | 0.48175 |
| H | 5.26702 | -2.15164 | 0.53222 |
| H | 5.39884 | 2.11484 | 0.52023 |
| C | -2.19996 | -1.74173 | -1.06016 |
| C | -2.68591 | -2.42826 | -2.19641 |
| C | -2.48944 | -2.24003 | 0.22533 |
| C | -3.43506 | -3.58271 | -2.00198 |
| C | -3.24740 | -3.39791 | 0.35433 |
| C | -3.72523 | -4.09107 | -0.74467 |
| H | -3.80901 | -4.10235 | -2.87885 |
| H | -3.46710 | -3.76477 | 1.35264 |
| O | -0.87795 | 0.12346 | -2.67849 |
| Pb | 1.46811 | -0.24999 | -2.53495 |
| Cl | 1.33453 | -2.74237 | -2.90906 |
| C | -2.32667 | 1.13719 | -0.65384 |
| H | -3.17842 | 1.19874 | -1.33454 |
| H | -2.69120 | 0.98467 | 0.36083 |
| H | -1.76180 | 2.06955 | -0.70314 |
| C | 2.77724 | 2.58978 | 0.81267 |
| H | 2.20719 | 2.81065 | -0.09517 |
| H | 2.07016 | 2.63228 | 1.64685 |
| H | 3.50821 | 3.38813 | 0.94852 |
| C | 2.63498 | -2.47927 | 0.84307 |
| H | 1.91311 | -2.45685 | 1.66482 |
| H | 2.07557 | -2.70891 | -0.06825 |
| H | 3.32960 | -3.30038 | 1.02566 |
| C | 6.98799 | -0.07368 | 0.28390 |
| H | 7.23581 | -0.16442 | -0.77843 |
| H | 7.47020 | 0.83175 | 0.65649 |
| H | 7.42913 | -0.93230 | 0.79378 |
| C | -1.99522 | -1.62332 | 1.50133 |
| H | -1.00207 | -2.00570 | 1.75287 |
| H | -1.90824 | -0.53874 | 1.47313 |
| H | -2.66467 | -1.87954 | 2.32406 |
| C | -2.44993 | -2.01438 | -3.62102 |
| H | -2.71160 | -0.97390 | -3.80766 |
| H | -1.39769 | -2.12733 | -3.88799 |
| H | -3.04095 | -2.64883 | -4.28281 |
| C | -4.51137 | -5.35525 | -0.58684 |
| H | -3.86658 | -6.22872 | -0.72491 |
| H | -4.95624 | -5.42764 | 0.40688 |

H -5.31004 -5.42214 -1.32837

R = Mes*

P 0.82879 1.48234 1.26754
C 0.15935 0.63147 0.01926
P -1.45955 0.32219 -0.61474
Cl 1.67199 -2.84891 -0.07728
O -1.25105 -0.98729 -1.38820
C -3.08183 0.19408 0.25944
C -3.63270 -1.11172 0.40286
C -3.97380 1.29703 0.30215
C -4.99368 -1.26983 0.18050
C -5.33101 1.05765 0.09719
C -5.85718 -0.21192 -0.06789
H -5.39764 -2.27353 0.21254
H -5.99904 1.90761 0.07744
C 2.62795 1.12244 1.00267
C 3.26592 0.17884 1.83984
C 3.32212 1.63929 -0.12069
C 4.43929 -0.41617 1.38043
C 4.48278 0.98548 -0.52307
C 5.02677 -0.08803 0.17016
H 4.89841 -1.18254 1.98356
H 4.99852 1.34015 -1.40540
C 2.76682 -0.17687 3.25533
C 2.95125 2.94504 -0.86230
C 6.24919 -0.81535 -0.38155
C -3.63076 2.73747 0.73828
C -2.88525 -2.35548 0.92280
C -7.31982 -0.47282 -0.40753
C 4.22596 3.65241 -1.35072
H 3.96097 4.64546 -1.72192
H 4.95295 3.77304 -0.54449
H 4.71176 3.12726 -2.17477
C 2.25397 3.94538 0.06207
H 1.26039 3.61718 0.38156
H 2.84694 4.13623 0.95950
H 2.11380 4.89371 -0.46414
C 2.07235 2.69297 -2.09112
H 2.54913 1.98494 -2.77486
H 1.09740 2.29986 -1.80384
H 1.91471 3.62785 -2.63776
C 7.41974 0.16446 -0.52156
H 8.29744 -0.35138 -0.92134
H 7.18233 0.98876 -1.19737
H 7.68865 0.59212 0.44756
C 6.69149 -1.96709 0.51736
H 7.54797 -2.47318 0.06510
H 7.00110 -1.61758 1.50566
H 5.89733 -2.70654 0.64503
C 5.90128 -1.39316 -1.75898
H 5.07536 -2.10489 -1.68350
H 5.61111 -0.61009 -2.46320
H 6.76531 -1.91617 -2.17879
C 3.78167 -1.03746 4.01368
H 4.76534 -0.56471 4.06871
H 3.42372 -1.17689 5.03635
H 3.89345 -2.03001 3.57128
C 2.59566 1.11514 4.06641
H 3.53812 1.66591 4.12339
H 1.84143 1.77820 3.63824
H 2.28003 0.87316 5.08533
C 1.45283 -0.96379 3.24384
H 0.60810 -0.36069 2.90585
H 1.51835 -1.83496 2.58984
H 1.22111 -1.30011 4.25908

C -2.17991 2.94255 1.15139
H -1.86963 2.20070 1.88964
H -1.47194 2.91051 0.32627
H -2.07210 3.92666 1.61449
C -4.45159 3.00013 2.01823
H -4.21318 3.99519 2.40423
H -5.52641 2.95788 1.84080
H -4.20824 2.26773 2.79136
C -4.03293 3.78733 -0.30241
H -5.09968 3.74289 -0.52980
H -3.82057 4.78836 0.08309
H -3.49278 3.66942 -1.24237
C -1.54802 -2.01268 1.57050
H -1.14484 -2.90247 2.05946
H -0.78958 -1.69615 0.86101
H -1.67138 -1.23841 2.33244
C -2.70707 -3.42238 -0.16058
H -2.08859 -3.05239 -0.97502
H -2.22839 -4.30669 0.26901
H -3.67461 -3.72916 -0.56760
C -3.73529 -2.96400 2.05709
H -3.95165 -2.22485 2.83259
H -4.68185 -3.37936 1.70950
H -3.17278 -3.78132 2.51530
C -8.09528 0.81794 -0.65736
H -8.14123 1.44660 0.23562
H -7.65596 1.40353 -1.46896
H -9.12290 0.57736 -0.94023
C -7.99340 -1.22418 0.74688
H -7.51366 -2.18558 0.93989
H -7.95518 -0.63919 1.66909
H -9.04327 -1.41681 0.50860
C -7.38813 -1.32911 -1.67759
H -6.92846 -0.81149 -2.52310
H -6.87196 -2.28253 -1.54971
H -8.42986 -1.54219 -1.93329
Pb 1.13139 -0.88917 -1.57129
C -1.76499 1.55736 -1.91062
H -2.71105 1.30804 -2.39403
H -1.78183 2.58960 -1.57571
H -0.96158 1.43475 -2.64012

R-P=C(Pb (II)Cl)-P(S)ClR

R= H

P 0.74871 0.04774 0.96749
C 0.51241 -0.19479 -0.65348
P -1.01470 -0.17429 -1.46940
Cl 1.34246 -2.39598 -3.30894
S -0.77704 0.89634 -3.12061
Pb 1.83625 -0.02934 -2.65369
Cl -2.61637 0.40895 -0.36347
H -1.37814 -1.50343 -1.74085
H 2.18077 -0.01977 0.97674

R = Me

P 0.85708 0.09546 0.86656
C 0.40926 -0.14225 -0.70699
P -1.21792 -0.05270 -1.29730
Cl 1.06477 -2.44622 -3.42202
S -1.12784 0.85769 -3.06996
Pb 1.48879 -0.02731 -2.85354
Cl -2.51752 0.91357 -0.04756
C -1.93483 -1.69563 -1.40454
H -2.00721 -2.12524 -0.40437
H -2.92301 -1.62015 -1.85971

| | | | |
|---|----------|----------|----------|
| H | -1.27399 | -2.29825 | -2.03309 |
| C | 2.68576 | -0.10864 | 0.86956 |
| H | 2.95232 | -0.81893 | 1.65732 |
| H | 3.08700 | -0.46168 | -0.08088 |
| H | 3.14858 | 0.84675 | 1.13478 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.79418 | -0.23939 | 0.99108 |
| C | 0.55038 | -0.37410 | -0.64262 |
| P | -1.04871 | -0.28939 | -1.33460 |
| Cl | 2.12840 | -2.46651 | -3.29289 |
| S | -0.84605 | 0.33942 | -3.22114 |
| Pb | 1.83257 | -0.04787 | -2.66087 |
| C | 2.63854 | -0.43504 | 1.29686 |
| C | 2.79055 | -0.50598 | 2.81750 |
| H | 2.25692 | -1.36385 | 3.23533 |
| H | 3.84744 | -0.60844 | 3.08255 |
| H | 2.40674 | 0.39448 | 3.30471 |
| C | 3.17796 | -1.71261 | 0.66518 |
| H | 2.67116 | -2.59746 | 1.05903 |
| H | 3.05926 | -1.73175 | -0.41980 |
| H | 4.24527 | -1.81458 | 0.89071 |
| C | 3.37613 | 0.79575 | 0.77570 |
| H | 3.33262 | 0.87246 | -0.31340 |
| H | 2.96921 | 1.72203 | 1.19073 |
| H | 4.43294 | 0.74052 | 1.05887 |
| C | -1.99417 | -1.88315 | -1.21767 |
| C | -2.22666 | -2.24282 | 0.24611 |
| H | -2.74477 | -3.20533 | 0.28362 |
| H | -1.28828 | -2.34941 | 0.79399 |
| H | -2.84537 | -1.50507 | 0.75834 |
| C | -1.15651 | -2.96280 | -1.90098 |
| H | -0.96189 | -2.72922 | -2.94831 |
| H | -0.19431 | -3.11290 | -1.40973 |
| H | -1.71316 | -3.90361 | -1.85870 |
| C | -3.32365 | -1.70931 | -1.94821 |
| H | -3.85348 | -2.66585 | -1.92902 |
| H | -3.95847 | -0.96115 | -1.47082 |
| H | -3.17399 | -1.42780 | -2.99212 |
| Cl | -2.25111 | 1.02764 | -0.31575 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78402 | 0.16093 | 0.70147 |
| C | 0.21854 | 0.05726 | -0.85205 |
| P | -1.45817 | 0.20272 | -1.29328 |
| C | 2.58883 | -0.01337 | 0.53080 |
| C | 3.24827 | -0.88530 | 1.39721 |
| C | 3.34223 | 0.73113 | -0.37871 |
| C | 4.62189 | -1.05362 | 1.31591 |
| C | 4.71789 | 0.57616 | -0.44687 |
| C | 5.35798 | -0.32527 | 0.39260 |
| H | 5.12017 | -1.75072 | 1.97987 |
| H | 5.29386 | 1.16578 | -1.15122 |
| C | -2.31243 | -1.37778 | -1.15393 |
| C | -2.84874 | -1.98644 | -2.28101 |
| C | -2.40940 | -1.99284 | 0.09329 |
| C | -3.49226 | -3.20900 | -2.15820 |
| C | -3.05205 | -3.21162 | 0.20726 |
| C | -3.59439 | -3.81941 | -0.91892 |
| H | -3.90642 | -3.68682 | -3.03804 |
| H | -3.12899 | -3.69136 | 1.17595 |
| Cl | 0.61905 | -2.41693 | -3.47393 |
| S | -1.50499 | 0.96637 | -3.12798 |
| Pb | 1.13363 | 0.00447 | -3.07471 |
| Cl | -2.50116 | 1.38942 | 0.00996 |

| | | | |
|---|----------|----------|----------|
| H | 2.85190 | 1.46457 | -1.01051 |
| H | 6.43330 | -0.44910 | 0.33643 |
| H | 2.67941 | -1.44782 | 2.13107 |
| H | -4.09452 | -4.77683 | -0.82682 |
| H | -2.75075 | -1.50798 | -3.24757 |
| H | -1.98519 | -1.51969 | 0.97220 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.89425 | -0.84034 | 0.25596 |
| C | 0.34399 | -0.24001 | -1.18742 |
| P | -1.33442 | -0.14580 | -1.68059 |
| C | 2.68921 | -0.48949 | 0.17647 |
| C | 3.58419 | -1.53631 | -0.08576 |
| C | 3.17111 | 0.79516 | 0.47456 |
| C | 4.94824 | -1.27173 | -0.08052 |
| C | 4.54361 | 1.01247 | 0.46899 |
| C | 5.44854 | -0.00403 | 0.18579 |
| H | 5.63894 | -2.08356 | -0.28977 |
| H | 4.91728 | 2.00450 | 0.70684 |
| C | -2.46420 | -1.43862 | -1.07568 |
| C | -2.05574 | -2.75577 | -1.40517 |
| C | -3.65173 | -1.24372 | -0.33507 |
| C | -2.78349 | -3.82800 | -0.90562 |
| C | -4.33432 | -2.36495 | 0.12415 |
| C | -3.91273 | -3.66144 | -0.12206 |
| H | -2.45325 | -4.83088 | -1.15718 |
| H | -5.24421 | -2.20828 | 0.69482 |
| Cl | 2.21253 | -1.68861 | -3.91736 |
| S | -1.33557 | 0.04714 | -3.65942 |
| Pb | 1.39308 | 0.57502 | -3.16811 |
| C | 2.24485 | 1.92475 | 0.82280 |
| H | 1.63890 | 2.23731 | -0.03183 |
| H | 1.54049 | 1.63870 | 1.61016 |
| H | 2.80767 | 2.79087 | 1.17350 |
| C | 3.09103 | -2.91502 | -0.40292 |
| H | 2.26114 | -3.20765 | 0.24914 |
| H | 2.73082 | -2.96343 | -1.43529 |
| H | 3.88682 | -3.65244 | -0.28778 |
| C | 6.92236 | 0.26348 | 0.15515 |
| H | 7.49226 | -0.61057 | 0.47593 |
| H | 7.25051 | 0.51132 | -0.85928 |
| H | 7.18912 | 1.10296 | 0.79969 |
| C | -4.29499 | 0.07703 | -0.01792 |
| H | -3.74189 | 0.63696 | 0.73733 |
| H | -4.38689 | 0.71608 | -0.89549 |
| H | -5.29749 | -0.10282 | 0.37092 |
| C | -0.92453 | -3.09295 | -2.33143 |
| H | -1.22134 | -2.92523 | -3.36971 |
| H | -0.02166 | -2.50587 | -2.17380 |
| H | -0.65887 | -4.14491 | -2.22213 |
| C | -4.65132 | -4.83650 | 0.43647 |
| H | -5.71065 | -4.61329 | 0.57406 |
| H | -4.56249 | -5.70869 | -0.21341 |
| H | -4.24517 | -5.11429 | 1.41421 |
| Cl | -1.85083 | 1.66595 | -0.86403 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.74522 | 0.93626 | 1.54586 |
| C | 0.16324 | 0.40292 | 0.08533 |
| P | -1.47077 | 0.22155 | -0.50518 |
| Cl | 1.93334 | -2.81819 | -0.60362 |
| C | -3.09872 | 0.08853 | 0.35677 |
| C | -3.66458 | -1.21958 | 0.42708 |
| C | -3.97027 | 1.20243 | 0.47962 |
| C | -5.02286 | -1.34279 | 0.17796 |

| | | | |
|---|----------|----------|----------|
| C | -5.32352 | 0.99238 | 0.22565 |
| C | -5.86145 | -0.25630 | -0.03582 |
| H | -5.44687 | -2.33919 | 0.16849 |
| H | -5.97972 | 1.85129 | 0.24946 |
| C | 2.56555 | 0.80541 | 1.25494 |
| C | 3.28936 | -0.23331 | 1.88704 |
| C | 3.20392 | 1.59657 | 0.26805 |
| C | 4.49906 | -0.62485 | 1.31965 |
| C | 4.39965 | 1.12537 | -0.26667 |
| C | 5.03540 | -0.01933 | 0.19418 |
| H | 5.02808 | -1.45546 | 1.75784 |
| H | 4.86553 | 1.68936 | -1.06487 |
| C | 2.83560 | -0.90650 | 3.19659 |
| C | 2.75583 | 3.00822 | -0.17337 |
| C | 6.29293 | -0.53102 | -0.50122 |
| C | -3.62566 | 2.58412 | 1.07672 |
| C | -2.97194 | -2.48717 | 0.97350 |
| C | -7.31545 | -0.47127 | -0.43573 |
| C | 3.99154 | 3.92599 | -0.20857 |
| H | 3.67021 | 4.95322 | -0.39856 |
| H | 4.52630 | 3.90642 | 0.74384 |
| H | 4.69555 | 3.66044 | -0.99770 |
| C | 1.78942 | 3.66725 | 0.80980 |
| H | 0.79827 | 3.20823 | 0.80851 |
| H | 2.17850 | 3.64675 | 1.83078 |
| H | 1.64211 | 4.71310 | 0.52658 |
| C | 2.12869 | 3.00242 | -1.56969 |
| H | 2.79525 | 2.53686 | -2.30046 |
| H | 1.17546 | 2.47138 | -1.57626 |
| H | 1.93705 | 4.02764 | -1.90035 |
| C | 7.38432 | 0.54474 | -0.46646 |
| H | 8.28601 | 0.18224 | -0.96808 |
| H | 7.07012 | 1.46115 | -0.97037 |
| H | 7.64760 | 0.80116 | 0.56275 |
| C | 6.84280 | -1.79505 | 0.15443 |
| H | 7.72274 | -2.13664 | -0.39613 |
| H | 7.15089 | -1.61759 | 1.18807 |
| H | 6.10977 | -2.60514 | 0.14559 |
| C | 5.94780 | -0.86112 | -1.95875 |
| H | 5.17768 | -1.63496 | -2.00868 |
| H | 5.58178 | 0.01738 | -2.49519 |
| H | 6.83479 | -1.22718 | -2.48360 |
| C | 3.91881 | -1.82599 | 3.76705 |
| H | 4.86458 | -1.30194 | 3.92506 |
| H | 3.58215 | -2.20053 | 4.73647 |
| H | 4.10056 | -2.69386 | 3.12903 |
| C | 2.57443 | 0.17734 | 4.25173 |
| H | 3.47212 | 0.77643 | 4.42453 |
| H | 1.76731 | 0.85278 | 3.96141 |
| H | 2.28827 | -0.28880 | 5.19886 |
| C | 1.58318 | -1.76656 | 3.01334 |
| H | 0.69710 | -1.16393 | 2.80219 |
| H | 1.70362 | -2.47566 | 2.19283 |
| H | 1.37910 | -2.31872 | 3.93582 |
| C | -2.17906 | 2.74145 | 1.52560 |
| H | -1.86967 | 1.91576 | 2.16971 |
| H | -1.48075 | 2.82129 | 0.69633 |
| H | -2.08518 | 3.66037 | 2.11015 |
| C | -4.46423 | 2.68351 | 2.36966 |
| H | -4.23038 | 3.62320 | 2.87761 |
| H | -5.53655 | 2.66513 | 2.17350 |
| H | -4.23082 | 1.86144 | 3.05052 |
| C | -4.01544 | 3.75226 | 0.16723 |
| H | -5.07335 | 3.72503 | -0.10071 |
| H | -3.83431 | 4.69542 | 0.69010 |
| H | -3.43371 | 3.75847 | -0.75351 |

| | | | |
|----|----------|----------|----------|
| C | -1.53021 | -2.28470 | 1.42235 |
| H | -1.21527 | -3.15691 | 2.00054 |
| H | -0.82408 | -2.19131 | 0.59953 |
| H | -1.44165 | -1.41238 | 2.07451 |
| C | -3.04692 | -3.67806 | 0.01601 |
| H | -2.47203 | -3.49212 | -0.89024 |
| H | -2.63302 | -4.56329 | 0.50617 |
| H | -4.07533 | -3.90978 | -0.26941 |
| C | -3.75389 | -2.84621 | 2.25611 |
| H | -3.73320 | -2.02025 | 2.97160 |
| H | -4.79719 | -3.09244 | 2.05562 |
| H | -3.28727 | -3.71564 | 2.72680 |
| C | -8.06037 | 0.84549 | -0.63773 |
| H | -8.13106 | 1.42180 | 0.28835 |
| H | -7.58084 | 1.46897 | -1.39641 |
| H | -9.07989 | 0.63975 | -0.97237 |
| C | -8.03968 | -1.27480 | 0.65099 |
| H | -7.58602 | -2.25638 | 0.80127 |
| H | -8.02163 | -0.74574 | 1.60701 |
| H | -9.08433 | -1.43117 | 0.36800 |
| C | -7.35129 | -1.25349 | -1.75426 |
| H | -6.85124 | -0.69868 | -2.55164 |
| H | -6.85702 | -2.22257 | -1.66209 |
| H | -8.38661 | -1.43106 | -2.05818 |
| Pb | 1.33865 | -0.63325 | -1.74063 |
| S | -1.38011 | -1.22332 | -1.88202 |
| Cl | -1.72023 | 1.93682 | -1.64758 |

R-P=C(Pb (II)Cl)-P(S)MeR

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.79861 | 0.14024 | 0.92090 |
| C | 0.57712 | -0.11003 | -0.70244 |
| P | -0.96794 | 0.06825 | -1.51186 |
| Cl | 1.13412 | -2.53069 | -3.18031 |
| S | -0.54924 | 1.00005 | -3.23155 |
| Pb | 1.92382 | -0.19977 | -2.67023 |
| H | -1.44158 | -1.23828 | -1.74369 |
| H | 2.21951 | -0.03976 | 0.98483 |
| C | -2.29790 | 0.85387 | -0.58169 |
| H | -3.20337 | 0.86568 | -1.19090 |
| H | -2.48028 | 0.29559 | 0.33935 |
| H | -2.00818 | 1.87714 | -0.34111 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.83802 | 0.16745 | 0.73298 |
| C | 0.46929 | -0.09996 | -0.85651 |
| P | -1.16420 | 0.04982 | -1.48109 |
| Cl | 1.12237 | -2.66916 | -3.28127 |
| S | -0.94247 | 0.73910 | -3.35907 |
| Pb | 1.62251 | -0.21327 | -2.94781 |
| C | -1.93920 | -1.57735 | -1.46990 |
| H | -2.06955 | -1.91631 | -0.43988 |
| H | -2.90574 | -1.51949 | -1.97386 |
| H | -1.28505 | -2.26691 | -2.00735 |
| C | 2.65883 | -0.07042 | 0.85725 |
| H | 2.86192 | -0.81153 | 1.63543 |
| H | 3.11050 | -0.40168 | -0.07859 |
| H | 3.12239 | 0.86653 | 1.17936 |
| C | -2.25609 | 1.12380 | -0.52210 |
| H | -3.23905 | 1.15335 | -0.99608 |
| H | -2.34945 | 0.74444 | 0.49779 |
| H | -1.83552 | 2.12903 | -0.50019 |

R = t-Bu

| | | | |
|---|---------|----------|---------|
| P | 0.77519 | -0.32421 | 0.95824 |
|---|---------|----------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.54329 | -0.35273 | -0.68195 |
| P | -1.08895 | -0.24904 | -1.34722 |
| Cl | 2.15488 | -2.43787 | -3.27905 |
| S | -0.86274 | 0.31285 | -3.27332 |
| Pb | 1.81062 | -0.00590 | -2.69559 |
| C | -2.08973 | 0.98379 | -0.47499 |
| H | -3.08243 | 1.04922 | -0.92204 |
| H | -2.16700 | 0.73224 | 0.58378 |
| H | -1.58938 | 1.94645 | -0.58057 |
| C | 2.62489 | -0.44221 | 1.27854 |
| C | 2.77546 | -0.49504 | 2.79946 |
| H | 2.25929 | -1.36012 | 3.22429 |
| H | 3.83374 | -0.57158 | 3.06820 |
| H | 2.37104 | 0.40162 | 3.27727 |
| C | 3.19312 | -1.71447 | 0.65926 |
| H | 2.70552 | -2.60633 | 1.06205 |
| H | 3.07331 | -1.74449 | -0.42544 |
| H | 4.26236 | -1.79109 | 0.88647 |
| C | 3.33648 | 0.79686 | 0.74476 |
| H | 3.28800 | 0.86228 | -0.34459 |
| H | 2.91183 | 1.71819 | 1.15292 |
| H | 4.39539 | 0.76562 | 1.02430 |
| C | -2.00616 | -1.86205 | -1.22920 |
| C | -2.30854 | -2.17618 | 0.23387 |
| H | -2.77500 | -3.16415 | 0.28881 |
| H | -1.40283 | -2.20368 | 0.84392 |
| H | -3.00327 | -1.46007 | 0.67781 |
| C | -1.13636 | -2.96006 | -1.83402 |
| H | -0.88281 | -2.75168 | -2.87432 |
| H | -0.20136 | -3.09014 | -1.28743 |
| H | -1.68899 | -3.90371 | -1.79853 |
| C | -3.30638 | -1.73640 | -2.02221 |
| H | -3.82350 | -2.70004 | -1.99798 |
| H | -3.98328 | -0.99088 | -1.59825 |
| H | -3.11564 | -1.48120 | -3.06606 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78904 | -0.52126 | 0.40729 |
| C | 0.22750 | 0.09277 | -1.02558 |
| P | -1.49547 | 0.20393 | -1.37929 |
| C | 2.59729 | -0.36650 | 0.28535 |
| C | 3.37284 | -1.38676 | 0.83691 |
| C | 3.23909 | 0.73299 | -0.28851 |
| C | 4.75652 | -1.33540 | 0.76973 |
| C | 4.62216 | 0.79226 | -0.34056 |
| C | 5.38238 | -0.24713 | 0.17966 |
| H | 5.34799 | -2.14445 | 1.18287 |
| H | 5.11081 | 1.65397 | -0.78138 |
| C | -2.36875 | -1.34947 | -1.07576 |
| C | -1.97163 | -2.47181 | -1.80363 |
| C | -3.39932 | -1.45644 | -0.14622 |
| C | -2.60251 | -3.68552 | -1.59548 |
| C | -4.02990 | -2.67609 | 0.05413 |
| C | -3.63216 | -3.78938 | -0.66882 |
| H | -2.28881 | -4.55457 | -2.16200 |
| H | -4.83368 | -2.75319 | 0.77722 |
| Cl | 1.27534 | -1.91385 | -3.74520 |
| S | -1.61754 | 0.74869 | -3.31148 |
| Pb | 1.14305 | 0.54662 | -3.18277 |
| H | 2.64653 | 1.55976 | -0.66632 |
| H | 6.46452 | -0.20177 | 0.13532 |
| H | 2.88603 | -2.23512 | 1.30797 |
| H | -4.12571 | -4.74171 | -0.51117 |
| H | -1.16664 | -2.39445 | -2.52874 |
| H | -3.72134 | -0.59535 | 0.42654 |
| C | -2.26935 | 1.45261 | -0.32600 |

| | | | |
|---|----------|---------|----------|
| H | -1.73267 | 2.38781 | -0.48614 |
| H | -3.31358 | 1.58877 | -0.61176 |
| H | -2.19222 | 1.16790 | 0.72490 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.86270 | -0.67272 | 0.30732 |
| C | 0.31898 | -0.22374 | -1.19100 |
| P | -1.38536 | -0.10229 | -1.65174 |
| C | 2.67216 | -0.39787 | 0.20295 |
| C | 3.52273 | -1.48510 | -0.04291 |
| C | 3.20975 | 0.87038 | 0.46972 |
| C | 4.89663 | -1.27594 | -0.04970 |
| C | 4.58967 | 1.03322 | 0.45299 |
| C | 5.45063 | -0.02498 | 0.18767 |
| H | 5.55223 | -2.11987 | -0.24466 |
| H | 5.00431 | 2.01496 | 0.66448 |
| C | -2.45603 | -1.46090 | -1.06922 |
| C | -2.04595 | -2.76887 | -1.42345 |
| C | -3.63559 | -1.29278 | -0.31145 |
| C | -2.77285 | -3.85524 | -0.95373 |
| C | -4.32019 | -2.42243 | 0.12322 |
| C | -3.90259 | -3.71155 | -0.16566 |
| H | -2.44004 | -4.85103 | -1.22928 |
| H | -5.22418 | -2.28112 | 0.70742 |
| Cl | 2.14944 | -1.83145 | -3.92189 |
| S | -1.37577 | 0.07878 | -3.66218 |
| Pb | 1.35442 | 0.46426 | -3.22989 |
| C | -1.85554 | 1.51021 | -0.96759 |
| H | -1.07166 | 2.18771 | -1.31063 |
| H | -2.80817 | 1.85711 | -1.36125 |
| H | -1.85607 | 1.49758 | 0.12195 |
| C | 2.33142 | 2.04745 | 0.78214 |
| H | 1.77190 | 2.37909 | -0.09734 |
| H | 1.59081 | 1.80513 | 1.55071 |
| H | 2.92525 | 2.88984 | 1.13976 |
| C | 2.97509 | -2.85086 | -0.32515 |
| H | 2.13456 | -3.09420 | 0.33318 |
| H | 2.61319 | -2.91210 | -1.35629 |
| H | 3.74193 | -3.61535 | -0.19105 |
| C | 6.93416 | 0.18056 | 0.14391 |
| H | 7.46912 | -0.70534 | 0.49145 |
| H | 7.26813 | 0.38144 | -0.87897 |
| H | 7.23797 | 1.02869 | 0.76015 |
| C | -4.26380 | 0.02431 | 0.04969 |
| H | -3.66005 | 0.60416 | 0.74881 |
| H | -4.45245 | 0.64375 | -0.82796 |
| H | -5.22564 | -0.15534 | 0.52962 |
| C | -0.89350 | -3.06757 | -2.33155 |
| H | -1.12793 | -2.78932 | -3.36146 |
| H | 0.01614 | -2.52763 | -2.07216 |
| H | -0.66531 | -4.13353 | -2.31030 |
| C | -4.64122 | -4.90283 | 0.35815 |
| H | -5.69342 | -4.67410 | 0.53561 |
| H | -4.58217 | -5.74388 | -0.33493 |
| H | -4.21190 | -5.23309 | 1.30933 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.76078 | 1.19455 | 1.35349 |
| C | 0.16098 | 0.47638 | -0.01505 |
| P | -1.48978 | 0.29984 | -0.61429 |
| Cl | 1.83905 | -2.89642 | -0.26129 |
| C | -3.10703 | 0.22796 | 0.29657 |
| C | -3.68662 | -1.05472 | 0.51610 |
| C | -3.97532 | 1.35187 | 0.29244 |
| C | -5.04883 | -1.19597 | 0.29114 |

| | | | |
|---|----------|----------|----------|
| C | -5.33232 | 1.12969 | 0.06871 |
| C | -5.88257 | -0.13664 | -0.04072 |
| H | -5.47765 | -2.18508 | 0.39487 |
| H | -5.98209 | 1.99118 | -0.00301 |
| C | 2.58571 | 1.00069 | 1.10483 |
| C | 3.28400 | 0.03690 | 1.86984 |
| C | 3.26479 | 1.68482 | 0.06384 |
| C | 4.51132 | -0.41538 | 1.39043 |
| C | 4.48528 | 1.17029 | -0.36189 |
| C | 5.09727 | 0.07698 | 0.23621 |
| H | 5.01835 | -1.19761 | 1.93159 |
| H | 4.99142 | 1.65283 | -1.18714 |
| C | 2.79704 | -0.47681 | 3.23976 |
| C | 2.81350 | 3.02902 | -0.55410 |
| C | 6.38543 | -0.49439 | -0.34788 |
| C | -3.61065 | 2.79108 | 0.72011 |
| C | -2.99680 | -2.26058 | 1.18685 |
| C | -7.34229 | -0.38482 | -0.39988 |
| C | 4.04272 | 3.88181 | -0.90991 |
| H | 3.71016 | 4.88528 | -1.18676 |
| H | 4.72853 | 3.97143 | -0.06452 |
| H | 4.59863 | 3.48791 | -1.76221 |
| C | 2.00638 | 3.86972 | 0.43729 |
| H | 1.03379 | 3.43338 | 0.68215 |
| H | 2.55279 | 4.01272 | 1.37244 |
| H | 1.80580 | 4.85369 | 0.00428 |
| C | 2.00470 | 2.83895 | -1.84014 |
| H | 2.56538 | 2.24921 | -2.57052 |
| H | 1.05969 | 2.33562 | -1.63933 |
| H | 1.78544 | 3.81073 | -2.29336 |
| C | 7.47529 | 0.58352 | -0.36236 |
| H | 8.39969 | 0.17891 | -0.78424 |
| H | 7.18602 | 1.44765 | -0.96408 |
| H | 7.68912 | 0.93592 | 0.64982 |
| C | 6.90221 | -1.68907 | 0.44933 |
| H | 7.80569 | -2.07980 | -0.02531 |
| H | 7.16299 | -1.41326 | 1.47436 |
| H | 6.16870 | -2.49803 | 0.48489 |
| C | 6.11160 | -0.96109 | -1.78296 |
| H | 5.34500 | -1.73978 | -1.79775 |
| H | 5.77088 | -0.13888 | -2.41617 |
| H | 7.02302 | -1.37056 | -2.22788 |
| C | 3.85443 | -1.34217 | 3.93094 |
| H | 4.80552 | -0.81761 | 4.05070 |
| H | 3.49250 | -1.60182 | 4.92844 |
| H | 4.03403 | -2.27806 | 3.39678 |
| C | 2.54395 | 0.72770 | 4.15774 |
| H | 3.45090 | 1.32691 | 4.27267 |
| H | 1.75377 | 1.37836 | 3.77793 |
| H | 2.23709 | 0.38011 | 5.14841 |
| C | 1.53087 | -1.33015 | 3.14356 |
| H | 0.65863 | -0.74183 | 2.85308 |
| H | 1.64517 | -2.13370 | 2.41435 |
| H | 1.30889 | -1.76604 | 4.12253 |
| C | -2.17663 | 2.95659 | 1.20884 |
| H | -1.94056 | 2.23112 | 1.98951 |
| H | -1.42037 | 2.86356 | 0.43356 |
| H | -2.05757 | 3.95336 | 1.64132 |
| C | -4.48208 | 3.09120 | 1.95911 |
| H | -4.21963 | 4.07646 | 2.35439 |
| H | -5.54761 | 3.09600 | 1.72925 |
| H | -4.30876 | 2.35196 | 2.74435 |
| C | -3.94229 | 3.84249 | -0.34338 |
| H | -4.99615 | 3.80633 | -0.62634 |
| H | -3.74321 | 4.84183 | 0.05330 |
| H | -3.35447 | 3.72159 | -1.25300 |

| | | | |
|----|----------|----------|----------|
| C | -1.54976 | -2.01440 | 1.59021 |
| H | -1.22090 | -2.82479 | 2.24532 |
| H | -0.86139 | -2.00216 | 0.74767 |
| H | -1.45300 | -1.08059 | 2.14889 |
| C | -3.08834 | -3.54594 | 0.36168 |
| H | -2.52802 | -3.45639 | -0.56787 |
| H | -2.66675 | -4.37516 | 0.93606 |
| H | -4.12188 | -3.80427 | 0.12007 |
| C | -3.76452 | -2.47709 | 2.50883 |
| H | -3.73245 | -1.57988 | 3.13235 |
| H | -4.81111 | -2.73896 | 2.34793 |
| H | -3.29495 | -3.29355 | 3.06392 |
| C | -8.08222 | 0.90660 | -0.73816 |
| H | -8.13657 | 1.58314 | 0.11867 |
| H | -7.60983 | 1.43811 | -1.56814 |
| H | -9.10753 | 0.67278 | -1.03458 |
| C | -8.05957 | -1.05781 | 0.77635 |
| H | -7.60908 | -2.01918 | 1.03042 |
| H | -8.02836 | -0.42590 | 1.66736 |
| H | -9.10801 | -1.23824 | 0.52310 |
| C | -7.39840 | -1.30790 | -1.62301 |
| H | -6.90583 | -0.84789 | -2.48305 |
| H | -6.90699 | -2.26335 | -1.42973 |
| H | -8.43812 | -1.51219 | -1.89353 |
| Pb | 1.31043 | -0.85254 | -1.66332 |
| S | -1.39969 | -1.33777 | -1.81281 |
| C | -1.71781 | 1.63385 | -1.83583 |
| H | -1.62606 | 2.63771 | -1.43276 |
| H | -0.94884 | 1.47723 | -2.59245 |
| H | -2.69326 | 1.49862 | -2.30417 |

PCPX-E(II)-AuCl model systems

E = Si(II)

[R-P=C(Si(II)Cl)-P(O)ClR](AuCl)

Coordination through Si(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.80407 | -0.10260 | 1.11290 |
| C | 0.50080 | -0.30589 | -0.50484 |
| P | -1.00073 | -0.32247 | -1.38538 |
| Cl | 1.69669 | -2.37389 | -2.52939 |
| Si | 1.37961 | -0.34670 | -2.24607 |
| O | -0.37130 | -0.21508 | -2.78862 |
| H | 2.22854 | -0.13774 | 1.02508 |
| H | -1.79496 | -1.47465 | -1.26978 |
| Cl | -2.31334 | 1.12054 | -1.03045 |
| Au | 2.83535 | 1.22136 | -2.88237 |
| Cl | 4.31876 | 2.85901 | -3.47553 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.82454 | -0.12224 | 1.05780 |
| C | 0.48027 | -0.32854 | -0.55090 |
| P | -1.03768 | -0.35138 | -1.39582 |
| Cl | 1.67504 | -2.33087 | -2.66395 |
| Si | 1.31439 | -0.31188 | -2.29766 |
| O | -0.42140 | -0.18977 | -2.81182 |
| Cl | -2.29254 | 1.15329 | -1.00619 |
| Au | 2.79295 | 1.25840 | -2.89514 |
| Cl | 4.31676 | 2.89056 | -3.41386 |
| C | 2.65008 | -0.15651 | 1.09402 |
| H | 2.98031 | -1.20036 | 1.10023 |
| H | 3.08082 | 0.33854 | 0.22003 |

| | | | |
|---|----------|----------|----------|
| H | 3.00592 | 0.31765 | 2.00948 |
| C | -2.03198 | -1.82570 | -1.28546 |
| H | -2.44352 | -1.92052 | -0.27969 |
| H | -2.84048 | -1.77008 | -2.01651 |
| H | -1.38154 | -2.67362 | -1.51048 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.76569 | -0.03962 | 0.84767 |
| C | 0.55800 | -0.42678 | -0.75353 |
| P | -0.98118 | -0.57348 | -1.57706 |
| Cl | 1.99969 | -2.56584 | -2.65315 |
| Si | 1.37098 | -0.58957 | -2.50912 |
| O | -0.36383 | -0.74572 | -2.99486 |
| Au | 2.59243 | 1.07478 | -3.38614 |
| Cl | 3.83575 | 2.82682 | -4.19736 |
| C | 2.58651 | 0.13779 | 1.17507 |
| C | 3.49742 | -0.63361 | 0.23544 |
| C | 2.84616 | 1.64711 | 1.06486 |
| C | 2.79271 | -0.31895 | 2.62169 |
| H | 3.26333 | -1.69980 | 0.21596 |
| H | 3.44936 | -0.24727 | -0.78546 |
| H | 4.53517 | -0.52266 | 0.56647 |
| H | 2.17944 | 2.23007 | 1.70761 |
| H | 3.87252 | 1.85321 | 1.38539 |
| H | 2.73715 | 2.00096 | 0.03737 |
| H | 3.82356 | -0.11195 | 2.92363 |
| H | 2.12949 | 0.20610 | 3.31464 |
| H | 2.62169 | -1.39272 | 2.73532 |
| C | -2.13852 | -1.92498 | -1.17130 |
| C | -3.23135 | -1.96088 | -2.24050 |
| C | -1.32749 | -3.22338 | -1.19621 |
| C | -2.72517 | -1.68413 | 0.21800 |
| H | -3.84354 | -1.05801 | -2.23067 |
| H | -2.81340 | -2.09088 | -3.24051 |
| H | -3.88409 | -2.81323 | -2.03389 |
| H | -0.53183 | -3.22440 | -0.44947 |
| H | -2.00650 | -4.04959 | -0.96988 |
| H | -0.87951 | -3.40750 | -2.17330 |
| H | -3.36195 | -2.53461 | 0.47508 |
| H | -1.94840 | -1.60798 | 0.98312 |
| H | -3.33738 | -0.78195 | 0.25358 |
| Cl | -2.06603 | 1.11520 | -1.53047 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.93879 | -0.18396 | 0.70106 |
| C | 0.53424 | -0.29240 | -0.91017 |
| P | -1.09367 | -0.42231 | -1.52120 |
| Cl | 1.67461 | -2.40355 | -2.95525 |
| Si | 1.10730 | -0.41007 | -2.75416 |
| O | -0.67633 | -0.53517 | -3.01338 |
| Au | 2.27660 | 1.18478 | -3.81122 |
| Cl | 3.50922 | 2.83124 | -4.83190 |
| C | -2.12875 | -1.78760 | -1.03988 |
| C | -1.95913 | -2.99210 | -1.72317 |
| C | -3.02002 | -1.69629 | 0.02790 |
| C | -2.69475 | -4.10017 | -1.33729 |
| H | -1.26149 | -3.05659 | -2.54964 |
| C | -3.74319 | -2.81323 | 0.40800 |
| H | -3.15545 | -0.75820 | 0.55253 |
| C | -3.58199 | -4.01163 | -0.27443 |
| H | -2.57397 | -5.03504 | -1.87125 |
| H | -4.43986 | -2.74633 | 1.23498 |
| H | -4.15532 | -4.88200 | 0.02324 |
| C | 2.72270 | -0.09233 | 0.81766 |
| C | 3.22483 | -0.23745 | 2.11762 |
| C | 3.61267 | 0.13968 | -0.23659 |

| | | | |
|----|----------|----------|----------|
| C | 4.58744 | -0.18040 | 2.35470 |
| H | 2.53659 | -0.39851 | 2.94179 |
| C | 4.97041 | 0.21105 | 0.00656 |
| H | 3.24704 | 0.29440 | -1.24624 |
| C | 5.45859 | 0.04392 | 1.29863 |
| H | 4.96919 | -0.30242 | 3.36144 |
| H | 5.65172 | 0.40283 | -0.81391 |
| H | 6.52586 | 0.09796 | 1.48133 |
| Cl | -2.19706 | 1.22262 | -1.22782 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.88492 | 0.52359 | 0.43753 |
| C | 0.61208 | -0.55016 | -0.80048 |
| P | -0.79120 | -0.94799 | -1.77807 |
| Cl | 1.92308 | -3.37468 | -1.45422 |
| Si | 1.67504 | -1.42166 | -2.15124 |
| O | 0.05429 | -1.55069 | -2.93643 |
| Au | 3.34454 | -0.38296 | -3.22925 |
| Cl | 5.04133 | 0.78597 | -4.25397 |
| C | -2.04278 | -2.06314 | -1.16229 |
| C | -2.28611 | -3.31349 | -1.77471 |
| C | -2.77131 | -1.66879 | -0.01971 |
| C | -3.22732 | -4.14659 | -1.18259 |
| C | -3.68892 | -2.55365 | 0.52352 |
| C | -3.92562 | -3.80236 | -0.03410 |
| H | -3.42049 | -5.10787 | -1.64751 |
| H | -4.24182 | -2.24976 | 1.40662 |
| C | 2.67832 | 0.41568 | 0.69298 |
| C | 3.22976 | -0.62090 | 1.45892 |
| C | 3.48476 | 1.44324 | 0.18306 |
| C | 4.60191 | -0.62448 | 1.66885 |
| C | 4.85173 | 1.39029 | 0.41274 |
| C | 5.43088 | 0.36009 | 1.14303 |
| H | 5.03675 | -1.42207 | 2.26396 |
| H | 5.48176 | 2.17066 | -0.00290 |
| C | 2.37727 | -1.70342 | 2.05168 |
| H | 1.49064 | -1.29546 | 2.54862 |
| H | 2.02793 | -2.40073 | 1.28539 |
| H | 2.93813 | -2.27431 | 2.79268 |
| C | 2.90238 | 2.55069 | -0.64020 |
| H | 2.77278 | 2.23166 | -1.67942 |
| H | 1.92115 | 2.86725 | -0.26633 |
| H | 3.55573 | 3.42380 | -0.64466 |
| C | 6.91407 | 0.30412 | 1.33826 |
| H | 7.40048 | -0.09627 | 0.44359 |
| H | 7.33016 | 1.29802 | 1.51475 |
| H | 7.18339 | -0.33758 | 2.17852 |
| C | -2.64196 | -0.31619 | 0.61043 |
| H | -1.60639 | 0.01365 | 0.72179 |
| H | -3.15825 | 0.44187 | 0.01549 |
| H | -3.08788 | -0.31886 | 1.60509 |
| C | -1.62192 | -3.81172 | -3.02472 |
| H | -1.68705 | -3.09595 | -3.84402 |
| H | -0.56201 | -4.01496 | -2.86430 |
| H | -2.10139 | -4.73778 | -3.34126 |
| C | -4.89526 | -4.75398 | 0.59095 |
| H | -5.69616 | -4.22483 | 1.10965 |
| H | -5.34028 | -5.41607 | -0.15320 |
| H | -4.38754 | -5.38395 | 1.32809 |
| Cl | -1.75350 | 0.65949 | -2.51627 |

R = Mes *

| | | | |
|----|----------|----------|----------|
| P | -0.57086 | 1.64882 | 1.52737 |
| C | 0.08893 | 0.57309 | 0.43669 |
| P | 1.68449 | -0.13496 | 0.19918 |
| Cl | -0.97120 | 0.54341 | -2.64108 |

| | | | |
|---|----------|----------|----------|
| O | 1.26660 | -0.83898 | -1.13079 |
| C | 3.39257 | 0.45935 | 0.07751 |
| C | 3.97455 | 0.54943 | -1.22286 |
| C | 4.24692 | 0.37500 | 1.20778 |
| C | 5.29586 | 0.14977 | -1.34774 |
| C | 5.56988 | 0.00853 | 0.99157 |
| C | 6.09389 | -0.21685 | -0.27091 |
| H | 5.73003 | 0.14764 | -2.33855 |
| H | 6.21285 | -0.09863 | 1.85380 |
| C | -2.33436 | 1.60591 | 1.04066 |
| C | -2.82573 | 2.57239 | 0.13455 |
| C | -3.17033 | 0.54577 | 1.47611 |
| C | -4.02593 | 2.29449 | -0.51602 |
| C | -4.34610 | 0.33129 | 0.77085 |
| C | -4.76218 | 1.14552 | -0.27500 |
| H | -4.38999 | 2.99531 | -1.25013 |
| H | -4.96062 | -0.51485 | 1.03980 |
| C | -2.16154 | 3.94772 | -0.08289 |
| C | -2.96273 | -0.21797 | 2.79883 |
| C | -6.00566 | 0.77434 | -1.07526 |
| C | 3.90846 | 0.83193 | 2.63900 |
| C | 3.33022 | 1.20328 | -2.46046 |
| C | 7.50388 | -0.74286 | -0.50364 |
| C | -3.92949 | -1.39668 | 2.94575 |
| H | -3.72673 | -1.90072 | 3.89349 |
| H | -4.97154 | -1.07200 | 2.97609 |
| H | -3.81059 | -2.13184 | 2.14573 |
| C | -3.26524 | 0.78532 | 3.92459 |
| H | -2.56717 | 1.62708 | 3.90915 |
| H | -4.27681 | 1.18641 | 3.82885 |
| H | -3.18236 | 0.29273 | 4.89782 |
| C | -1.55959 | -0.77598 | 3.02505 |
| H | -1.23147 | -1.41534 | 2.20407 |
| H | -0.80900 | 0.01148 | 3.17495 |
| H | -1.55589 | -1.36509 | 3.94629 |
| C | -7.21455 | 0.65888 | -0.13937 |
| H | -8.10672 | 0.39381 | -0.71331 |
| H | -7.07013 | -0.11235 | 0.61930 |
| H | -7.40755 | 1.60557 | 0.37213 |
| C | -6.33215 | 1.80680 | -2.15094 |
| H | -7.21481 | 1.48340 | -2.70775 |
| H | -6.55452 | 2.78839 | -1.72330 |
| H | -5.51408 | 1.91831 | -2.86697 |
| C | -5.75975 | -0.57687 | -1.75907 |
| H | -4.91496 | -0.51668 | -2.44930 |
| H | -5.53917 | -1.36807 | -1.04001 |
| H | -6.64511 | -0.87485 | -2.32795 |
| C | -3.01865 | 4.85827 | -0.96620 |
| H | -4.02306 | 4.99786 | -0.56096 |
| H | -2.54453 | 5.84099 | -1.02031 |
| H | -3.10430 | 4.48003 | -1.98752 |
| C | -2.02904 | 4.64693 | 1.27732 |
| H | -3.00515 | 4.75523 | 1.75567 |
| H | -1.37853 | 4.09951 | 1.96427 |
| H | -1.59891 | 5.64388 | 1.14528 |
| C | -0.78531 | 3.86814 | -0.74886 |
| H | -0.02792 | 3.42223 | -0.09926 |
| H | -0.81893 | 3.28248 | -1.66867 |
| H | -0.43768 | 4.87731 | -0.98872 |
| C | 2.48638 | 1.34405 | 2.81708 |
| H | 2.22591 | 2.08720 | 2.05926 |
| H | 1.74151 | 0.54900 | 2.81463 |
| H | 2.39883 | 1.83797 | 3.78757 |
| C | 4.82692 | 2.04147 | 2.91024 |
| H | 4.61251 | 2.44030 | 3.90526 |
| H | 5.88356 | 1.77488 | 2.87534 |

| | | | |
|----|----------|----------|----------|
| H | 4.65420 | 2.83608 | 2.18039 |
| C | 4.19581 | -0.24153 | 3.69208 |
| H | 5.23452 | -0.57498 | 3.66448 |
| H | 4.00979 | 0.16808 | 4.68832 |
| H | 3.55677 | -1.11450 | 3.56127 |
| C | 2.16849 | 2.11504 | -2.07327 |
| H | 1.78618 | 2.61523 | -2.96593 |
| H | 1.31764 | 1.59714 | -1.63930 |
| H | 2.50041 | 2.88514 | -1.37176 |
| C | 2.92294 | 0.18408 | -3.52880 |
| H | 2.13704 | -0.48282 | -3.18607 |
| H | 2.56474 | 0.71079 | -4.41721 |
| H | 3.78265 | -0.42267 | -3.82481 |
| C | 4.37450 | 2.14227 | -3.09809 |
| H | 4.79901 | 2.83076 | -2.36374 |
| H | 5.19231 | 1.60622 | -3.58075 |
| H | 3.88053 | 2.73401 | -3.87252 |
| C | 8.20649 | -1.10962 | 0.80075 |
| H | 8.35962 | -0.23840 | 1.44281 |
| H | 7.64849 | -1.86145 | 1.36437 |
| H | 9.19132 | -1.52635 | 0.57821 |
| C | 8.34028 | 0.32317 | -1.22188 |
| H | 7.91712 | 0.58767 | -2.19280 |
| H | 8.40997 | 1.23572 | -0.62478 |
| H | 9.35370 | -0.05017 | -1.39135 |
| C | 7.42086 | -1.99982 | -1.37846 |
| H | 6.83767 | -2.78212 | -0.88706 |
| H | 6.95566 | -1.79213 | -2.34401 |
| H | 8.42426 | -2.39039 | -1.56721 |
| Au | -1.84543 | -2.37137 | -0.56216 |
| Cl | -3.29839 | -4.09862 | -0.06114 |
| Si | -0.51494 | -0.60301 | -0.96522 |
| Cl | 1.86216 | -1.68829 | 1.49720 |

Coordination through O atom

| | | | |
|-------------|----------|----------|----------|
| R= H | | | |
| P | 0.68754 | -0.15581 | 1.15403 |
| C | 0.43909 | -0.31608 | -0.47915 |
| P | -1.02055 | -0.12697 | -1.38122 |
| Cl | 1.15080 | -2.49278 | -2.52264 |
| Si | 1.50603 | -0.43793 | -2.15362 |
| O | -0.36606 | 0.18671 | -2.74918 |
| H | 2.09225 | -0.42595 | 1.14571 |
| H | -1.80826 | -1.28441 | -1.45998 |
| Cl | -2.33763 | 1.25860 | -0.83945 |
| Au | -1.44027 | 0.28583 | -4.57949 |
| Cl | -2.59636 | 0.38737 | -6.47005 |

| | | | |
|---------------|----------|----------|----------|
| R = Me | | | |
| P | 0.67263 | -0.18041 | 1.09828 |
| C | 0.41603 | -0.30856 | -0.53571 |
| P | -1.05964 | -0.15948 | -1.41429 |
| Cl | 1.36178 | -2.39356 | -2.63029 |
| Si | 1.46371 | -0.30744 | -2.21448 |
| O | -0.39866 | 0.13043 | -2.79982 |
| Cl | -2.28473 | 1.34444 | -0.91938 |
| Au | -1.42885 | 0.21114 | -4.65056 |
| Cl | -2.54662 | 0.28742 | -6.56721 |
| C | 2.46628 | -0.51910 | 1.25565 |
| H | 2.84036 | -0.09053 | 2.18641 |
| H | 2.61619 | -1.60244 | 1.29637 |
| H | 3.03223 | -0.12511 | 0.40805 |
| C | -2.09106 | -1.60886 | -1.47780 |
| H | -2.88214 | -1.45457 | -2.21446 |
| H | -1.45545 | -2.44559 | -1.77608 |

H -2.52244 -1.78900 -0.49179

R = t-Bu

P 0.81298 -0.33896 0.88213
C 0.43413 -0.19882 -0.73109
P -1.19134 -0.29069 -1.35024
Cl 1.77440 -1.56249 -3.20515
Si 1.14071 0.34838 -2.50655
O -0.82221 0.08063 -2.82118
Au -2.01945 0.44993 -4.52668
Cl -3.27989 0.82397 -6.31724
C 2.66798 -0.26596 1.05175
C 3.10524 -1.71694 1.28446
C 3.40412 0.33110 -0.13358
C 2.93005 0.55867 2.31553
H 2.56858 -2.17928 2.11820
H 2.95209 -2.32877 0.39264
H 4.17237 -1.73609 1.52982
H 3.05766 1.34051 -0.36653
H 4.47437 0.39341 0.09114
H 3.30491 -0.29082 -1.02704
H 3.99819 0.53505 2.55161
H 2.63981 1.60410 2.18330
H 2.38782 0.16386 3.17897
C -2.12379 -1.86110 -1.22351
C -3.45857 -1.73407 -1.95818
C -1.26005 -2.94611 -1.87096
C -2.35208 -2.16486 0.25693
H -4.10837 -0.98508 -1.50416
H -3.32871 -1.48670 -3.01441
H -3.96584 -2.70101 -1.90100
H -0.29164 -3.05234 -1.37979
H -1.79391 -3.89597 -1.78313
H -1.08513 -2.75091 -2.92957
H -2.86425 -3.12785 0.32916
H -1.41523 -2.24314 0.81305
H -2.98087 -1.41351 0.73749
Cl -2.40998 1.13193 -0.61718

R = Ph

P 0.86686 -0.38279 1.11932
C 0.41255 -0.35394 -0.48444
P -1.20409 -0.29234 -1.07620
Cl 1.35101 -1.67007 -3.18668
Si 1.12206 0.22610 -2.23484
O -0.84738 0.35558 -2.45783
Au -2.21078 0.75282 -4.02709
Cl -3.67947 1.16569 -5.64350
C 2.66276 -0.42540 1.08917
C 3.29756 -0.00964 2.26580
C 3.44334 -0.83442 0.00220
C 4.67877 0.03554 2.34062
H 2.69790 0.29103 3.11953
C 4.82390 -0.79492 0.08380
H 2.97136 -1.22437 -0.89284
C 5.44126 -0.35388 1.24787
H 5.16209 0.37019 3.25098
H 5.42208 -1.11548 -0.76109
H 6.52335 -0.32530 1.30660
C -2.06292 -1.84157 -1.24450
C -3.39881 -1.86953 -1.64796
C -1.36095 -3.02644 -1.03146
C -4.02533 -3.08755 -1.83704
H -3.94243 -0.94834 -1.82220
C -2.00271 -4.24004 -1.21611
H -0.31999 -2.99648 -0.73518

C -3.32941 -4.26960 -1.61824
H -5.05927 -3.11362 -2.15889
H -1.46126 -5.16368 -1.05096
H -3.82671 -5.22136 -1.76591
Cl -2.48109 0.93364 -0.13140

R = Mes

P 1.19827 -1.31270 1.37492
C 0.27535 -0.73093 0.12291
P -1.42967 -0.69968 -0.19785
Cl 0.81560 -0.44804 -2.93785
Si 0.61945 0.72509 -1.15946
O -1.38680 0.61227 -1.04663
Au -2.67739 2.30984 -1.09913
Cl -4.00278 4.09258 -1.16585
C 2.86378 -0.71464 0.93351
C 3.36821 0.41582 1.59198
C 3.66466 -1.43479 0.03475
C 4.66621 0.82531 1.31809
C 4.95789 -0.98918 -0.20354
C 5.47519 0.14052 0.42007
H 5.05576 1.70430 1.82323
H 5.58307 -1.54687 -0.89470
C -2.14641 -2.09699 -1.05313
C -2.80313 -1.96542 -2.29831
C -2.03288 -3.36020 -0.43380
C -3.30212 -3.11838 -2.88934
C -2.55834 -4.46914 -1.07985
C -3.18777 -4.37507 -2.31158
H -3.81194 -3.02146 -3.84231
H -2.47568 -5.43687 -0.59533
C 2.51696 1.19661 2.54699
H 1.76729 1.78717 2.01087
H 1.97635 0.54168 3.23948
H 3.12014 1.88449 3.14057
C 6.86186 0.61743 0.11587
H 6.85555 1.29705 -0.74205
H 7.29104 1.16038 0.95962
H 7.52423 -0.21394 -0.13189
C 3.15640 -2.66279 -0.66010
H 2.69422 -3.36271 0.04408
H 2.40179 -2.41009 -1.41023
H 3.96911 -3.18751 -1.16365
C -1.35846 -3.58642 0.88534
H -0.27520 -3.67209 0.76095
H -1.53912 -2.79239 1.61077
H -1.71176 -4.51796 1.32855
C -3.01688 -0.67596 -3.03117
H -2.07212 -0.22576 -3.33813
H -3.61209 -0.85988 -3.92509
H -3.54715 0.06361 -2.42633
C -3.71844 -5.58943 -3.00457
H -2.98567 -5.96734 -3.72437
H -3.93027 -6.39276 -2.29770
H -4.63117 -5.36391 -3.55867
Cl -2.61132 -0.32193 1.39631

R = Mes*

P 2.08237 1.96568 -0.28892
C 1.08578 0.63266 -0.25310
P -0.64875 0.48119 -0.37291
C 3.73676 1.16585 -0.24052
C 4.45456 1.15274 0.98779
C 4.23307 0.44908 -1.34766
C 5.48555 0.23842 1.12263
C 5.26818 -0.46290 -1.12441

| | | | | | | | |
|---|----------|----------|----------|-----------------------------------------------------|----------|----------|----------|
| C | 5.86974 | -0.63263 | 0.10579 | H | -3.90736 | 3.28505 | -2.89145 |
| H | 6.01383 | 0.18599 | 2.06318 | H | -2.48312 | 4.23225 | -3.31066 |
| H | 5.61416 | -1.05209 | -1.96208 | C | -6.39869 | 0.89993 | 0.41482 |
| C | 3.86194 | 0.66466 | -2.82982 | C | -7.03004 | 1.43745 | 1.70502 |
| C | 4.18665 | 2.14542 | 2.13533 | C | -6.62948 | -0.61397 | 0.32365 |
| C | 6.94535 | -1.68069 | 0.36869 | H | -6.87628 | 2.51541 | 1.80079 |
| C | 2.82492 | 1.92377 | 2.79835 | H | -8.10644 | 1.24657 | 1.69873 |
| H | 1.99066 | 2.16576 | 2.13497 | H | -6.61353 | 0.95657 | 2.59224 |
| H | 2.70100 | 0.88645 | 3.11420 | H | -6.17860 | -1.03510 | -0.57723 |
| H | 2.73121 | 2.57288 | 3.67399 | H | -6.20203 | -1.14437 | 1.17630 |
| C | 4.27763 | 3.57879 | 1.59389 | H | -7.70225 | -0.82367 | 0.30267 |
| H | 5.26083 | 3.76507 | 1.15521 | Cl | 1.88027 | -1.68525 | 1.74949 |
| H | 3.52396 | 3.78790 | 0.83158 | O | -0.66822 | -1.02546 | 0.06680 |
| H | 4.12530 | 4.29410 | 2.40701 | Au | -2.27872 | -2.34899 | -0.37539 |
| C | 5.23427 | 2.02994 | 3.24577 | Cl | -3.97989 | -3.71780 | -0.82591 |
| H | 5.18756 | 1.06682 | 3.75934 | C | -0.84076 | 3.51240 | -1.30073 |
| H | 6.24966 | 2.17826 | 2.87118 | H | -0.46707 | 3.49781 | -0.27384 |
| H | 5.04066 | 2.80499 | 3.99077 | H | -0.29826 | 2.77180 | -1.88665 |
| C | 3.37048 | -0.63259 | -3.47959 | H | -0.57893 | 4.48631 | -1.72139 |
| H | 2.46415 | -1.00204 | -2.99496 | C | -0.56512 | 0.78582 | 2.78602 |
| H | 3.14898 | -0.45656 | -4.53600 | H | 0.10449 | 0.27385 | 2.09819 |
| H | 4.11846 | -1.42551 | -3.42712 | H | -0.51638 | 1.86204 | 2.59988 |
| C | 2.82423 | 1.75150 | -3.09786 | H | -0.15858 | 0.60101 | 3.78325 |
| H | 1.81391 | 1.44941 | -2.82099 | C | -7.08510 | 1.56661 | -0.77426 |
| H | 3.07276 | 2.69384 | -2.59761 | H | -7.01881 | 2.65712 | -0.73034 |
| H | 2.80349 | 1.96429 | -4.17070 | H | -6.66288 | 1.23018 | -1.72432 |
| C | 5.14568 | 1.12709 | -3.54468 | H | -8.14563 | 1.30538 | -0.77301 |
| H | 5.51321 | 2.06425 | -3.11860 | Si | 1.30948 | -1.33955 | -0.27353 |
| H | 5.94712 | 0.39134 | -3.47486 | Cl | -1.04904 | 0.35312 | -2.36750 |
| H | 4.93589 | 1.29316 | -4.60490 | | | | |
| C | 7.22288 | -2.54550 | -0.85782 | Coordination through P (sp²) atom | | | |
| H | 7.60989 | -1.95697 | -1.69383 | R = H | | | |
| H | 7.97645 | -3.29687 | -0.61035 | P | 0.50562 | 0.13284 | 1.11549 |
| H | 6.32668 | -3.07395 | -1.19213 | C | 0.30871 | -0.25356 | -0.46491 |
| C | 6.47621 | -2.59651 | 1.50610 | P | -1.09919 | -0.29801 | -1.46341 |
| H | 6.30729 | -2.03958 | 2.42987 | Cl | 1.29170 | -2.62781 | -2.18597 |
| H | 5.54137 | -3.09768 | 1.24488 | Si | 1.36906 | -0.49748 | -2.16982 |
| H | 7.23141 | -3.36103 | 1.70875 | O | -0.40343 | -0.18808 | -2.82264 |
| C | 8.25173 | -0.99022 | 0.77733 | H | 1.88508 | -0.03306 | 1.36561 |
| H | 8.12919 | -0.39057 | 1.68154 | H | -1.81760 | -1.49504 | -1.32603 |
| H | 9.02503 | -1.73740 | 0.97625 | Cl | -2.51617 | 1.07677 | -1.21270 |
| H | 8.61156 | -0.33138 | -0.01699 | Au | -0.90029 | 0.77800 | 2.67214 |
| C | -2.10731 | 1.30370 | 0.29904 | Cl | -2.35271 | 1.43037 | 4.26430 |
| C | -2.72087 | 0.68486 | 1.42925 | | | | |
| C | -2.88873 | 2.14927 | -0.53105 | R = Me | | | |
| C | -4.10294 | 0.59474 | 1.42135 | P | 0.54920 | 0.11872 | 1.06651 |
| C | -4.26926 | 2.02133 | -0.45504 | C | 0.33194 | -0.24855 | -0.51360 |
| C | -4.89963 | 1.16052 | 0.43274 | P | -1.09593 | -0.33666 | -1.48565 |
| H | -4.58006 | 0.06143 | 2.23346 | Cl | 1.45597 | -2.62511 | -2.15980 |
| H | -4.87322 | 2.62564 | -1.11773 | Si | 1.37370 | -0.48052 | -2.21334 |
| C | -2.00174 | 0.28133 | 2.72986 | O | -0.39480 | -0.30957 | -2.85565 |
| C | -2.04753 | -1.22211 | 3.00945 | Cl | -2.38232 | 1.19163 | -1.32325 |
| C | -2.73950 | 1.00298 | 3.87639 | Au | -0.96062 | 0.65608 | 2.57678 |
| H | -1.42808 | -1.78471 | 2.31257 | Cl | -2.52622 | 1.17073 | 4.12013 |
| H | -1.67443 | -1.41522 | 4.01886 | C | 2.29767 | -0.03737 | 1.49236 |
| H | -3.06640 | -1.61004 | 2.94737 | H | 2.44342 | -0.97657 | 2.03315 |
| H | -2.79159 | 2.08014 | 3.70032 | H | 2.91326 | -0.03850 | 0.59222 |
| H | -3.75413 | 0.63271 | 4.02465 | H | 2.58254 | 0.78172 | 2.15446 |
| H | -2.19067 | 0.83593 | 4.80661 | C | -2.07892 | -1.80154 | -1.24358 |
| C | -2.35422 | 3.33693 | -1.35312 | H | -2.84969 | -1.84470 | -2.01510 |
| C | -2.94332 | 4.59002 | -0.67144 | H | -1.40739 | -2.65822 | -1.33281 |
| C | -2.81959 | 3.31996 | -2.81108 | H | -2.53991 | -1.77564 | -0.25491 |
| H | -2.63858 | 4.64607 | 0.37635 | | | | |
| H | -2.57590 | 5.48438 | -1.18187 | | | | |
| H | -4.03297 | 4.60423 | -0.70742 | | | | |
| H | -2.41434 | 2.46747 | -3.35518 | | | | |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.80873 | 0.10291 | 0.86099 |
| C | 0.50413 | -0.41203 | -0.67193 |
| P | -1.02254 | -0.60216 | -1.48595 |
| Cl | 1.93274 | -2.65788 | -2.41991 |
| Si | 1.36609 | -0.59616 | -2.47454 |
| O | -0.44872 | -0.79014 | -2.90736 |
| Au | -0.67063 | 0.79048 | 2.35410 |
| Cl | -2.20687 | 1.47791 | 3.86775 |
| C | 2.61823 | 0.05224 | 1.24977 |
| C | 2.81121 | 0.61142 | 2.65685 |
| C | 3.08321 | -1.40429 | 1.18748 |
| C | 3.36994 | 0.90828 | 0.23190 |
| H | 2.47490 | 1.64771 | 2.73526 |
| H | 2.27490 | 0.02516 | 3.40651 |
| H | 3.87586 | 0.58256 | 2.90501 |
| H | 2.95043 | -1.83435 | 0.19370 |
| H | 4.14782 | -1.44300 | 1.43886 |
| H | 2.54944 | -2.02942 | 1.90788 |
| H | 4.43942 | 0.86820 | 0.46004 |
| H | 3.23682 | 0.55334 | -0.79309 |
| H | 3.05725 | 1.95421 | 0.27311 |
| C | -2.13248 | -1.97826 | -1.01521 |
| C | -1.29265 | -3.25707 | -1.00435 |
| C | -2.74058 | -1.72514 | 0.36061 |
| C | -3.21896 | -2.06975 | -2.08968 |
| H | -0.84181 | -3.46130 | -1.97569 |
| H | -0.49454 | -3.21715 | -0.26136 |
| H | -1.95300 | -4.09012 | -0.74894 |
| H | -3.35015 | -0.82117 | 0.38733 |
| H | -3.38397 | -2.57292 | 0.61088 |
| H | -1.97918 | -1.64981 | 1.13991 |
| H | -3.84361 | -2.93863 | -1.86595 |
| H | -3.86109 | -1.18784 | -2.09886 |
| H | -2.79288 | -2.20655 | -3.08521 |
| Cl | -2.16281 | 1.05753 | -1.43919 |

R= Ph

| | | | |
|----|----------|----------|----------|
| P | 0.81466 | -0.13222 | 1.00890 |
| C | 0.42910 | -0.20230 | -0.58750 |
| P | -1.14443 | -0.25436 | -1.31192 |
| Cl | 1.64467 | -1.88714 | -2.96444 |
| Si | 1.15416 | 0.12923 | -2.41377 |
| O | -0.69823 | 0.04669 | -2.75464 |
| Au | -0.58989 | 0.01867 | 2.70897 |
| Cl | -2.08320 | 0.11480 | 4.40598 |
| C | -2.03668 | -1.78921 | -1.18994 |
| C | -2.77942 | -2.09811 | -0.05049 |
| C | -1.92638 | -2.70004 | -2.23871 |
| C | -3.41335 | -3.32455 | 0.03376 |
| H | -2.86750 | -1.38761 | 0.76401 |
| C | -2.57276 | -3.92214 | -2.14402 |
| H | -1.33928 | -2.45157 | -3.11402 |
| C | -3.31128 | -4.23326 | -1.01218 |
| H | -3.99120 | -3.56937 | 0.91678 |
| H | -2.49596 | -4.63280 | -2.95820 |
| H | -3.81346 | -5.19143 | -0.94276 |
| C | 2.57107 | -0.20116 | 1.26780 |
| C | 3.46115 | -0.60349 | 0.26713 |
| C | 3.05631 | 0.17424 | 2.52414 |
| C | 4.82028 | -0.60712 | 0.52216 |
| H | 3.09037 | -0.94394 | -0.69243 |
| C | 4.41782 | 0.16934 | 2.76844 |
| H | 2.36114 | 0.47396 | 3.30171 |
| C | 5.29848 | -0.21761 | 1.76728 |
| H | 5.50966 | -0.92299 | -0.25173 |
| H | 4.79262 | 0.46557 | 3.74085 |

| | | | |
|----|----------|----------|----------|
| H | 6.36507 | -0.22484 | 1.96083 |
| Cl | -2.40972 | 1.15699 | -0.65158 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.79940 | -0.30541 | 1.63752 |
| C | 0.27375 | -0.40067 | 0.08643 |
| P | -1.24804 | -0.32366 | -0.75250 |
| Cl | 1.44551 | -1.66115 | -2.54563 |
| Si | 1.13880 | 0.25001 | -1.59870 |
| O | -0.69603 | 0.43729 | -1.97561 |
| Au | -0.32417 | -0.23514 | 3.53876 |
| Cl | -1.45433 | -0.16398 | 5.49812 |
| C | -2.06760 | -1.85648 | -1.17698 |
| C | -2.34889 | -2.78531 | -0.15535 |
| C | -2.44506 | -2.12257 | -2.51245 |
| C | -2.96403 | -3.98155 | -0.49135 |
| C | -3.05807 | -3.33984 | -2.77938 |
| C | -3.31544 | -4.28657 | -1.79800 |
| H | -3.18196 | -4.69137 | 0.30029 |
| H | -3.35486 | -3.54771 | -3.80236 |
| C | 2.59472 | -0.21280 | 1.62795 |
| C | 3.35474 | -1.37097 | 1.40490 |
| C | 3.20911 | 1.02207 | 1.88764 |
| C | 4.73796 | -1.26248 | 1.44496 |
| C | 4.59492 | 1.07536 | 1.91056 |
| C | 5.37635 | -0.05378 | 1.69573 |
| H | 5.33513 | -2.15315 | 1.27522 |
| H | 5.07763 | 2.02947 | 2.09861 |
| C | -2.01145 | -2.55232 | 1.28433 |
| H | -0.95391 | -2.75051 | 1.47727 |
| H | -2.21922 | -1.53256 | 1.61359 |
| H | -2.59073 | -3.22024 | 1.92194 |
| C | -2.25093 | -1.18683 | -3.66932 |
| H | -2.62371 | -0.18326 | -3.46385 |
| H | -1.19485 | -1.08766 | -3.92490 |
| H | -2.77972 | -1.57614 | -4.53941 |
| C | -3.94622 | -5.59860 | -2.14135 |
| H | -4.61261 | -5.50806 | -3.00060 |
| H | -3.17767 | -6.33394 | -2.39948 |
| H | -4.51452 | -6.00039 | -1.30110 |
| C | 6.86998 | 0.02449 | 1.76118 |
| H | 7.21947 | -0.14598 | 2.78434 |
| H | 7.33644 | -0.73016 | 1.12594 |
| H | 7.23092 | 1.00683 | 1.45216 |
| C | 2.71749 | -2.69925 | 1.12845 |
| H | 1.93150 | -2.92864 | 1.85505 |
| H | 2.26315 | -2.72105 | 0.13392 |
| H | 3.45760 | -3.49830 | 1.17881 |
| C | 2.40240 | 2.26656 | 2.09919 |
| H | 1.85823 | 2.54126 | 1.19021 |
| H | 1.66432 | 2.13993 | 2.89796 |
| H | 3.04403 | 3.10547 | 2.36927 |
| Cl | -2.64437 | 0.83837 | 0.13426 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.22485 | 0.73325 | 0.01613 |
| C | -0.26043 | -0.53321 | 0.42510 |
| P | 1.42508 | -0.92817 | 0.70319 |
| Cl | -1.24208 | -3.26331 | -0.99783 |
| O | 1.21304 | -2.45381 | 0.60882 |
| C | 3.05570 | -0.52420 | 0.02176 |
| C | 3.60028 | -1.48158 | -0.88375 |
| C | 3.93524 | 0.35768 | 0.70237 |
| C | 4.94939 | -1.77292 | -0.75839 |
| C | 5.27893 | 0.00566 | 0.75870 |
| C | 5.79606 | -1.11171 | 0.12285 |

| | | | |
|----|----------|----------|----------|
| H | 5.36037 | -2.54615 | -1.39437 |
| H | 5.94549 | 0.64799 | 1.31682 |
| C | -2.92430 | 0.09930 | 0.11216 |
| C | -3.59323 | -0.33082 | -1.06593 |
| C | -3.47345 | -0.17927 | 1.38784 |
| C | -4.66563 | -1.20044 | -0.91056 |
| C | -4.53952 | -1.07089 | 1.44513 |
| C | -5.11861 | -1.63907 | 0.32508 |
| H | -5.15786 | -1.57018 | -1.79433 |
| H | -4.93319 | -1.32945 | 2.41954 |
| C | -3.27500 | 0.17546 | -2.48719 |
| C | -3.10698 | 0.47461 | 2.73840 |
| C | -6.22669 | -2.67528 | 0.47873 |
| C | 3.59155 | 1.76879 | 1.21204 |
| C | 2.86963 | -2.10252 | -2.08805 |
| C | 7.24203 | -1.56304 | 0.28208 |
| C | -4.38371 | 1.14834 | 3.27603 |
| H | -4.16595 | 1.62732 | 4.23427 |
| H | -4.73936 | 1.91681 | 2.58515 |
| H | -5.19675 | 0.44059 | 3.43717 |
| C | -2.05783 | 1.58140 | 2.68470 |
| H | -1.04874 | 1.20679 | 2.50649 |
| H | -2.29805 | 2.34853 | 1.94331 |
| H | -2.02865 | 2.08276 | 3.65617 |
| C | -2.63410 | -0.58196 | 3.74226 |
| H | -3.39312 | -1.34582 | 3.91970 |
| H | -1.73463 | -1.09018 | 3.38854 |
| H | -2.40991 | -0.10604 | 4.70105 |
| C | -7.40584 | -2.06290 | 1.24336 |
| H | -8.20124 | -2.80388 | 1.36137 |
| H | -7.11464 | -1.72781 | 2.24086 |
| H | -7.81758 | -1.20431 | 0.70708 |
| C | -6.73921 | -3.18166 | -0.86696 |
| H | -7.51289 | -3.93482 | -0.70009 |
| H | -7.18454 | -2.38070 | -1.46282 |
| H | -5.94455 | -3.64876 | -1.45375 |
| C | -5.67432 | -3.87135 | 1.26406 |
| H | -4.82743 | -4.32337 | 0.74268 |
| H | -5.33436 | -3.57938 | 2.25973 |
| H | -6.45057 | -4.63218 | 1.38436 |
| C | -4.15748 | -0.49205 | -3.54713 |
| H | -5.22015 | -0.29884 | -3.38627 |
| H | -3.89841 | -0.07627 | -4.52311 |
| H | -3.99815 | -1.57204 | -3.59510 |
| C | -3.58286 | 1.67808 | -2.53888 |
| H | -4.63276 | 1.86482 | -2.30041 |
| H | -2.97414 | 2.25216 | -1.83674 |
| H | -3.38424 | 2.06832 | -3.54069 |
| C | -1.83139 | -0.08578 | -2.92459 |
| H | -1.09802 | 0.51387 | -2.38023 |
| H | -1.56472 | -1.13684 | -2.80837 |
| H | -1.71852 | 0.19223 | -3.97622 |
| C | 2.14346 | 2.17816 | 0.98428 |
| H | 1.84182 | 1.98443 | -0.04832 |
| H | 1.44094 | 1.69372 | 1.66039 |
| H | 2.03860 | 3.25341 | 1.14284 |
| C | 4.43122 | 2.72934 | 0.34257 |
| H | 4.19816 | 3.76021 | 0.62044 |
| H | 5.50301 | 2.57710 | 0.47368 |
| H | 4.19643 | 2.60525 | -0.71704 |
| C | 3.97227 | 1.99090 | 2.67769 |
| H | 5.03142 | 1.79726 | 2.85796 |
| H | 3.77894 | 3.03236 | 2.94716 |
| H | 3.39360 | 1.35555 | 3.34743 |
| C | 1.54421 | -1.41233 | -2.39537 |
| H | 1.16324 | -1.78004 | -3.35118 |
| H | 0.76229 | -1.62507 | -1.67059 |
| H | 1.67213 | -0.32998 | -2.48360 |
| C | 2.67189 | -3.61277 | -1.93435 |
| H | 2.01585 | -3.84829 | -1.09925 |
| H | 2.22647 | -4.01867 | -2.84644 |
| H | 3.62842 | -4.11754 | -1.77684 |
| C | 3.75289 | -1.85600 | -3.32796 |
| H | 3.97390 | -0.79341 | -3.45419 |
| H | 4.69773 | -2.39887 | -3.29313 |
| H | 3.21419 | -2.19819 | -4.21502 |
| C | 8.00195 | -0.72137 | 1.30368 |
| H | 8.08994 | 0.32203 | 0.99043 |
| H | 7.52486 | -0.74836 | 2.28652 |
| H | 9.01513 | -1.11391 | 1.41633 |
| C | 7.96671 | -1.45988 | -1.06543 |
| H | 7.50254 | -2.08922 | -1.82715 |
| H | 7.96690 | -0.43092 | -1.43312 |
| H | 9.00566 | -1.78215 | -0.95569 |
| C | 7.25166 | -3.02206 | 0.75465 |
| H | 6.75054 | -3.12462 | 1.72008 |
| H | 6.74816 | -3.68120 | 0.04478 |
| H | 8.28127 | -3.37248 | 0.86575 |
| Au | -0.71677 | 2.81365 | -0.57849 |
| Cl | -0.21178 | 4.95191 | -1.15149 |
| Si | -0.65744 | -2.46756 | 0.90978 |
| Cl | 1.67207 | -0.61904 | 2.70834 |

| Coordination through $\pi(\text{C}=\text{P})$ bond | | | |
|----------------------------------------------------|----------|----------|----------|
| R = H | | | |
| P | 0.69472 | 0.17989 | 1.10190 |
| C | 0.33114 | 0.00754 | -0.57998 |
| P | -1.16640 | -0.34682 | -1.38664 |
| Cl | 1.24536 | -2.59254 | -2.00106 |
| Si | 1.19657 | -0.48193 | -2.35779 |
| O | -0.64833 | -0.35774 | -2.82862 |
| H | 2.09460 | -0.08498 | 1.00090 |
| H | -1.67450 | -1.59472 | -0.99565 |
| Cl | -2.75954 | 0.83730 | -1.17799 |
| Au | 0.71809 | 2.10029 | -0.29106 |
| Cl | 1.06215 | 4.30588 | -0.51413 |

| R = Me | | | |
|--------|----------|----------|----------|
| P | 0.71426 | 0.20744 | 0.99808 |
| C | 0.32776 | 0.02436 | -0.67444 |
| P | -1.17263 | -0.42007 | -1.44272 |
| Cl | 1.50355 | -2.55792 | -1.97888 |
| Si | 1.19939 | -0.47209 | -2.43381 |
| O | -0.63116 | -0.55768 | -2.87746 |
| Cl | -2.68862 | 0.89829 | -1.40704 |
| Au | 0.61786 | 2.13712 | -0.39252 |
| Cl | 0.88043 | 4.36420 | -0.55661 |
| C | 2.50831 | -0.16477 | 1.05017 |
| H | 2.96691 | 0.40145 | 1.86285 |
| H | 2.60661 | -1.23074 | 1.28108 |
| H | 3.02399 | 0.03857 | 0.11190 |
| C | -1.87753 | -1.93861 | -0.83012 |
| H | -2.24642 | -1.79010 | 0.18583 |
| H | -2.69723 | -2.23736 | -1.48564 |
| H | -1.08865 | -2.69353 | -0.84841 |

| R = <i>t</i> -Bu | | | |
|------------------|----------|----------|----------|
| P | 0.64331 | 0.17443 | 0.96019 |
| C | 0.35142 | 0.11982 | -0.74698 |
| P | -1.15511 | -0.34988 | -1.52999 |
| Cl | 2.02724 | -1.93812 | -2.56224 |

| | | | |
|----|----------|----------|----------|
| Si | 1.18140 | 0.03639 | -2.59356 |
| O | -0.60172 | -0.44604 | -2.96499 |
| Au | 0.41969 | 2.21959 | -0.22544 |
| Cl | 0.51006 | 4.46610 | -0.08256 |
| C | 2.47825 | -0.02039 | 1.24597 |
| C | 2.67352 | -1.53350 | 1.40299 |
| C | 3.39248 | 0.52626 | 0.16312 |
| C | 2.75273 | 0.68162 | 2.57767 |
| H | 2.00073 | -1.96003 | 2.15371 |
| H | 2.52162 | -2.05597 | 0.45604 |
| H | 3.69797 | -1.72759 | 1.73670 |
| H | 3.26258 | 1.60186 | 0.02549 |
| H | 4.43494 | 0.35096 | 0.45008 |
| H | 3.23867 | 0.02922 | -0.79644 |
| H | 3.78809 | 0.49638 | 2.87865 |
| H | 2.61420 | 1.76267 | 2.49817 |
| H | 2.10172 | 0.31305 | 3.37529 |
| C | -1.98747 | -1.89021 | -0.99219 |
| C | -3.03809 | -2.23579 | -2.04991 |
| C | -0.93347 | -2.99626 | -0.92193 |
| C | -2.63114 | -1.67871 | 0.37641 |
| H | -3.82274 | -1.48020 | -2.11093 |
| H | -2.58993 | -2.35717 | -3.03760 |
| H | -3.50446 | -3.18411 | -1.76954 |
| H | -0.17210 | -2.79155 | -0.16756 |
| H | -1.43943 | -3.92538 | -0.64587 |
| H | -0.43155 | -3.14907 | -1.87739 |
| H | -3.06409 | -2.62858 | 0.70150 |
| H | -1.90192 | -1.37156 | 1.13020 |
| H | -3.43009 | -0.93721 | 0.34386 |
| Cl | -2.60452 | 1.05661 | -1.49595 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.70624 | 0.17366 | 1.09576 |
| C | 0.22841 | 0.18574 | -0.56754 |
| P | -1.37738 | -0.08097 | -1.19255 |
| Cl | 1.23581 | -1.68238 | -3.02672 |
| Si | 0.78478 | 0.35331 | -2.50956 |
| O | -1.08439 | 0.23993 | -2.67051 |
| Au | 0.57242 | 2.26222 | -0.06606 |
| Cl | 0.89611 | 4.48694 | 0.08177 |
| C | 2.48346 | -0.14403 | 1.11432 |
| C | 3.13237 | 0.15556 | 2.31650 |
| C | 3.21352 | -0.69432 | 0.05919 |
| C | 4.49310 | -0.05956 | 2.44928 |
| H | 2.56634 | 0.57107 | 3.14461 |
| C | 4.57195 | -0.91839 | 0.20157 |
| H | 2.71685 | -0.97188 | -0.86255 |
| C | 5.21324 | -0.59556 | 1.39064 |
| H | 4.99203 | 0.18770 | 3.37896 |
| H | 5.13311 | -1.34828 | -0.61996 |
| H | 6.27817 | -0.76967 | 1.49460 |
| C | -1.99556 | -1.73854 | -0.97898 |
| C | -2.10217 | -2.56964 | -2.09000 |
| C | -2.35225 | -2.19449 | 0.28944 |
| C | -2.57366 | -3.86309 | -1.92589 |
| H | -1.81096 | -2.20629 | -3.06724 |
| C | -2.81521 | -3.48852 | 0.44180 |
| H | -2.27092 | -1.54237 | 1.15259 |
| C | -2.92699 | -4.32040 | -0.66590 |
| H | -2.65964 | -4.51505 | -2.78689 |
| H | -3.09211 | -3.84966 | 1.42502 |
| H | -3.29234 | -5.33350 | -0.54270 |
| Cl | -2.84047 | 1.11256 | -0.49672 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.70795 | 0.14859 | 1.51674 |
| C | 0.10204 | 0.17174 | -0.11185 |
| P | -1.48872 | -0.08167 | -0.80565 |
| Cl | 1.27374 | -0.92560 | -3.01509 |
| Si | 0.63613 | 0.82495 | -1.95385 |
| O | -1.19236 | 0.60767 | -2.15715 |
| Au | 0.28214 | 2.26425 | 0.45187 |
| Cl | 0.43409 | 4.49138 | 0.82501 |
| C | 2.50847 | -0.07254 | 1.35050 |
| C | 3.37540 | 0.83875 | 1.97893 |
| C | 3.02402 | -1.24410 | 0.76091 |
| C | 4.74560 | 0.61687 | 1.90865 |
| C | 4.39919 | -1.42022 | 0.72617 |
| C | 5.28026 | -0.49079 | 1.26797 |
| H | 5.41241 | 1.33178 | 2.38148 |
| H | 4.79507 | -2.32522 | 0.27485 |
| C | -2.02474 | -1.78324 | -0.97683 |
| C | -2.35525 | -2.31650 | -2.24490 |
| C | -2.13051 | -2.58018 | 0.18052 |
| C | -2.70870 | -3.65755 | -2.30897 |
| C | -2.49304 | -3.91272 | 0.04410 |
| C | -2.76553 | -4.47886 | -1.19115 |
| H | -2.96503 | -4.07083 | -3.27918 |
| H | -2.57638 | -4.52020 | 0.93997 |
| C | 2.87902 | 2.04205 | 2.72126 |
| H | 2.67217 | 2.88113 | 2.05028 |
| H | 1.95090 | 1.83850 | 3.26320 |
| H | 3.62389 | 2.37407 | 3.44605 |
| C | 2.14458 | -2.34135 | 0.23760 |
| H | 1.36392 | -2.60654 | 0.95720 |
| H | 1.65144 | -2.06646 | -0.69557 |
| H | 2.73541 | -3.23874 | 0.05012 |
| C | 6.76076 | -0.68782 | 1.16870 |
| H | 7.28858 | -0.15522 | 1.96140 |
| H | 7.02753 | -1.74498 | 1.22537 |
| H | 7.13493 | -0.30888 | 0.21239 |
| C | -1.88590 | -2.07729 | 1.57155 |
| H | -0.84555 | -2.22878 | 1.87162 |
| H | -2.10863 | -1.01881 | 1.70152 |
| H | -2.50850 | -2.62950 | 2.27718 |
| C | -2.38890 | -1.54121 | -3.52958 |
| H | -2.96195 | -0.61810 | -3.44238 |
| H | -1.38638 | -1.26426 | -3.85766 |
| H | -2.84616 | -2.15480 | -4.30590 |
| C | -3.11568 | -5.92731 | -1.31973 |
| H | -3.84840 | -6.09091 | -2.11190 |
| H | -2.22630 | -6.51253 | -1.57347 |
| H | -3.51717 | -6.32626 | -0.38719 |
| Cl | -3.04979 | 0.90887 | 0.02587 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.68548 | 0.31836 | 1.04893 |
| C | 0.40885 | 0.05722 | -0.66620 |
| P | -1.11961 | -0.16336 | -1.59247 |
| O | -0.42902 | -0.00202 | -2.97679 |
| Cl | 2.51777 | -0.83105 | -3.21163 |
| Au | 0.65550 | 2.23171 | -0.51523 |
| Cl | 0.73431 | 4.50259 | -0.26653 |
| C | 2.51059 | 0.09287 | 1.21706 |
| C | 3.16106 | -1.08485 | 0.75290 |
| C | 3.31518 | 1.17272 | 1.66464 |
| C | 4.49825 | -0.99465 | 0.39932 |
| C | 4.65306 | 1.19017 | 1.26659 |
| C | 5.24810 | 0.16509 | 0.55477 |
| H | 4.98601 | -1.87733 | 0.00605 |
| H | 5.24989 | 2.04719 | 1.54327 |

| | | | |
|---|----------|----------|----------|
| C | 2.94124 | 2.25286 | 2.70395 |
| C | 2.60539 | -2.52048 | 0.86097 |
| C | 6.67635 | 0.23418 | 0.02761 |
| C | 3.78157 | 1.91431 | 3.95227 |
| H | 3.53382 | 0.92031 | 4.33425 |
| H | 4.85197 | 1.93633 | 3.74305 |
| H | 3.57448 | 2.64448 | 4.73962 |
| C | 3.30750 | 3.66468 | 2.23580 |
| H | 2.75247 | 3.94869 | 1.34156 |
| H | 3.05674 | 4.38086 | 3.02328 |
| H | 4.37382 | 3.77187 | 2.03078 |
| C | 1.48908 | 2.27402 | 3.17222 |
| H | 1.41212 | 2.95914 | 4.02121 |
| H | 0.80260 | 2.63889 | 2.40827 |
| H | 1.15208 | 1.29365 | 3.51881 |
| C | 2.90172 | -3.35583 | -0.38806 |
| H | 2.50663 | -2.88171 | -1.28544 |
| H | 3.97110 | -3.51354 | -0.53583 |
| H | 2.44418 | -4.34390 | -0.28574 |
| C | 3.34654 | -3.15116 | 2.05669 |
| H | 4.42707 | -3.14661 | 1.90621 |
| H | 3.13438 | -2.60572 | 2.97979 |
| H | 3.02302 | -4.18798 | 2.18905 |
| C | 1.11848 | -2.64928 | 1.17336 |
| H | 0.82419 | -2.05275 | 2.04300 |
| H | 0.48850 | -2.37522 | 0.32962 |
| H | 0.90197 | -3.69309 | 1.41870 |
| C | 7.32847 | 1.58683 | 0.30054 |
| H | 6.76135 | 2.40673 | -0.14674 |
| H | 7.43130 | 1.78249 | 1.37109 |
| H | 8.33152 | 1.60180 | -0.13264 |
| C | 6.64976 | 0.00840 | -1.48898 |
| H | 7.66564 | 0.04242 | -1.89284 |
| H | 6.21689 | -0.96070 | -1.74517 |
| H | 6.05678 | 0.77791 | -1.98858 |
| C | 7.53064 | -0.85422 | 0.68804 |
| H | 7.55989 | -0.72472 | 1.77286 |
| H | 7.14824 | -1.85528 | 0.47852 |
| H | 8.55636 | -0.80602 | 0.31171 |
| C | -2.36730 | -1.49681 | -1.68738 |
| C | -2.35683 | -2.33340 | -2.84649 |
| C | -3.57812 | -1.36894 | -0.95377 |
| C | -3.58403 | -2.65362 | -3.40646 |
| C | -1.13646 | -3.05294 | -3.45154 |
| C | -4.75932 | -1.76671 | -1.56912 |
| C | -3.71976 | -0.98136 | 0.52843 |
| C | -4.80450 | -2.31329 | -2.83979 |
| H | -3.58132 | -3.22524 | -4.32471 |
| C | -0.69866 | -2.45906 | -4.79395 |
| C | -1.52579 | -4.52316 | -3.71218 |
| C | 0.01382 | -3.12991 | -2.45598 |
| H | -5.68168 | -1.63401 | -1.02214 |
| C | -2.41473 | -0.59617 | 1.20092 |
| C | -4.21266 | -2.25497 | 1.24415 |
| C | -4.74205 | 0.13624 | 0.75621 |
| C | -6.10534 | -2.62459 | -3.56746 |
| H | 0.10268 | -3.06985 | -5.21804 |
| H | -1.53176 | -2.46342 | -5.50182 |
| H | -0.33757 | -1.43959 | -4.69802 |
| H | -2.21494 | -4.64238 | -4.54890 |
| H | -0.62000 | -5.08000 | -3.96458 |
| H | -1.97239 | -4.98455 | -2.82840 |
| H | 0.40819 | -2.16366 | -2.15391 |
| H | -0.29392 | -3.67453 | -1.55979 |
| H | 0.85036 | -3.66832 | -2.90585 |
| H | -1.64028 | -1.34929 | 1.04165 |

| | | | |
|----|----------|----------|----------|
| H | -2.04370 | 0.37856 | 0.88506 |
| H | -2.56695 | -0.52009 | 2.28007 |
| H | -4.30880 | -2.05251 | 2.31419 |
| H | -5.18353 | -2.58761 | 0.87510 |
| H | -3.50263 | -3.07555 | 1.11543 |
| H | -5.73426 | -0.12608 | 0.38579 |
| H | -4.83382 | 0.32770 | 1.82841 |
| H | -4.43389 | 1.06418 | 0.27431 |
| C | -7.33071 | -2.15779 | -2.78633 |
| C | -6.22121 | -4.13715 | -3.79236 |
| C | -6.09366 | -1.90777 | -4.92314 |
| H | -7.43276 | -2.68214 | -1.83274 |
| H | -7.30067 | -1.08336 | -2.58893 |
| H | -8.23226 | -2.36235 | -3.36820 |
| H | -5.39835 | -4.52369 | -4.39671 |
| H | -6.22315 | -4.67626 | -2.84184 |
| H | -7.15391 | -4.36605 | -4.31475 |
| H | -6.02166 | -0.82535 | -4.79365 |
| H | -5.25399 | -2.22730 | -5.54342 |
| H | -7.01545 | -2.12542 | -5.46908 |
| Cl | -2.35696 | 1.45806 | -1.50700 |
| Si | 1.19989 | 0.61508 | -2.42064 |

[R-P=C(Si(II)Cl)-P(O)MeR](AuCl)

Coordination through Si(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.77632 | -0.24722 | 1.12673 |
| C | 0.47308 | -0.35419 | -0.49894 |
| P | -1.03242 | -0.30820 | -1.39698 |
| Cl | 1.73654 | -2.36604 | -2.54415 |
| Si | 1.36436 | -0.35031 | -2.23004 |
| O | -0.35426 | -0.22164 | -2.79512 |
| H | 2.20179 | -0.26832 | 1.04949 |
| H | -1.79886 | -1.48584 | -1.29275 |
| Au | 2.80107 | 1.26105 | -2.81441 |
| Cl | 4.23783 | 2.96510 | -3.35313 |
| C | -2.16382 | 1.03726 | -1.10499 |
| H | -2.95615 | 1.01586 | -1.85628 |
| H | -2.60140 | 0.93143 | -0.10937 |
| H | -1.61807 | 1.97964 | -1.17083 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.80059 | -0.03016 | 1.03831 |
| C | 0.41483 | -0.23519 | -0.55892 |
| P | -1.13949 | -0.29909 | -1.36303 |
| Cl | 1.67991 | -2.23722 | -2.63814 |
| Si | 1.19721 | -0.23265 | -2.32588 |
| O | -0.53244 | -0.20615 | -2.80486 |
| C | -2.25849 | 1.06238 | -1.06428 |
| H | -3.10364 | 1.00416 | -1.75349 |
| H | -2.62247 | 1.02209 | -0.03543 |
| H | -1.72119 | 1.99790 | -1.22400 |
| C | 2.62884 | 0.00658 | 1.03178 |
| H | 3.02048 | 0.49355 | 0.13572 |
| H | 2.98778 | 0.51863 | 1.92564 |
| H | 2.99840 | -1.02343 | 1.05977 |
| C | -2.04163 | -1.82943 | -1.15786 |
| H | -2.41378 | -1.90705 | -0.13420 |
| H | -2.87982 | -1.86084 | -1.85727 |
| H | -1.36153 | -2.65695 | -1.36451 |
| Au | 2.56413 | 1.40921 | -3.00621 |
| Cl | 3.95121 | 3.13850 | -3.60955 |

R = t-Bu

| | | | |
|---|---------|----------|---------|
| P | 0.76300 | -0.03880 | 0.82836 |
|---|---------|----------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.55116 | -0.43035 | -0.76897 |
| P | -1.00035 | -0.53460 | -1.60277 |
| Cl | 2.02813 | -2.57538 | -2.66434 |
| Si | 1.35726 | -0.61159 | -2.52340 |
| O | -0.35372 | -0.76831 | -3.01632 |
| C | -1.90681 | 1.01209 | -1.61024 |
| H | -2.76036 | 0.95704 | -2.28739 |
| H | -2.24525 | 1.25747 | -0.60253 |
| H | -1.22150 | 1.78749 | -1.95699 |
| Au | 2.53894 | 1.09120 | -3.39371 |
| Cl | 3.69751 | 2.91044 | -4.19545 |
| C | 2.58597 | 0.12180 | 1.17053 |
| C | 3.49208 | -0.63428 | 0.21441 |
| C | 2.86485 | 1.62901 | 1.10090 |
| C | 2.78307 | -0.37446 | 2.60513 |
| H | 3.25175 | -1.69839 | 0.17287 |
| H | 3.44313 | -0.22716 | -0.79840 |
| H | 4.53116 | -0.53597 | 0.54581 |
| H | 2.20152 | 2.20231 | 1.75579 |
| H | 3.89218 | 1.81678 | 1.42971 |
| H | 2.76342 | 2.01002 | 0.08229 |
| H | 3.81490 | -0.18629 | 2.91651 |
| H | 2.12236 | 0.13901 | 3.30921 |
| H | 2.60014 | -1.44895 | 2.68992 |
| C | -2.12178 | -1.91021 | -1.16772 |
| C | -3.20215 | -2.00353 | -2.24817 |
| C | -1.30781 | -3.20327 | -1.13074 |
| C | -2.73843 | -1.62831 | 0.20252 |
| H | -3.84847 | -1.12356 | -2.26743 |
| H | -2.76839 | -2.14170 | -3.24058 |
| H | -3.83489 | -2.86940 | -2.03480 |
| H | -0.52868 | -3.17110 | -0.36750 |
| H | -1.98182 | -4.03124 | -0.89495 |
| H | -0.83320 | -3.41201 | -2.09044 |
| H | -3.34972 | -2.48615 | 0.49526 |
| H | -1.97614 | -1.48772 | 0.97361 |
| H | -3.38829 | -0.75068 | 0.19215 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.93615 | -0.19721 | 0.69149 |
| C | 0.53096 | -0.30173 | -0.91648 |
| P | -1.11197 | -0.39119 | -1.53769 |
| Cl | 1.72020 | -2.40185 | -2.96468 |
| Si | 1.10279 | -0.42302 | -2.75750 |
| O | -0.65893 | -0.55351 | -3.03058 |
| C | -2.06695 | 1.10831 | -1.33495 |
| H | -3.00435 | 1.03260 | -1.88886 |
| H | -2.27286 | 1.28940 | -0.27862 |
| H | -1.47048 | 1.93444 | -1.72560 |
| Au | 2.23100 | 1.21772 | -3.79805 |
| Cl | 3.38096 | 2.94068 | -4.79828 |
| C | -2.11350 | -1.78387 | -1.04101 |
| C | -1.91486 | -3.00802 | -1.67897 |
| C | -3.04191 | -1.67597 | -0.00611 |
| C | -2.65067 | -4.11280 | -1.28456 |
| H | -1.19020 | -3.08871 | -2.48081 |
| C | -3.76868 | -2.78793 | 0.38541 |
| H | -3.20343 | -0.73043 | 0.49851 |
| C | -3.57412 | -4.00390 | -0.25434 |
| H | -2.50160 | -5.06243 | -1.78448 |
| H | -4.49087 | -2.70382 | 1.18877 |
| H | -4.14714 | -4.87165 | 0.05151 |
| C | 2.72431 | -0.10960 | 0.81488 |
| C | 3.22800 | -0.26791 | 2.11157 |
| C | 3.61305 | 0.12977 | -0.23769 |
| C | 4.59147 | -0.21598 | 2.34766 |

| | | | |
|---|---------|----------|----------|
| H | 2.54075 | -0.43621 | 2.93521 |
| C | 4.97195 | 0.19513 | 0.00379 |
| H | 3.24542 | 0.29334 | -1.24528 |
| C | 5.46224 | 0.01553 | 1.29305 |
| H | 4.97396 | -0.34868 | 3.35288 |
| H | 5.65232 | 0.39170 | -0.81641 |
| H | 6.52993 | 0.06487 | 1.47468 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.88169 | 0.37527 | 0.64358 |
| C | 0.57907 | -0.48163 | -0.74454 |
| P | -0.87631 | -0.80595 | -1.70176 |
| Cl | 2.01843 | -3.17841 | -1.63890 |
| Si | 1.58579 | -1.21667 | -2.21148 |
| O | -0.05187 | -1.39207 | -2.90285 |
| C | -1.71930 | 0.65469 | -2.31426 |
| H | -2.42267 | 0.34781 | -3.09149 |
| H | -2.25622 | 1.17219 | -1.52115 |
| H | -0.96672 | 1.31794 | -2.74411 |
| Au | 3.09181 | -0.00599 | -3.35752 |
| Cl | 4.59086 | 1.34263 | -4.47358 |
| C | -2.08405 | -1.97595 | -1.05920 |
| C | -2.31686 | -3.23045 | -1.66684 |
| C | -2.80605 | -1.60333 | 0.09109 |
| C | -3.25376 | -4.07220 | -1.07979 |
| C | -3.72111 | -2.49386 | 0.63378 |
| C | -3.95713 | -3.73761 | 0.06895 |
| H | -3.43611 | -5.03532 | -1.54577 |
| H | -4.26574 | -2.19991 | 1.52580 |
| C | 2.69195 | 0.31237 | 0.80398 |
| C | 3.29460 | -0.75283 | 1.48590 |
| C | 3.45719 | 1.38585 | 0.32728 |
| C | 4.67390 | -0.73953 | 1.64574 |
| C | 4.83263 | 1.35160 | 0.50659 |
| C | 5.46113 | 0.29431 | 1.15323 |
| H | 5.14686 | -1.56317 | 2.17253 |
| H | 5.42973 | 2.17246 | 0.12118 |
| C | 2.48531 | -1.89209 | 2.03000 |
| H | 1.60485 | -1.53870 | 2.57784 |
| H | 2.12775 | -2.54232 | 1.22668 |
| H | 3.07966 | -2.49911 | 2.71413 |
| C | 2.82200 | 2.53409 | -0.39539 |
| H | 2.59587 | 2.26106 | -1.43138 |
| H | 1.88468 | 2.84637 | 0.07943 |
| H | 3.48763 | 3.39730 | -0.42318 |
| C | 6.95146 | 0.26378 | 1.29549 |
| H | 7.41646 | -0.09122 | 0.37073 |
| H | 7.35270 | 1.25886 | 1.49772 |
| H | 7.26269 | -0.40399 | 2.10036 |
| C | -2.67495 | -0.26351 | 0.75559 |
| H | -1.67841 | 0.17490 | 0.67929 |
| H | -3.38953 | 0.45030 | 0.33372 |
| H | -2.89820 | -0.34712 | 1.81984 |
| C | -1.63596 | -3.73031 | -2.90841 |
| H | -1.71733 | -3.03104 | -3.74039 |
| H | -0.57076 | -3.89907 | -2.74391 |
| H | -2.08768 | -4.67498 | -3.21104 |
| C | -4.92192 | -4.69935 | 0.68743 |
| H | -5.43217 | -5.29435 | -0.07195 |
| H | -4.39625 | -5.39599 | 1.34784 |
| H | -5.67346 | -4.18264 | 1.28603 |

R = Mes*

| | | | |
|---|----------|----------|---------|
| P | -0.54787 | 1.62204 | 1.53692 |
| C | 0.11914 | 0.55453 | 0.44723 |
| P | 1.71358 | -0.21546 | 0.25686 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| Cl | -0.93069 | 0.50772 | -2.66550 | H | 1.73506 | 0.52865 | 2.82532 |
| O | 1.28793 | -0.87375 | -1.11675 | H | 2.41139 | 1.77806 | 3.82922 |
| C | 1.83872 | -1.64882 | 1.34508 | C | 4.84777 | 1.96978 | 2.96678 |
| H | 2.64556 | -2.27896 | 0.96586 | H | 4.63015 | 2.37086 | 3.96035 |
| H | 2.01972 | -1.40972 | 2.38746 | H | 5.90245 | 1.69497 | 2.93765 |
| H | 0.89054 | -2.18399 | 1.25006 | H | 4.68503 | 2.76462 | 2.23525 |
| C | 3.41877 | 0.41507 | 0.12335 | C | 4.20493 | -0.30365 | 3.74546 |
| C | 4.01638 | 0.51114 | -1.16675 | H | 5.24964 | -0.61861 | 3.73789 |
| C | 4.26821 | 0.30766 | 1.25608 | H | 3.99205 | 0.09935 | 4.73888 |
| C | 5.33702 | 0.10225 | -1.28770 | H | 3.59357 | -1.19715 | 3.61149 |
| C | 5.59078 | -0.06931 | 1.04986 | C | 2.21351 | 2.07581 | -2.02557 |
| C | 6.12512 | -0.28233 | -0.21074 | H | 1.84199 | 2.58437 | -2.91805 |
| H | 5.77693 | 0.10499 | -2.27617 | H | 1.36210 | 1.54725 | -1.60770 |
| H | 6.22693 | -0.18768 | 1.91607 | H | 2.53207 | 2.83974 | -1.31115 |
| C | -2.30917 | 1.59170 | 1.03372 | C | 2.99298 | 0.15987 | -3.48488 |
| C | -2.79241 | 2.53375 | 0.10004 | H | 2.21084 | -0.51552 | -3.14967 |
| C | -3.15065 | 0.54678 | 1.49515 | H | 2.63458 | 0.69002 | -4.37122 |
| C | -3.98812 | 2.23986 | -0.55286 | H | 3.85979 | -0.43683 | -3.78125 |
| C | -4.31879 | 0.31166 | 0.78357 | C | 4.43284 | 2.12150 | -3.02231 |
| C | -4.72489 | 1.09684 | -0.28881 | H | 4.84200 | 2.80821 | -2.27750 |
| H | -4.34749 | 2.92302 | -1.30586 | H | 5.26153 | 1.59321 | -3.49508 |
| H | -4.93692 | -0.52662 | 1.06787 | H | 3.94757 | 2.71533 | -3.80067 |
| C | -2.12906 | 3.90618 | -0.14088 | C | 8.22558 | -1.19781 | 0.86670 |
| C | -2.94578 | -0.18565 | 2.83952 | H | 8.37635 | -0.33565 | 1.52144 |
| C | -5.96124 | 0.70338 | -1.08985 | H | 7.65997 | -1.95472 | 1.41597 |
| C | 3.92365 | 0.76657 | 2.68654 | H | 9.21079 | -1.61548 | 0.64748 |
| C | 3.38430 | 1.17352 | -2.40552 | C | 8.38216 | 0.26104 | -1.13500 |
| C | 7.53542 | -0.81123 | -0.43864 | H | 7.96753 | 0.54058 | -2.10536 |
| C | -4.02943 | -1.23957 | 3.08396 | H | 8.44967 | 1.16506 | -0.52485 |
| H | -3.86020 | -1.69424 | 4.06277 | H | 9.39579 | -0.11323 | -1.30147 |
| H | -5.03053 | -0.80372 | 3.10036 | C | 7.45739 | -2.05597 | -1.33094 |
| H | -3.99992 | -2.03835 | 2.33818 | H | 6.87054 | -2.84467 | -0.85402 |
| C | -3.06835 | 0.87606 | 3.94400 | H | 6.99842 | -1.83468 | -2.29644 |
| H | -2.28579 | 1.63583 | 3.86200 | H | 8.46138 | -2.44560 | -1.51878 |
| H | -4.03455 | 1.38342 | 3.89315 | Au | -1.80941 | -2.36449 | -0.51742 |
| H | -2.97909 | 0.40582 | 4.92772 | Cl | -3.25039 | -4.07732 | 0.07719 |
| C | -1.60514 | -0.90464 | 3.00934 | Si | -0.46820 | -0.60837 | -0.97211 |
| H | -1.39642 | -1.56711 | 2.16678 | | | | |
| H | -0.76672 | -0.21191 | 3.12786 | | | | |
| H | -1.63974 | -1.50734 | 3.92102 | | | | |
| C | -7.17856 | 0.61090 | -0.16238 | | | | |
| H | -8.06547 | 0.33017 | -0.73716 | | | | |
| H | -7.04034 | -0.14018 | 0.61742 | | | | |
| H | -7.37673 | 1.57035 | 0.32272 | | | | |
| C | -6.27913 | 1.70720 | -2.19478 | | | | |
| H | -7.15627 | 1.36838 | -2.75126 | | | | |
| H | -6.50637 | 2.69916 | -1.79451 | | | | |
| H | -5.45439 | 1.80146 | -2.90559 | | | | |
| C | -5.70857 | -0.66473 | -1.73639 | | | | |
| H | -4.85785 | -0.62125 | -2.42059 | | | | |
| H | -5.49314 | -1.43668 | -0.99514 | | | | |
| H | -6.58871 | -0.97855 | -2.30499 | | | | |
| C | -3.00294 | 4.80999 | -1.01497 | | | | |
| H | -4.00242 | 4.94565 | -0.59616 | | | | |
| H | -2.53390 | 5.79460 | -1.07952 | | | | |
| H | -3.10109 | 4.42846 | -2.03390 | | | | |
| C | -1.97080 | 4.61840 | 1.20962 | | | | |
| H | -2.93683 | 4.72868 | 1.70771 | | | | |
| H | -1.30404 | 4.07994 | 1.88825 | | | | |
| H | -1.54601 | 5.61505 | 1.05898 | | | | |
| C | -0.76531 | 3.82107 | -0.83123 | | | | |
| H | -0.00181 | 3.36216 | -0.20015 | | | | |
| H | -0.82124 | 3.24333 | -1.75489 | | | | |
| H | -0.41614 | 4.82978 | -1.07117 | | | | |
| C | 2.50625 | 1.29790 | 2.85262 | | | | |
| H | 2.27014 | 2.05417 | 2.10076 | | | | |

| Coordination through O atom | | | |
|-----------------------------|----------|----------|----------|
| R = H | | | |
| P | 0.66476 | -0.20823 | 1.17026 |
| C | 0.42206 | -0.32631 | -0.46596 |
| P | -1.04642 | -0.14557 | -1.38115 |
| Cl | 1.23265 | -2.50103 | -2.44499 |
| Si | 1.51237 | -0.41935 | -2.12395 |
| O | -0.34044 | 0.11039 | -2.75288 |
| H | 2.08225 | -0.40387 | 1.16541 |
| H | -1.78134 | -1.34331 | -1.43844 |
| Au | -1.45558 | 0.31553 | -4.53488 |
| Cl | -2.69771 | 0.55381 | -6.35902 |
| C | -2.21451 | 1.13390 | -0.96080 |
| H | -3.01271 | 1.15892 | -1.70602 |
| H | -2.63661 | 0.91374 | 0.02341 |
| H | -1.70167 | 2.09616 | -0.93469 |

| R = Me | | | |
|--------|----------|----------|----------|
| P | 0.73750 | 0.04541 | 1.01710 |
| C | 0.42074 | -0.22652 | -0.58646 |
| P | -1.11673 | -0.23587 | -1.39784 |
| Cl | 1.45825 | -2.47678 | -2.43161 |
| Si | 1.39273 | -0.34591 | -2.30303 |
| O | -0.49768 | -0.14628 | -2.84527 |
| C | -2.22760 | 1.13556 | -1.11144 |
| H | -3.07756 | 1.07155 | -1.79463 |
| H | -2.58204 | 1.10237 | -0.07849 |

| | | | |
|----|----------|----------|----------|
| H | -1.69094 | 2.06944 | -1.28130 |
| C | 2.55995 | -0.13128 | 1.12440 |
| H | 3.05770 | 0.20822 | 0.21334 |
| H | 2.93403 | 0.42603 | 1.98455 |
| H | 2.79963 | -1.18817 | 1.27616 |
| C | -2.03262 | -1.75689 | -1.20553 |
| H | -2.40762 | -1.82809 | -0.18208 |
| H | -2.86718 | -1.77423 | -1.91029 |
| H | -1.35697 | -2.58846 | -1.41081 |
| Au | -1.68137 | -0.16862 | -4.58965 |
| Cl | -2.99755 | -0.17541 | -6.37895 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.80650 | -0.34616 | 0.84989 |
| C | 0.42923 | -0.23448 | -0.76387 |
| P | -1.20940 | -0.30006 | -1.38588 |
| Cl | 1.81631 | -1.66666 | -3.17556 |
| Si | 1.13785 | 0.25972 | -2.55165 |
| O | -0.78421 | -0.03453 | -2.88503 |
| C | -2.25468 | 1.04504 | -0.82437 |
| H | -3.18714 | 1.07169 | -1.39037 |
| H | -2.46351 | 0.93403 | 0.24107 |
| H | -1.71053 | 1.97658 | -0.98681 |
| Au | -2.03134 | 0.59854 | -4.46316 |
| Cl | -3.37892 | 1.26771 | -6.09895 |
| C | 2.66249 | -0.26451 | 1.03258 |
| C | 3.11251 | -1.71265 | 1.25473 |
| C | 3.39687 | 0.34694 | -0.14672 |
| C | 2.91572 | 0.55287 | 2.30207 |
| H | 2.57799 | -2.18570 | 2.08386 |
| H | 2.96431 | -2.31816 | 0.35781 |
| H | 4.17963 | -1.72603 | 1.50109 |
| H | 3.04011 | 1.35333 | -0.37659 |
| H | 4.46586 | 0.41826 | 0.08211 |
| H | 3.30614 | -0.27004 | -1.04423 |
| H | 3.98315 | 0.53569 | 2.54237 |
| H | 2.61845 | 1.59722 | 2.17586 |
| H | 2.37293 | 0.14869 | 3.16095 |
| C | -2.10954 | -1.88671 | -1.21967 |
| C | -3.41392 | -1.81702 | -2.01723 |
| C | -1.22248 | -3.00649 | -1.76203 |
| C | -2.40575 | -2.11284 | 0.26415 |
| H | -4.10344 | -1.06700 | -1.62509 |
| H | -3.24216 | -1.60806 | -3.07551 |
| H | -3.91095 | -2.78850 | -1.94559 |
| H | -0.28092 | -3.08347 | -1.21640 |
| H | -1.75933 | -3.95300 | -1.65550 |
| H | -0.98852 | -2.86354 | -2.81756 |
| H | -2.88177 | -3.09085 | 0.37441 |
| H | -1.49770 | -2.11544 | 0.87209 |
| H | -3.09337 | -1.36682 | 0.66854 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.86202 | -0.43387 | 1.07052 |
| C | 0.41336 | -0.37308 | -0.53141 |
| P | -1.22288 | -0.28649 | -1.11301 |
| Cl | 1.38649 | -1.70789 | -3.19999 |
| Si | 1.12269 | 0.20497 | -2.27999 |
| O | -0.82224 | 0.30533 | -2.52424 |
| C | -2.33176 | 0.85155 | -0.28983 |
| H | -3.27406 | 0.92907 | -0.83525 |
| H | -2.52427 | 0.48982 | 0.72258 |
| H | -1.85529 | 1.83178 | -0.24868 |
| Au | -2.22651 | 0.88335 | -3.98196 |
| Cl | -3.77311 | 1.49387 | -5.45818 |
| C | 2.66220 | -0.44483 | 1.06251 |

| | | | |
|---|----------|----------|----------|
| C | 3.28163 | -0.03689 | 2.24898 |
| C | 3.45628 | -0.82952 | -0.02248 |
| C | 4.66186 | 0.02415 | 2.33663 |
| H | 2.67132 | 0.24443 | 3.10184 |
| C | 4.83592 | -0.77406 | 0.07131 |
| H | 2.99597 | -1.21117 | -0.92712 |
| C | 5.43869 | -0.34133 | 1.24585 |
| H | 5.13308 | 0.35240 | 3.25575 |
| H | 5.44452 | -1.07556 | -0.77324 |
| H | 6.51984 | -0.30029 | 1.31420 |
| C | -2.05077 | -1.86255 | -1.26844 |
| C | -3.35725 | -1.91449 | -1.75950 |
| C | -1.38345 | -3.03833 | -0.93285 |
| C | -3.98728 | -3.13749 | -1.90678 |
| H | -3.87668 | -1.00900 | -2.05373 |
| C | -2.02501 | -4.25783 | -1.07595 |
| H | -0.36359 | -2.99568 | -0.57125 |
| C | -3.32324 | -4.30687 | -1.56088 |
| H | -4.99672 | -3.17729 | -2.29804 |
| H | -1.50522 | -5.17205 | -0.81547 |
| H | -3.82069 | -5.26296 | -1.67697 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.09250 | -1.00675 | 1.31746 |
| C | 0.43175 | -0.85324 | -0.19863 |
| P | -1.26966 | -0.77431 | -0.61907 |
| Cl | 1.08389 | -1.46917 | -3.16032 |
| Si | 0.96419 | 0.17787 | -1.78574 |
| O | -1.02565 | 0.29058 | -1.77344 |
| C | -2.27387 | -0.09074 | 0.70097 |
| H | -3.30483 | 0.06314 | 0.38719 |
| H | -2.25008 | -0.80423 | 1.52971 |
| H | -1.84017 | 0.85641 | 1.02406 |
| Au | -1.71464 | 2.30091 | -1.79244 |
| Cl | -2.45435 | 4.39807 | -1.80076 |
| C | 2.83593 | -0.53048 | 1.07370 |
| C | 3.25389 | 0.71284 | 1.57254 |
| C | 3.76322 | -1.41241 | 0.50048 |
| C | 4.59237 | 1.06358 | 1.46577 |
| C | 5.09340 | -1.02020 | 0.42087 |
| C | 5.52790 | 0.21372 | 0.88880 |
| H | 4.91255 | 2.02950 | 1.84542 |
| H | 5.81399 | -1.70526 | -0.01635 |
| C | -2.13190 | -2.21598 | -1.27735 |
| C | -3.37265 | -2.00034 | -1.91449 |
| C | -1.62454 | -3.52755 | -1.15522 |
| C | -4.06320 | -3.09402 | -2.42152 |
| C | -2.36881 | -4.57783 | -1.67304 |
| C | -3.58461 | -4.38924 | -2.31506 |
| H | -5.01046 | -2.91661 | -2.92145 |
| H | -1.97251 | -5.58364 | -1.57736 |
| C | 2.27440 | 1.67517 | 2.17455 |
| H | 1.65664 | 2.14179 | 1.40083 |
| H | 1.59456 | 1.17885 | 2.87588 |
| H | 2.78763 | 2.47185 | 2.71437 |
| C | 6.96175 | 0.62539 | 0.75687 |
| H | 7.12096 | 1.17131 | -0.17833 |
| H | 7.26458 | 1.28325 | 1.57352 |
| H | 7.62623 | -0.24027 | 0.74721 |
| C | 3.35674 | -2.75768 | -0.02318 |
| H | 2.67298 | -3.27072 | 0.65989 |
| H | 2.84673 | -2.66893 | -0.98699 |
| H | 4.22921 | -3.39667 | -0.16572 |
| C | -0.31775 | -3.87144 | -0.50779 |
| H | 0.51425 | -3.37657 | -1.01009 |
| H | -0.28588 | -3.58018 | 0.54402 |

| | | | |
|---|----------|----------|----------|
| H | -0.15492 | -4.94810 | -0.56011 |
| C | -4.03797 | -0.66234 | -2.07621 |
| H | -3.35154 | 0.18171 | -2.11419 |
| H | -4.61139 | -0.64668 | -3.00377 |
| H | -4.74948 | -0.48353 | -1.26363 |
| C | -4.33393 | -5.54420 | -2.90014 |
| H | -3.94404 | -5.78794 | -3.89324 |
| H | -4.23158 | -6.43842 | -2.28263 |
| H | -5.39535 | -5.31779 | -3.00970 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 2.05797 | 1.94983 | -0.47768 |
| C | 1.05099 | 0.63354 | -0.34499 |
| P | -0.69688 | 0.47391 | -0.50853 |
| C | 3.71769 | 1.16036 | -0.34934 |
| C | 4.41265 | 1.23405 | 0.89063 |
| C | 4.24225 | 0.37337 | -1.39406 |
| C | 5.44252 | 0.33460 | 1.10939 |
| C | 5.27613 | -0.51627 | -1.08799 |
| C | 5.85065 | -0.60198 | 0.16314 |
| H | 5.95077 | 0.34817 | 2.06221 |
| H | 5.64237 | -1.15929 | -1.87594 |
| C | 3.90483 | 0.47630 | -2.89685 |
| C | 4.12483 | 2.30215 | 1.96426 |
| C | 6.92105 | -1.62754 | 0.51962 |
| C | 2.76220 | 2.11011 | 2.63504 |
| H | 1.92940 | 2.30150 | 1.95515 |
| H | 2.64752 | 1.09297 | 3.01419 |
| H | 2.66073 | 2.81033 | 3.46957 |
| C | 4.20379 | 3.69624 | 1.32691 |
| H | 5.18843 | 3.86385 | 0.88373 |
| H | 3.45376 | 3.84454 | 0.54716 |
| H | 4.03732 | 4.46304 | 2.08880 |
| C | 5.16740 | 2.27785 | 3.08568 |
| H | 5.12381 | 1.35643 | 3.67102 |
| H | 6.18403 | 2.40405 | 2.70628 |
| H | 4.96405 | 3.10566 | 3.76883 |
| C | 3.44612 | -0.87325 | -3.45876 |
| H | 2.54852 | -1.23010 | -2.94834 |
| H | 3.22576 | -0.77591 | -4.52573 |
| H | 4.21114 | -1.64370 | -3.35006 |
| C | 2.86075 | 1.52394 | -3.27352 |
| H | 1.85028 | 1.22968 | -2.99148 |
| H | 3.08084 | 2.50443 | -2.83868 |
| H | 2.86513 | 1.65202 | -4.35990 |
| C | 5.19920 | 0.90357 | -3.61437 |
| H | 5.54012 | 1.87785 | -3.25464 |
| H | 6.01002 | 0.19044 | -3.46504 |
| H | 5.01559 | 0.98157 | -4.68961 |
| C | 7.22429 | -2.57416 | -0.63852 |
| H | 7.62945 | -2.04402 | -1.50451 |
| H | 7.97188 | -3.30635 | -0.32415 |
| H | 6.33487 | -3.12471 | -0.95481 |
| C | 6.42852 | -2.46398 | 1.70711 |
| H | 6.24000 | -1.84488 | 2.58642 |
| H | 5.49923 | -2.98304 | 1.46151 |
| H | 7.17945 | -3.21155 | 1.97785 |
| C | 8.21853 | -0.90867 | 0.90702 |
| H | 8.07656 | -0.24833 | 1.76492 |
| H | 8.98785 | -1.63894 | 1.17315 |
| H | 8.59465 | -0.30529 | 0.07695 |
| C | -2.13555 | 1.32394 | 0.20192 |
| C | -2.73750 | 0.75489 | 1.36089 |
| C | -2.93652 | 2.12579 | -0.65260 |
| C | -4.12092 | 0.65712 | 1.37389 |
| C | -4.31659 | 1.99782 | -0.55879 |

| | | | |
|----|----------|----------|----------|
| C | -4.93374 | 1.17544 | 0.37388 |
| H | -4.58452 | 0.15416 | 2.21287 |
| H | -4.93061 | 2.57196 | -1.23935 |
| C | -2.00359 | 0.40492 | 2.66810 |
| C | -2.03581 | -1.08745 | 3.00375 |
| C | -2.73472 | 1.16207 | 3.79588 |
| H | -1.41973 | -1.67054 | 2.32145 |
| H | -1.65036 | -1.24073 | 4.01538 |
| H | -3.05315 | -1.48329 | 2.96823 |
| H | -2.80055 | 2.23122 | 3.57983 |
| H | -3.74335 | 0.78749 | 3.97254 |
| H | -2.17186 | 1.03650 | 4.72425 |
| C | -2.41279 | 3.27594 | -1.53415 |
| C | -3.03547 | 4.56025 | -0.94793 |
| C | -2.85479 | 3.16468 | -2.99596 |
| H | -2.76082 | 4.68280 | 0.10223 |
| H | -2.66518 | 5.42766 | -1.50118 |
| H | -4.12361 | 4.55801 | -1.01440 |
| H | -2.44990 | 2.28166 | -3.49075 |
| H | -3.94169 | 3.11917 | -3.08399 |
| H | -2.51688 | 4.04402 | -3.55057 |
| C | -6.43256 | 0.91024 | 0.38802 |
| C | -7.04820 | 1.49994 | 1.66276 |
| C | -6.66113 | -0.60641 | 0.36398 |
| H | -6.89659 | 2.58139 | 1.71050 |
| H | -8.12396 | 1.30586 | 1.68056 |
| H | -6.61678 | 1.05871 | 2.56334 |
| H | -6.22175 | -1.06425 | -0.52475 |
| H | -6.22013 | -1.09870 | 1.23248 |
| H | -7.73340 | -0.81985 | 0.36706 |
| Cl | 1.84433 | -1.60238 | 1.77940 |
| O | -0.68593 | -1.01531 | 0.05972 |
| Au | -2.26854 | -2.36218 | -0.35500 |
| Cl | -3.95834 | -3.74426 | -0.80804 |
| C | -0.90449 | 3.48864 | -1.45070 |
| H | -0.56895 | 3.57308 | -0.41472 |
| H | -0.30993 | 2.71575 | -1.93595 |
| H | -0.64460 | 4.42347 | -1.95311 |
| C | -0.57160 | 0.92336 | 2.68802 |
| H | 0.08944 | 0.40173 | 2.00039 |
| H | -0.53828 | 1.99442 | 2.47130 |
| H | -0.14732 | 0.77018 | 3.68318 |
| C | -7.13762 | 1.52473 | -0.81819 |
| H | -7.07221 | 2.61619 | -0.82184 |
| H | -6.72905 | 1.14864 | -1.75943 |
| H | -8.19769 | 1.26300 | -0.79050 |
| C | -1.06784 | 0.22128 | -2.26015 |
| H | -2.10765 | -0.09096 | -2.36957 |
| H | -0.86902 | 1.09098 | -2.87881 |
| H | -0.41524 | -0.59731 | -2.57585 |
| Si | 1.24843 | -1.33114 | -0.24689 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.52080 | 0.09607 | 1.12056 |
| C | 0.31683 | -0.25053 | -0.46524 |
| P | -1.12466 | -0.26803 | -1.44637 |
| Cl | 1.30083 | -2.61348 | -2.16580 |
| Si | 1.34907 | -0.47598 | -2.18798 |
| O | -0.41220 | -0.20463 | -2.81415 |
| H | 1.90287 | -0.03317 | 1.37824 |
| H | -1.80225 | -1.49011 | -1.27632 |
| Au | -0.93798 | 0.68391 | 2.66256 |
| Cl | -2.49413 | 1.29589 | 4.17703 |
| C | -2.35559 | 1.00400 | -1.23253 |
| H | -2.80502 | 0.90924 | -0.24055 |

| | | | |
|---|----------|---------|----------|
| H | -1.88523 | 1.98312 | -1.33055 |
| H | -3.12828 | 0.88794 | -1.99586 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.82918 | 0.00873 | 0.94003 |
| C | 0.39670 | -0.23576 | -0.61622 |
| P | -1.18321 | -0.27650 | -1.35940 |
| Cl | 1.34077 | -2.46986 | -2.53786 |
| Si | 1.15781 | -0.32684 | -2.47059 |
| O | -0.67038 | -0.20607 | -2.82336 |
| C | -2.28874 | 1.08064 | -0.99246 |
| H | -3.17497 | 1.00870 | -1.62701 |
| H | -2.58710 | 1.04300 | 0.05783 |
| H | -1.77527 | 2.02179 | -1.19127 |
| C | 2.62266 | -0.10691 | 1.13138 |
| H | 3.11056 | -0.07939 | 0.15677 |
| H | 2.97364 | 0.71209 | 1.76150 |
| H | 2.86322 | -1.04747 | 1.63389 |
| C | -2.04758 | -1.80621 | -1.03330 |
| H | -2.34234 | -1.84689 | 0.01764 |
| H | -2.93444 | -1.86574 | -1.66798 |
| H | -1.37311 | -2.63178 | -1.26460 |
| Au | -0.51342 | 0.39698 | 2.65179 |
| Cl | -1.96349 | 0.78708 | 4.34374 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.81316 | 0.08370 | 0.86464 |
| C | 0.47748 | -0.38505 | -0.67373 |
| P | -1.08177 | -0.52828 | -1.46909 |
| Cl | 1.91785 | -2.56672 | -2.51193 |
| Si | 1.29247 | -0.51764 | -2.49714 |
| O | -0.49917 | -0.72602 | -2.90273 |
| C | -2.07039 | 0.96744 | -1.40086 |
| H | -2.97115 | 0.86162 | -2.00749 |
| H | -2.34288 | 1.19548 | -0.36870 |
| H | -1.46271 | 1.78143 | -1.79875 |
| Au | -0.66543 | 0.77376 | 2.36842 |
| Cl | -2.24204 | 1.49165 | 3.83140 |
| C | 2.62677 | 0.01955 | 1.23731 |
| C | 2.83485 | 0.54899 | 2.65335 |
| C | 3.08453 | -1.43716 | 1.14039 |
| C | 3.37323 | 0.89095 | 0.22915 |
| H | 2.50427 | 1.58517 | 2.75553 |
| H | 2.30136 | -0.04971 | 3.39533 |
| H | 3.90123 | 0.50992 | 2.89291 |
| H | 2.93676 | -1.84522 | 0.13939 |
| H | 4.15205 | -1.48666 | 1.37764 |
| H | 2.55586 | -2.07426 | 1.85408 |
| H | 4.44566 | 0.83628 | 0.44040 |
| H | 3.22082 | 0.56019 | -0.80122 |
| H | 3.07062 | 1.93844 | 0.29855 |
| C | -2.12266 | -1.95989 | -0.99524 |
| C | -1.24212 | -3.20242 | -0.87865 |
| C | -2.82349 | -1.67829 | 0.33214 |
| C | -3.14747 | -2.15305 | -2.11776 |
| H | -0.70691 | -3.41371 | -1.80494 |
| H | -0.50591 | -3.10308 | -0.07942 |
| H | -1.88197 | -4.05849 | -0.64722 |
| H | -3.51603 | -0.83673 | 0.27128 |
| H | -3.40313 | -2.56175 | 0.61327 |
| H | -2.11607 | -1.48115 | 1.14136 |
| H | -3.74757 | -3.03749 | -1.88709 |
| H | -3.83359 | -1.30776 | -2.20579 |
| H | -2.66310 | -2.31359 | -3.08236 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.81940 | -0.13983 | 0.99360 |
| C | 0.42602 | -0.20031 | -0.59811 |
| P | -1.17527 | -0.21895 | -1.30536 |
| Cl | 1.64605 | -1.88500 | -2.97264 |
| Si | 1.12525 | 0.12909 | -2.43115 |
| O | -0.70303 | 0.04074 | -2.76307 |
| C | -2.29129 | 1.06512 | -0.75043 |
| H | -3.19149 | 1.04847 | -1.36807 |
| H | -2.56286 | 0.91150 | 0.29599 |
| H | -1.78767 | 2.02738 | -0.85260 |
| Au | -0.61829 | 0.03786 | 2.67204 |
| Cl | -2.20266 | 0.19504 | 4.28472 |
| C | -2.02087 | -1.78819 | -1.17697 |
| C | -2.72546 | -2.12232 | -0.01990 |
| C | -1.94813 | -2.68440 | -2.24067 |
| C | -3.35848 | -3.35019 | 0.06594 |
| H | -2.77646 | -1.43864 | 0.82119 |
| C | -2.58998 | -3.90920 | -2.14640 |
| H | -1.38841 | -2.42046 | -3.12953 |
| C | -3.29239 | -4.24097 | -0.99743 |
| H | -3.90328 | -3.61097 | 0.96542 |
| H | -2.53657 | -4.60733 | -2.97336 |
| H | -3.79058 | -5.20117 | -0.92714 |
| C | 2.57554 | -0.20944 | 1.26677 |
| C | 3.46890 | -0.59846 | 0.26451 |
| C | 3.05532 | 0.14947 | 2.52919 |
| C | 4.82722 | -0.60636 | 0.52534 |
| H | 3.10075 | -0.92246 | -0.70184 |
| C | 4.41599 | 0.13958 | 2.77974 |
| H | 2.35707 | 0.43999 | 3.30760 |
| C | 5.30083 | -0.23478 | 1.77758 |
| H | 5.51952 | -0.91149 | -0.25034 |
| H | 4.78676 | 0.42226 | 3.75780 |
| H | 6.36657 | -0.24574 | 1.97565 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.81724 | -0.24990 | 1.54774 |
| C | 0.31489 | -0.39943 | -0.00462 |
| P | -1.22637 | -0.29338 | -0.84164 |
| Cl | 1.47166 | -1.77354 | -2.57772 |
| Si | 1.19284 | 0.18326 | -1.70544 |
| O | -0.61233 | 0.39173 | -2.09718 |
| C | -2.45031 | 0.80408 | -0.12109 |
| H | -3.24697 | 0.95922 | -0.85221 |
| H | -2.87840 | 0.37524 | 0.78571 |
| H | -1.97531 | 1.75737 | 0.11442 |
| Au | -0.38219 | -0.05373 | 3.40107 |
| Cl | -1.64133 | 0.17738 | 5.27133 |
| C | -2.03891 | -1.85276 | -1.24310 |
| C | -2.31001 | -2.77794 | -0.21722 |
| C | -2.44983 | -2.12598 | -2.56660 |
| C | -2.96037 | -3.96338 | -0.53060 |
| C | -3.09602 | -3.33050 | -2.81546 |
| C | -3.35295 | -4.26703 | -1.82473 |
| H | -3.16794 | -4.66705 | 0.26952 |
| H | -3.41613 | -3.53774 | -3.83173 |
| C | 2.61407 | -0.17755 | 1.59096 |
| C | 3.36441 | -1.35052 | 1.41811 |
| C | 3.23996 | 1.05450 | 1.83617 |
| C | 4.74767 | -1.26006 | 1.49554 |
| C | 4.62503 | 1.08973 | 1.89916 |
| C | 5.39616 | -0.05498 | 1.73560 |
| H | 5.33646 | -2.16265 | 1.36367 |
| H | 5.11579 | 2.04183 | 2.07654 |
| C | -1.91235 | -2.56700 | 1.21156 |

| | | | |
|---|----------|----------|----------|
| H | -0.85639 | -2.80536 | 1.36264 |
| H | -2.05923 | -1.54424 | 1.56284 |
| H | -2.49396 | -3.21495 | 1.86763 |
| C | -2.24709 | -1.20999 | -3.73934 |
| H | -2.57863 | -0.18973 | -3.54459 |
| H | -1.19274 | -1.14976 | -4.01326 |
| H | -2.80481 | -1.59070 | -4.59530 |
| C | -4.02004 | -5.56698 | -2.14702 |
| H | -4.72506 | -5.45921 | -2.97306 |
| H | -3.27745 | -6.31298 | -2.44688 |
| H | -4.55529 | -5.96592 | -1.28397 |
| C | 6.88834 | 0.00509 | 1.84257 |
| H | 7.20492 | -0.11542 | 2.88341 |
| H | 7.36143 | -0.78843 | 1.26203 |
| H | 7.27380 | 0.96456 | 1.49345 |
| C | 2.71895 | -2.67722 | 1.15287 |
| H | 1.91199 | -2.88209 | 1.86353 |
| H | 2.28939 | -2.71459 | 0.14784 |
| H | 3.44858 | -3.48290 | 1.23898 |
| C | 2.44790 | 2.31706 | 1.98798 |
| H | 1.94124 | 2.57471 | 1.05266 |
| H | 1.68056 | 2.22378 | 2.76329 |
| H | 3.09451 | 3.15230 | 2.25780 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.19686 | 0.73093 | 0.04173 |
| C | -0.20913 | -0.49676 | 0.50350 |
| P | 1.48836 | -0.84662 | 0.87492 |
| Cl | -1.17471 | -3.34440 | -0.71975 |
| O | 1.26194 | -2.39433 | 0.86411 |
| C | 3.10251 | -0.52324 | 0.08483 |
| C | 3.64058 | -1.55560 | -0.73465 |
| C | 3.99925 | 0.40148 | 0.68158 |
| C | 4.98979 | -1.84709 | -0.59311 |
| C | 5.34199 | 0.04868 | 0.76432 |
| C | 5.84881 | -1.12187 | 0.22212 |
| H | 5.38894 | -2.67690 | -1.16200 |
| H | 6.01603 | 0.73284 | 1.26106 |
| C | -2.89266 | 0.07419 | 0.11071 |
| C | -3.51175 | -0.41369 | -1.07262 |
| C | -3.49316 | -0.15421 | 1.37319 |
| C | -4.58075 | -1.28854 | -0.92348 |
| C | -4.55427 | -1.05282 | 1.42547 |
| C | -5.08068 | -1.67752 | 0.31027 |
| H | -5.03236 | -1.70231 | -1.80935 |
| H | -4.98740 | -1.27137 | 2.39287 |
| C | -3.14658 | 0.03645 | -2.50214 |
| C | -3.19620 | 0.55626 | 2.71315 |
| C | -6.18370 | -2.71903 | 0.46493 |
| C | 3.66326 | 1.85223 | 1.07159 |
| C | 2.89925 | -2.27613 | -1.87397 |
| C | 7.29413 | -1.56708 | 0.40640 |
| C | -4.49366 | 1.26604 | 3.14423 |
| H | -4.33117 | 1.77633 | 4.09745 |
| H | -4.79172 | 2.01387 | 2.40519 |
| H | -5.32594 | 0.57457 | 3.27511 |
| C | -2.13129 | 1.64838 | 2.68131 |
| H | -1.12091 | 1.25629 | 2.56190 |
| H | -2.31981 | 2.39305 | 1.90342 |
| H | -2.14923 | 2.18003 | 3.63683 |
| C | -2.79812 | -0.46169 | 3.78766 |
| H | -3.58950 | -1.18845 | 3.97830 |
| H | -1.90890 | -1.02194 | 3.48933 |
| H | -2.59047 | 0.05575 | 4.72862 |
| C | -7.40160 | -2.08655 | 1.14805 |
| H | -8.19363 | -2.83109 | 1.26692 |

| | | | |
|----|----------|----------|----------|
| H | -7.15757 | -1.70122 | 2.14012 |
| H | -7.79856 | -1.25929 | 0.55442 |
| C | -6.63131 | -3.29415 | -0.87629 |
| H | -7.40305 | -4.04902 | -0.70792 |
| H | -7.05898 | -2.52763 | -1.52779 |
| H | -5.80630 | -3.77709 | -1.40554 |
| C | -5.65390 | -3.87023 | 1.32887 |
| H | -4.77945 | -4.33434 | 0.86702 |
| H | -5.36170 | -3.52766 | 2.32360 |
| H | -6.42628 | -4.63482 | 1.45074 |
| C | -3.98508 | -0.68281 | -3.56421 |
| H | -5.05463 | -0.49527 | -3.44851 |
| H | -3.69568 | -0.30333 | -4.54647 |
| H | -3.81366 | -1.76205 | -3.56338 |
| C | -3.46512 | 1.53224 | -2.62940 |
| H | -4.52471 | 1.71844 | -2.43784 |
| H | -2.88769 | 2.14188 | -1.93083 |
| H | -3.23304 | 1.88111 | -3.63933 |
| C | -1.68612 | -0.22881 | -2.87698 |
| H | -0.97902 | 0.41121 | -2.34488 |
| H | -1.41123 | -1.26757 | -2.68997 |
| H | -1.54270 | -0.01263 | -3.93941 |
| C | 2.22884 | 2.25508 | 0.75675 |
| H | 1.98210 | 2.02786 | -0.28272 |
| H | 1.47642 | 1.79360 | 1.39484 |
| H | 2.11263 | 3.33356 | 0.88161 |
| C | 4.53591 | 2.74417 | 0.16314 |
| H | 4.29240 | 3.79348 | 0.34788 |
| H | 5.60174 | 2.60719 | 0.34786 |
| H | 4.34324 | 2.53382 | -0.89110 |
| C | 4.01068 | 2.18357 | 2.52568 |
| H | 5.06745 | 2.00739 | 2.73598 |
| H | 3.80914 | 3.24045 | 2.71768 |
| H | 3.43245 | 1.59814 | 3.24088 |
| C | 1.57917 | -1.60186 | -2.23002 |
| H | 1.17443 | -2.06160 | -3.13480 |
| H | 0.81175 | -1.72075 | -1.47027 |
| H | 1.72287 | -0.53699 | -2.43237 |
| C | 2.69113 | -3.76486 | -1.58455 |
| H | 2.04179 | -3.91785 | -0.72570 |
| H | 2.23328 | -4.24682 | -2.45244 |
| H | 3.64565 | -4.26158 | -1.39182 |
| C | 3.77500 | -2.14967 | -3.13695 |
| H | 4.00834 | -1.10498 | -3.35658 |
| H | 4.71336 | -2.70019 | -3.06304 |
| H | 3.22416 | -2.55988 | -3.98700 |
| C | 8.06705 | -0.64777 | 1.34828 |
| H | 8.15665 | 0.36571 | 0.94905 |
| H | 7.59871 | -0.59066 | 2.33416 |
| H | 9.07956 | -1.03455 | 1.48467 |
| C | 8.00765 | -1.57912 | -0.95090 |
| H | 7.53246 | -2.26543 | -1.65435 |
| H | 8.00973 | -0.58371 | -1.40159 |
| H | 9.04594 | -1.89773 | -0.82474 |
| C | 7.30324 | -2.98209 | 0.99736 |
| H | 6.81372 | -3.00226 | 1.97407 |
| H | 6.78773 | -3.69442 | 0.35036 |
| H | 8.33237 | -3.32843 | 1.12505 |
| Au | -0.73324 | 2.82226 | -0.56201 |
| Cl | -0.26242 | 4.97400 | -1.12399 |
| C | 1.71792 | -0.48292 | 2.63245 |
| H | 2.66615 | -0.91972 | 2.95034 |
| H | 1.68727 | 0.56963 | 2.89285 |
| H | 0.89973 | -1.00344 | 3.13732 |
| Si | -0.58214 | -2.38851 | 1.10888 |

Coordination through $\pi(\text{C}=\text{P})$ bond**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.79512 | 0.12658 | 1.06714 |
| C | 0.34430 | -0.00946 | -0.59215 |
| P | -1.20474 | -0.34908 | -1.34696 |
| Cl | 1.26030 | -2.61556 | -1.91988 |
| Si | 1.15467 | -0.52025 | -2.38355 |
| O | -0.68647 | -0.46554 | -2.79591 |
| H | 2.19726 | -0.08607 | 0.89072 |
| H | -1.68258 | -1.58526 | -0.87188 |
| Au | 0.67599 | 2.09378 | -0.26566 |
| Cl | 0.83791 | 4.31669 | -0.56531 |
| C | -2.58142 | 0.77938 | -1.20671 |
| H | -3.40643 | 0.41199 | -1.82150 |
| H | -2.90089 | 0.83430 | -0.16337 |
| H | -2.28014 | 1.76981 | -1.55079 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.73399 | 0.02117 | 1.11523 |
| C | 0.28023 | 0.15562 | -0.54015 |
| P | -1.25573 | -0.17984 | -1.33383 |
| Cl | 1.53725 | -2.14233 | -2.19419 |
| Si | 1.11113 | -0.02851 | -2.37439 |
| O | -0.70323 | -0.15935 | -2.78399 |
| C | -2.59740 | 0.99304 | -1.15811 |
| H | -3.42207 | 0.69269 | -1.80899 |
| H | -2.94083 | 1.01708 | -0.12199 |
| H | -2.25139 | 1.98605 | -1.44741 |
| C | 2.54700 | -0.24168 | 1.03764 |
| H | 3.00821 | 0.18011 | 0.14475 |
| H | 3.00959 | 0.17431 | 1.93449 |
| H | 2.71303 | -1.32399 | 1.03817 |
| C | -1.88404 | -1.79593 | -0.89291 |
| H | -2.21962 | -1.79338 | 0.14640 |
| H | -2.71787 | -2.05371 | -1.54931 |
| H | -1.07851 | -2.51992 | -1.02323 |
| Au | 0.46610 | 2.18956 | 0.15146 |
| Cl | 0.50659 | 4.43691 | 0.31490 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.65291 | 0.12625 | 0.95636 |
| C | 0.34309 | 0.11622 | -0.74378 |
| P | -1.19409 | -0.30341 | -1.53242 |
| Cl | 2.03136 | -1.92027 | -2.57186 |
| Si | 1.15213 | 0.04541 | -2.59630 |
| O | -0.60021 | -0.44549 | -2.96400 |
| C | -2.44785 | 0.98463 | -1.53822 |
| H | -3.30897 | 0.66378 | -2.12749 |
| H | -2.76437 | 1.22802 | -0.52360 |
| H | -2.01526 | 1.87383 | -1.99931 |
| Au | 0.39782 | 2.20913 | -0.16990 |
| Cl | 0.38161 | 4.46506 | -0.09682 |
| C | 2.49249 | -0.05388 | 1.22998 |
| C | 2.71155 | -1.56676 | 1.34959 |
| C | 3.39004 | 0.53179 | 0.15343 |
| C | 2.76795 | 0.61968 | 2.57578 |
| H | 2.05135 | -2.01987 | 2.09598 |
| H | 2.55765 | -2.06882 | 0.39211 |
| H | 3.74167 | -1.75423 | 1.66979 |
| H | 3.24613 | 1.60922 | 0.04553 |
| H | 4.43746 | 0.36180 | 0.42554 |
| H | 3.23128 | 0.05976 | -0.81765 |
| H | 3.80796 | 0.44178 | 2.86528 |
| H | 2.61426 | 1.70048 | 2.52365 |

| | | | |
|---|----------|----------|----------|
| H | 2.12769 | 0.22350 | 3.36891 |
| C | -1.98348 | -1.86322 | -0.97792 |
| C | -2.97847 | -2.28084 | -2.06490 |
| C | -0.92248 | -2.94912 | -0.81339 |
| C | -2.69971 | -1.61754 | 0.35049 |
| H | -3.79321 | -1.56356 | -2.18447 |
| H | -2.48556 | -2.41341 | -3.02955 |
| H | -3.42466 | -3.23688 | -1.77747 |
| H | -0.21243 | -2.70823 | -0.02067 |
| H | -1.42337 | -3.88300 | -0.54307 |
| H | -0.35873 | -3.11392 | -1.73206 |
| H | -3.10759 | -2.56701 | 0.70801 |
| H | -2.01948 | -1.24195 | 1.11977 |
| H | -3.53312 | -0.91940 | 0.25006 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.70787 | 0.10921 | 1.06131 |
| C | 0.23806 | 0.17027 | -0.59914 |
| P | -1.39641 | -0.05408 | -1.22169 |
| Cl | 1.28160 | -1.69721 | -3.02206 |
| Si | 0.79280 | 0.34200 | -2.53314 |
| O | -1.05219 | 0.20509 | -2.71308 |
| C | -2.69387 | 1.05016 | -0.66641 |
| H | -3.60874 | 0.82537 | -1.21889 |
| H | -2.87346 | 0.90855 | 0.40118 |
| H | -2.39086 | 2.08224 | -0.84835 |
| Au | 0.55256 | 2.23973 | -0.02696 |
| Cl | 0.76380 | 4.48273 | 0.11155 |
| C | 2.49179 | -0.17711 | 1.09666 |
| C | 3.11695 | 0.08316 | 2.32006 |
| C | 3.24845 | -0.66529 | 0.03013 |
| C | 4.47981 | -0.11073 | 2.46513 |
| H | 2.52999 | 0.45064 | 3.15635 |
| C | 4.60917 | -0.86786 | 0.18379 |
| H | 2.77090 | -0.91171 | -0.91030 |
| C | 5.22639 | -0.58527 | 1.39561 |
| H | 4.95974 | 0.10520 | 3.41253 |
| H | 5.19097 | -1.24960 | -0.64717 |
| H | 6.29307 | -0.74256 | 1.50840 |
| C | -1.99050 | -1.72608 | -0.98206 |
| C | -2.10542 | -2.57675 | -2.07720 |
| C | -2.34516 | -2.16792 | 0.29218 |
| C | -2.58465 | -3.86517 | -1.89506 |
| H | -1.80927 | -2.23038 | -3.05953 |
| C | -2.81875 | -3.45669 | 0.46567 |
| H | -2.23964 | -1.51571 | 1.15344 |
| C | -2.94062 | -4.30335 | -0.62881 |
| H | -2.67248 | -4.52982 | -2.74629 |
| H | -3.09053 | -3.80297 | 1.45582 |
| H | -3.31093 | -5.31267 | -0.49034 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.68804 | 0.13128 | 1.43370 |
| C | 0.05059 | 0.22346 | -0.18946 |
| P | -1.59992 | -0.03189 | -0.78819 |
| Cl | 1.42934 | -0.10540 | -3.26185 |
| Si | 0.36921 | 1.13173 | -1.91808 |
| O | -1.34122 | 0.63043 | -2.18553 |
| C | -2.96584 | 0.87373 | -0.04952 |
| H | -3.87366 | 0.66980 | -0.62174 |
| H | -3.12187 | 0.60022 | 0.99196 |
| H | -2.72500 | 1.93669 | -0.11161 |
| Au | 0.35107 | 2.30928 | 0.35255 |
| Cl | 0.71241 | 4.45003 | 1.06130 |
| C | 2.48223 | -0.12355 | 1.25270 |
| C | 3.35046 | 0.68140 | 2.01378 |

| | | | |
|---|----------|----------|----------|
| C | 2.99684 | -1.20462 | 0.50992 |
| C | 4.71856 | 0.44934 | 1.94146 |
| C | 4.37081 | -1.39652 | 0.47937 |
| C | 5.25218 | -0.56897 | 1.16542 |
| H | 5.38447 | 1.08256 | 2.52030 |
| H | 4.76500 | -2.23413 | -0.08888 |
| C | -2.04563 | -1.77445 | -0.92831 |
| C | -2.15591 | -2.42557 | -2.17843 |
| C | -2.28649 | -2.49279 | 0.26102 |
| C | -2.46690 | -3.78040 | -2.18369 |
| C | -2.58206 | -3.84674 | 0.18630 |
| C | -2.66820 | -4.51531 | -1.02459 |
| H | -2.55361 | -4.27908 | -3.14378 |
| H | -2.75551 | -4.39034 | 1.10994 |
| C | 2.85096 | 1.78461 | 2.89615 |
| H | 2.59312 | 2.68139 | 2.32443 |
| H | 1.94781 | 1.49561 | 3.44139 |
| H | 3.61261 | 2.06065 | 3.62687 |
| C | 2.12181 | -2.19530 | -0.20073 |
| H | 1.26126 | -2.48672 | 0.40762 |
| H | 1.73259 | -1.79505 | -1.13818 |
| H | 2.69045 | -3.09742 | -0.43160 |
| C | 6.73205 | -0.77569 | 1.07114 |
| H | 7.24611 | -0.38881 | 1.95266 |
| H | 6.98143 | -1.83306 | 0.96235 |
| H | 7.13886 | -0.25398 | 0.19899 |
| C | -2.29516 | -1.87223 | 1.62848 |
| H | -2.05968 | -2.62438 | 2.38229 |
| H | -1.57150 | -1.06522 | 1.75558 |
| H | -3.28873 | -1.48000 | 1.86670 |
| C | -1.98279 | -1.77018 | -3.51887 |
| H | -2.62132 | -0.89539 | -3.63893 |
| H | -0.95777 | -1.43462 | -3.67978 |
| H | -2.23259 | -2.48574 | -4.30239 |
| C | -2.95248 | -5.98304 | -1.08168 |
| H | -3.51719 | -6.24452 | -1.97814 |
| H | -2.01805 | -6.55229 | -1.10720 |
| H | -3.51504 | -6.31552 | -0.20797 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.69548 | 0.30887 | 1.03399 |
| C | 0.42064 | 0.04818 | -0.68126 |
| P | -1.14090 | -0.11502 | -1.60902 |
| O | -0.40206 | -0.00921 | -2.99495 |
| Cl | 2.55122 | -0.81734 | -3.24373 |
| Au | 0.70342 | 2.22329 | -0.54862 |
| Cl | 0.73816 | 4.50505 | -0.31847 |
| C | 2.52143 | 0.08518 | 1.21392 |
| C | 3.17739 | -1.09024 | 0.75286 |
| C | 3.32209 | 1.16717 | 1.66389 |
| C | 4.51653 | -0.99728 | 0.40587 |
| C | 4.66208 | 1.18760 | 1.27298 |
| C | 5.26346 | 0.16340 | 0.56522 |
| H | 5.00741 | -1.87859 | 0.01319 |
| H | 5.25543 | 2.04644 | 1.55177 |
| C | 2.94133 | 2.25047 | 2.69828 |
| C | 2.62373 | -2.52768 | 0.84781 |
| C | 6.69432 | 0.23534 | 0.04525 |
| C | 3.78369 | 1.92518 | 3.94868 |
| H | 3.54275 | 0.93149 | 4.33581 |
| H | 4.85408 | 1.95343 | 3.74024 |
| H | 3.57111 | 2.65808 | 4.73210 |
| C | 3.29732 | 3.66210 | 2.22171 |
| H | 2.73529 | 3.93918 | 1.32953 |
| H | 3.04774 | 4.38084 | 3.00733 |
| H | 4.36163 | 3.77380 | 2.00877 |

| | | | |
|---|----------|----------|----------|
| C | 1.48920 | 2.26585 | 3.16749 |
| H | 1.41014 | 2.95216 | 4.01546 |
| H | 0.80146 | 2.62483 | 2.40209 |
| H | 1.15674 | 1.28422 | 3.51470 |
| C | 2.91386 | -3.34622 | -0.41372 |
| H | 2.51108 | -2.86182 | -1.30208 |
| H | 3.98281 | -3.49774 | -0.57111 |
| H | 2.46021 | -4.33712 | -0.32118 |
| C | 3.37119 | -3.17349 | 2.03138 |
| H | 4.45096 | -3.16830 | 1.87568 |
| H | 3.16433 | -2.63922 | 2.96219 |
| H | 3.04752 | -4.21164 | 2.15282 |
| C | 1.13857 | -2.66112 | 1.16739 |
| H | 0.85123 | -2.07789 | 2.04792 |
| H | 0.50362 | -2.37224 | 0.33228 |
| H | 0.92372 | -3.70913 | 1.39624 |
| C | 7.34250 | 1.58915 | 0.32185 |
| H | 6.77623 | 2.40798 | -0.12848 |
| H | 7.43883 | 1.78493 | 1.39300 |
| H | 8.34796 | 1.60607 | -0.10576 |
| C | 6.67619 | 0.01009 | -1.47152 |
| H | 7.69403 | 0.04654 | -1.87037 |
| H | 6.24668 | -0.95985 | -1.73015 |
| H | 6.08375 | 0.77829 | -1.97378 |
| C | 7.54753 | -0.85146 | 0.70961 |
| H | 7.57130 | -0.72186 | 1.79457 |
| H | 7.16752 | -1.85309 | 0.49846 |
| H | 8.57500 | -0.80174 | 0.33813 |
| C | -2.36034 | -1.48995 | -1.68529 |
| C | -2.35803 | -2.33509 | -2.83554 |
| C | -3.57682 | -1.34904 | -0.96221 |
| C | -3.58609 | -2.65493 | -3.39850 |
| C | -1.13976 | -3.05978 | -3.43831 |
| C | -4.76118 | -1.74278 | -1.57643 |
| C | -3.71788 | -0.96127 | 0.52138 |
| C | -4.80693 | -2.30393 | -2.84107 |
| H | -3.58218 | -3.23290 | -4.31297 |
| C | -0.71171 | -2.47968 | -4.78982 |
| C | -1.52867 | -4.53357 | -3.67821 |
| C | 0.01813 | -3.12121 | -2.45107 |
| H | -5.68420 | -1.60332 | -1.03163 |
| C | -2.41025 | -0.58368 | 1.19428 |
| C | -4.21021 | -2.23378 | 1.23933 |
| C | -4.74576 | 0.15057 | 0.75546 |
| C | -6.10766 | -2.62137 | -3.56747 |
| H | 0.09141 | -3.09051 | -5.21064 |
| H | -1.54758 | -2.49695 | -5.49450 |
| H | -0.35569 | -1.45724 | -4.70480 |
| H | -2.22516 | -4.66468 | -4.50717 |
| H | -0.62417 | -5.09225 | -3.93122 |
| H | -1.96673 | -4.98476 | -2.78482 |
| H | 0.40721 | -2.14939 | -2.16249 |
| H | -0.28081 | -3.65729 | -1.54676 |
| H | 0.85263 | -3.66251 | -2.90134 |
| H | -1.64375 | -1.34481 | 1.03883 |
| H | -2.01386 | 0.38175 | 0.87997 |
| H | -2.56270 | -0.49834 | 2.27261 |
| H | -4.30605 | -2.03273 | 2.30979 |
| H | -5.18072 | -2.56644 | 0.86934 |
| H | -3.49962 | -3.05331 | 1.10900 |
| H | -5.74156 | -0.12627 | 0.40608 |
| H | -4.82109 | 0.35568 | 1.82629 |
| H | -4.46978 | 1.08215 | 0.25889 |
| C | -7.33320 | -2.14058 | -2.79507 |
| C | -6.22764 | -4.13659 | -3.77091 |
| C | -6.09339 | -1.92508 | -4.93357 |

| | | | |
|----|----------|----------|----------|
| H | -7.43822 | -2.65162 | -1.83460 |
| H | -7.30071 | -1.06360 | -2.61187 |
| H | -8.23457 | -2.35038 | -3.37541 |
| H | -5.40405 | -4.53368 | -4.36734 |
| H | -6.23261 | -4.66165 | -2.81260 |
| H | -7.15970 | -4.37124 | -4.29201 |
| H | -6.02356 | -0.84051 | -4.82029 |
| H | -5.25145 | -2.25264 | -5.54652 |
| H | -7.01322 | -2.15136 | -5.47936 |
| Si | 1.20264 | 0.57748 | -2.42095 |
| C | -2.23250 | 1.32893 | -1.62105 |
| H | -2.69199 | 1.53764 | -0.65973 |
| H | -1.63108 | 2.18764 | -1.92554 |
| H | -3.00931 | 1.14599 | -2.36611 |

[R-P=C(Si(II)Cl)-P(S)ClR](AuCl)

Coordination through Si(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.80758 | 0.23345 | 0.90815 |
| C | 0.45042 | -0.22531 | -0.64820 |
| P | -1.12771 | -0.40431 | -1.37393 |
| Cl | 1.62019 | -2.36199 | -2.58764 |
| Si | 1.44177 | -0.30935 | -2.29543 |
| H | 2.22214 | 0.31452 | 0.72733 |
| H | -1.62238 | -1.71540 | -1.25451 |
| Cl | -2.62195 | 0.62927 | -0.53398 |
| Au | 3.10492 | 1.10808 | -2.77799 |
| Cl | 4.80924 | 2.57396 | -3.19624 |
| S | -0.66480 | 0.10217 | -3.24505 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.76179 | -0.00067 | 0.91748 |
| C | 0.41357 | -0.26170 | -0.68802 |
| P | -1.17846 | -0.31583 | -1.40131 |
| Cl | 1.61948 | -2.32676 | -2.70947 |
| Si | 1.38539 | -0.28213 | -2.34017 |
| Cl | -2.51488 | 0.95595 | -0.59090 |
| Au | 3.07791 | 1.13023 | -2.76865 |
| Cl | 4.81971 | 2.57944 | -3.10920 |
| C | 2.58477 | -0.03790 | 0.97993 |
| H | 2.90913 | -1.07902 | 1.07861 |
| H | 3.03866 | 0.38429 | 0.07887 |
| H | 2.92410 | 0.50684 | 1.86197 |
| C | -1.98001 | -1.91411 | -1.25799 |
| H | -2.19869 | -2.11728 | -0.20825 |
| H | -2.90133 | -1.91045 | -1.84215 |
| H | -1.28757 | -2.65984 | -1.65389 |
| S | -0.67388 | 0.15939 | -3.28631 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.70253 | 0.01502 | 0.69331 |
| C | 0.51903 | -0.38683 | -0.91433 |
| P | -1.08418 | -0.50519 | -1.63609 |
| Cl | 2.08596 | -2.51099 | -2.69844 |
| Si | 1.52121 | -0.50793 | -2.55007 |
| Au | 2.95680 | 1.10034 | -3.19461 |
| Cl | 4.41786 | 2.77569 | -3.76863 |
| C | 2.51001 | 0.16017 | 1.10250 |
| C | 3.43605 | -0.76292 | 0.32686 |
| C | 2.85896 | 1.63254 | 0.84697 |
| C | 2.59877 | -0.13831 | 2.60235 |
| H | 3.13240 | -1.80938 | 0.39795 |
| H | 3.49675 | -0.48859 | -0.72828 |
| H | 4.44928 | -0.67825 | 0.73317 |
| H | 2.18364 | 2.31405 | 1.37325 |

| | | | |
|----|----------|----------|----------|
| H | 3.87128 | 1.82475 | 1.21706 |
| H | 2.83947 | 1.87465 | -0.21782 |
| H | 3.61979 | 0.04948 | 2.94681 |
| H | 1.92629 | 0.49588 | 3.18628 |
| H | 2.35892 | -1.18186 | 2.82354 |
| C | -2.12741 | -1.95376 | -1.15703 |
| C | -3.36068 | -1.96868 | -2.05785 |
| C | -1.28503 | -3.20833 | -1.38763 |
| C | -2.52237 | -1.83850 | 0.31264 |
| H | -3.99161 | -1.09180 | -1.90477 |
| H | -3.08959 | -2.02804 | -3.11419 |
| H | -3.95203 | -2.85568 | -1.81545 |
| H | -0.39017 | -3.22279 | -0.76370 |
| H | -1.89522 | -4.07752 | -1.12785 |
| H | -0.97571 | -3.30869 | -2.42874 |
| H | -3.08919 | -2.73323 | 0.58430 |
| H | -1.65103 | -1.78594 | 0.96921 |
| H | -3.15258 | -0.96916 | 0.50262 |
| Cl | -2.23617 | 1.10243 | -1.20304 |
| S | -0.53870 | -0.50535 | -3.57266 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.83732 | -0.27336 | 0.43446 |
| C | 0.47692 | -0.23906 | -1.19781 |
| P | -1.19827 | -0.36769 | -1.70291 |
| Cl | 1.98099 | -2.21196 | -3.10287 |
| Si | 1.25955 | -0.25932 | -2.94443 |
| Au | 2.47978 | 1.41744 | -3.81620 |
| Cl | 3.75887 | 3.13439 | -4.64503 |
| C | -2.13270 | -1.74526 | -1.02609 |
| C | -1.80242 | -3.01518 | -1.50175 |
| C | -3.09101 | -1.59450 | -0.02783 |
| C | -2.43712 | -4.12729 | -0.97739 |
| H | -1.05470 | -3.12973 | -2.27890 |
| C | -3.72021 | -2.71568 | 0.48925 |
| H | -3.34973 | -0.61044 | 0.34088 |
| C | -3.39537 | -3.97811 | 0.01602 |
| H | -2.18467 | -5.11300 | -1.34946 |
| H | -4.46990 | -2.59937 | 1.26279 |
| H | -3.89352 | -4.85133 | 0.42122 |
| C | 2.61112 | -0.19034 | 0.64956 |
| C | 3.03610 | -0.48469 | 1.95274 |
| C | 3.56172 | 0.16496 | -0.31381 |
| C | 4.38117 | -0.45507 | 2.27705 |
| H | 2.30084 | -0.74023 | 2.70967 |
| C | 4.90165 | 0.20866 | 0.01853 |
| H | 3.25932 | 0.43741 | -1.31963 |
| C | 5.31269 | -0.10834 | 1.30910 |
| H | 4.70221 | -0.69337 | 3.28414 |
| H | 5.62901 | 0.49551 | -0.73166 |
| H | 6.36659 | -0.07536 | 1.56125 |
| Cl | -2.26908 | 1.27079 | -1.20354 |
| S | -0.90406 | -0.48310 | -3.68576 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | -0.41725 | 1.47157 | 1.44297 |
| C | 0.14893 | 0.40405 | 0.28083 |
| P | 1.76859 | -0.27762 | 0.07630 |
| Cl | -1.20971 | 0.76900 | -2.62306 |
| C | 3.46693 | 0.39792 | 0.16124 |
| C | 4.09194 | 0.72275 | -1.08042 |
| C | 4.29397 | 0.11910 | 1.28266 |
| C | 5.41001 | 0.32717 | -1.24719 |
| C | 5.61329 | -0.24177 | 1.03208 |
| C | 6.16692 | -0.25676 | -0.23851 |
| H | 5.87436 | 0.51136 | -2.20793 |

| | | | | | | | |
|---|----------|----------|----------|-----------------|----------|----------|----------|
| H | 6.23155 | -0.51086 | 1.87706 | H | 2.17080 | 2.70168 | -0.81892 |
| C | -2.21104 | 1.52784 | 1.09096 | C | 3.49722 | 1.04816 | -3.55693 |
| C | -2.73555 | 2.57944 | 0.30413 | H | 2.77620 | 0.23395 | -3.61463 |
| C | -3.06373 | 0.48274 | 1.53491 | H | 3.20790 | 1.80888 | -4.28655 |
| C | -3.99723 | 2.39924 | -0.25677 | H | 4.47443 | 0.66182 | -3.85413 |
| C | -4.30329 | 0.36775 | 0.92095 | C | 4.50986 | 2.86688 | -2.19029 |
| C | -4.76384 | 1.26656 | -0.03268 | H | 4.58759 | 3.33614 | -1.20647 |
| H | -4.38834 | 3.16634 | -0.90559 | H | 5.51267 | 2.58090 | -2.50872 |
| H | -4.93404 | -0.46666 | 1.18871 | H | 4.13497 | 3.61406 | -2.89456 |
| C | -2.04088 | 3.94656 | 0.14673 | C | 8.22288 | -1.39357 | 0.70376 |
| C | -2.79727 | -0.35998 | 2.79849 | H | 8.38471 | -0.65536 | 1.49343 |
| C | -6.08240 | 1.00234 | -0.75020 | H | 7.62689 | -2.21312 | 1.11283 |
| C | 3.94630 | 0.38968 | 2.76032 | H | 9.20036 | -1.79841 | 0.43216 |
| C | 3.53244 | 1.67149 | -2.16027 | C | 8.45420 | 0.36977 | -1.02800 |
| C | 7.56759 | -0.77795 | -0.52958 | H | 8.06860 | 0.81300 | -1.94818 |
| C | -3.82441 | -1.48231 | 2.97404 | H | 8.53080 | 1.16118 | -0.27840 |
| H | -3.57785 | -2.04430 | 3.87780 | H | 9.46164 | -0.00068 | -1.23525 |
| H | -4.83674 | -1.09540 | 3.10723 | C | 7.47226 | -1.85598 | -1.61635 |
| H | -3.82126 | -2.18196 | 2.13436 | H | 6.85461 | -2.69384 | -1.28461 |
| C | -2.94270 | 0.60195 | 3.98999 | H | 7.03776 | -1.46431 | -2.53818 |
| H | -2.19369 | 1.39820 | 3.95604 | H | 8.46873 | -2.23912 | -1.85149 |
| H | -3.92996 | 1.06946 | 3.99673 | Au | -2.17665 | -2.25447 | -0.73624 |
| H | -2.81551 | 0.05570 | 4.92921 | Cl | -3.75426 | -3.88037 | -0.27157 |
| C | -1.41982 | -1.01196 | 2.88132 | Si | -0.70127 | -0.59297 | -1.11871 |
| H | -1.19876 | -1.62316 | 2.00510 | Cl | 1.87381 | -1.86933 | 1.35852 |
| H | -0.61241 | -0.27983 | 3.00739 | S | 1.42942 | -1.15707 | -1.71271 |
| H | -1.38145 | -1.65078 | 3.76796 | | | | |
| C | -7.21671 | 0.86335 | 0.27187 | | | | |
| H | -8.16200 | 0.67454 | -0.24421 | R = Mes* | | | |
| H | -7.04601 | 0.03318 | 0.95945 | P | -0.41725 | 1.47157 | 1.44297 |
| H | -7.32797 | 1.77633 | 0.86289 | C | 0.14893 | 0.40405 | 0.28083 |
| C | -6.44858 | 2.12261 | -1.72009 | P | 1.76859 | -0.27762 | 0.07630 |
| H | -7.38641 | 1.87448 | -2.22266 | Cl | -1.20971 | 0.76900 | -2.62306 |
| H | -6.59268 | 3.07809 | -1.20797 | C | 3.46693 | 0.39792 | 0.16124 |
| H | -5.68661 | 2.25501 | -2.49226 | C | 4.09194 | 0.72275 | -1.08042 |
| C | -5.94909 | -0.30356 | -1.54441 | C | 4.29397 | 0.11910 | 1.28266 |
| H | -5.15600 | -0.22547 | -2.29194 | C | 5.41001 | 0.32717 | -1.24719 |
| H | -5.71076 | -1.15425 | -0.90303 | C | 5.61329 | -0.24177 | 1.03208 |
| H | -6.88692 | -0.52317 | -2.06268 | C | 6.16692 | -0.25676 | -0.23851 |
| C | -2.89390 | 4.93397 | -0.65324 | H | 5.87436 | 0.51136 | -2.20793 |
| H | -3.87309 | 5.09599 | -0.19795 | H | 6.23155 | -0.51086 | 1.87706 |
| H | -2.38072 | 5.89801 | -0.68090 | C | -2.21104 | 1.52784 | 1.09096 |
| H | -3.03902 | 4.60911 | -1.68621 | C | -2.73555 | 2.57944 | 0.30413 |
| C | -1.84998 | 4.54861 | 1.54658 | C | -3.06373 | 0.48274 | 1.53491 |
| H | -2.80825 | 4.64670 | 2.06175 | C | -3.99723 | 2.39924 | -0.25677 |
| H | -1.19461 | 3.93656 | 2.17141 | C | -4.30329 | 0.36775 | 0.92095 |
| H | -1.39857 | 5.54199 | 1.46939 | C | -4.76384 | 1.26656 | -0.03268 |
| C | -0.68634 | 3.87222 | -0.55726 | H | -4.38834 | 3.16634 | -0.90559 |
| H | 0.06780 | 3.35602 | 0.04417 | H | -4.93404 | -0.46666 | 1.18871 |
| H | -0.75645 | 3.35629 | -1.51536 | C | -2.04088 | 3.94656 | 0.14673 |
| H | -0.30518 | 4.88348 | -0.72777 | C | -2.79727 | -0.35998 | 2.79849 |
| C | 2.54176 | 0.92968 | 2.99001 | C | -6.08240 | 1.00234 | -0.75020 |
| H | 2.32565 | 1.77690 | 2.33536 | C | 3.94630 | 0.38968 | 2.76032 |
| H | 1.76577 | 0.17702 | 2.86542 | C | 3.53244 | 1.67149 | -2.16027 |
| H | 2.45886 | 1.29140 | 4.01776 | C | 7.56759 | -0.77795 | -0.52958 |
| C | 4.90015 | 1.52659 | 3.18774 | C | -3.82441 | -1.48231 | 2.97404 |
| H | 4.67966 | 1.80975 | 4.22037 | H | -3.57785 | -2.04430 | 3.87780 |
| H | 5.94803 | 1.22986 | 3.13619 | H | -4.83674 | -1.09540 | 3.10723 |
| H | 4.76636 | 2.40872 | 2.55701 | H | -3.82126 | -2.18196 | 2.13436 |
| C | 4.19524 | -0.81136 | 3.67576 | C | -2.94270 | 0.60195 | 3.98999 |
| H | 5.22186 | -1.17488 | 3.60378 | H | -2.19369 | 1.39820 | 3.95604 |
| H | 4.02540 | -0.51566 | 4.71429 | H | -3.92996 | 1.06946 | 3.99673 |
| H | 3.52641 | -1.64035 | 3.44809 | H | -2.81551 | 0.05570 | 4.92921 |
| C | 2.17291 | 2.26896 | -1.82225 | C | -1.41982 | -1.01196 | 2.88132 |
| H | 1.95521 | 3.07604 | -2.52606 | H | -1.19876 | -1.62316 | 2.00510 |
| H | 1.35287 | 1.56064 | -1.90763 | H | -0.61241 | -0.27983 | 3.00739 |
| | | | | H | -1.38145 | -1.65078 | 3.76796 |

| | | | |
|----|----------|----------|----------|
| C | -7.21671 | 0.86335 | 0.27187 |
| H | -8.16200 | 0.67454 | -0.24421 |
| H | -7.04601 | 0.03318 | 0.95945 |
| H | -7.32797 | 1.77633 | 0.86289 |
| C | -6.44858 | 2.12261 | -1.72009 |
| H | -7.38641 | 1.87448 | -2.22266 |
| H | -6.59268 | 3.07809 | -1.20797 |
| H | -5.68661 | 2.25501 | -2.49226 |
| C | -5.94909 | -0.30356 | -1.54441 |
| H | -5.15600 | -0.22547 | -2.29194 |
| H | -5.71076 | -1.15425 | -0.90303 |
| H | -6.88692 | -0.52317 | -2.06268 |
| C | -2.89390 | 4.93397 | -0.65324 |
| H | -3.87309 | 5.09599 | -0.19795 |
| H | -2.38072 | 5.89801 | -0.68090 |
| H | -3.03902 | 4.60911 | -1.68621 |
| C | -1.84998 | 4.54861 | 1.54658 |
| H | -2.80825 | 4.64670 | 2.06175 |
| H | -1.19461 | 3.93656 | 2.17141 |
| H | -1.39857 | 5.54199 | 1.46939 |
| C | -0.68634 | 3.87222 | -0.55726 |
| H | 0.06780 | 3.35602 | 0.04417 |
| H | -0.75645 | 3.35629 | -1.51536 |
| H | -0.30518 | 4.88348 | -0.72777 |
| C | 2.54176 | 0.92968 | 2.99001 |
| H | 2.32565 | 1.77690 | 2.33536 |
| H | 1.76577 | 0.17702 | 2.86542 |
| H | 2.45886 | 1.29140 | 4.01776 |
| C | 4.90015 | 1.52659 | 3.18774 |
| H | 4.67966 | 1.80975 | 4.22037 |
| H | 5.94803 | 1.22986 | 3.13619 |
| H | 4.76636 | 2.40872 | 2.55701 |
| C | 4.19524 | -0.81136 | 3.67576 |
| H | 5.22186 | -1.17488 | 3.60378 |
| H | 4.02540 | -0.51566 | 4.71429 |
| H | 3.52641 | -1.64035 | 3.44809 |
| C | 2.17291 | 2.26896 | -1.82225 |
| H | 1.95521 | 3.07604 | -2.52606 |
| H | 1.35287 | 1.56064 | -1.90763 |
| H | 2.17080 | 2.70168 | -0.81892 |
| C | 3.49722 | 1.04816 | -3.55693 |
| H | 2.77620 | 0.23395 | -3.61463 |
| H | 3.20790 | 1.80888 | -4.28655 |
| H | 4.47443 | 0.66182 | -3.85413 |
| C | 4.50986 | 2.86688 | -2.19029 |
| H | 4.58759 | 3.33614 | -1.20647 |
| H | 5.51267 | 2.58090 | -2.50872 |
| H | 4.13497 | 3.61406 | -2.89456 |
| C | 8.22288 | -1.39357 | 0.70376 |
| H | 8.38471 | -0.65536 | 1.49343 |
| H | 7.62689 | -2.21312 | 1.11283 |
| H | 9.20036 | -1.79841 | 0.43216 |
| C | 8.45420 | 0.36977 | -1.02800 |
| H | 8.06860 | 0.81300 | -1.94818 |
| H | 8.53080 | 1.16118 | -0.27840 |
| H | 9.46164 | -0.00068 | -1.23525 |
| C | 7.47226 | -1.85598 | -1.61635 |
| H | 6.85461 | -2.69384 | -1.28461 |
| H | 7.03776 | -1.46431 | -2.53818 |
| H | 8.46873 | -2.23912 | -1.85149 |
| Au | -2.17665 | -2.25447 | -0.73624 |
| Cl | -3.75426 | -3.88037 | -0.27157 |
| Si | -0.70127 | -0.59297 | -1.11871 |
| Cl | 1.87381 | -1.86933 | 1.35852 |
| S | 1.42942 | -1.15707 | -1.71271 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.67279 | -0.20066 | 1.16497 |
| C | 0.44800 | -0.32977 | -0.47563 |
| P | -0.97740 | 0.06193 | -1.38101 |
| Cl | 0.89512 | -2.50126 | -2.61514 |
| Si | 1.67535 | -0.63102 | -1.99615 |
| H | 2.03934 | -0.62646 | 1.17921 |
| H | -1.66032 | -1.10827 | -1.73748 |
| Cl | -2.42535 | 1.14322 | -0.50417 |
| Au | -1.41067 | 0.36058 | -4.75462 |
| Cl | -2.72939 | -0.12431 | -6.50973 |
| S | -0.08309 | 0.90064 | -2.99328 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.67681 | -0.17002 | 1.11235 |
| C | 0.43945 | -0.22874 | -0.53344 |
| P | -1.05513 | 0.07553 | -1.35406 |
| Cl | 1.30900 | -2.31252 | -2.69608 |
| Si | 1.66345 | -0.31404 | -2.07018 |
| Cl | -2.34625 | 1.33202 | -0.42956 |
| Au | -1.49810 | 0.07268 | -4.80994 |
| Cl | -2.72340 | -0.67168 | -6.54508 |
| C | 2.42455 | -0.68402 | 1.29728 |
| H | 2.82669 | -0.27656 | 2.22602 |
| H | 2.46464 | -1.77572 | 1.36227 |
| H | 3.04089 | -0.36718 | 0.45106 |
| C | -2.01837 | -1.40834 | -1.62766 |
| H | -2.87639 | -1.16796 | -2.25691 |
| H | -1.37537 | -2.13596 | -2.12650 |
| H | -2.34656 | -1.78662 | -0.65728 |
| S | -0.27412 | 0.86586 | -3.06640 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.78161 | -0.09987 | 0.84218 |
| C | 0.42111 | 0.03957 | -0.78366 |
| P | -1.25226 | 0.00881 | -1.30077 |
| Cl | 1.81579 | -1.40873 | -3.20475 |
| Si | 1.34141 | 0.52221 | -2.45440 |
| Au | -1.98668 | -0.36572 | -4.83254 |
| Cl | -2.94074 | -1.46573 | -6.55261 |
| C | 2.62686 | -0.29410 | 1.04022 |
| C | 2.88745 | -1.80353 | 0.98024 |
| C | 3.47713 | 0.43658 | 0.01555 |
| C | 2.93569 | 0.22659 | 2.44673 |
| H | 2.27013 | -2.35600 | 1.69505 |
| H | 2.70104 | -2.20134 | -0.01945 |
| H | 3.93486 | -1.99703 | 1.23592 |
| H | 3.23461 | 1.49964 | -0.04409 |
| H | 4.53368 | 0.35111 | 0.29259 |
| H | 3.38302 | 0.00184 | -0.98342 |
| H | 3.98456 | 0.03002 | 2.68755 |
| H | 2.77053 | 1.30437 | 2.52408 |
| H | 2.31968 | -0.26333 | 3.20552 |
| C | -2.10952 | -1.63902 | -1.20615 |
| C | -3.51915 | -1.50612 | -1.77707 |
| C | -1.29251 | -2.65637 | -1.99784 |
| C | -2.17553 | -2.04922 | 0.26468 |
| H | -4.13064 | -0.80724 | -1.20501 |
| H | -3.51291 | -1.20018 | -2.82572 |
| H | -3.99298 | -2.48997 | -1.72768 |
| H | -0.27826 | -2.76147 | -1.61088 |
| H | -1.79433 | -3.62403 | -1.91335 |
| H | -1.23296 | -2.40438 | -3.05782 |
| H | -2.66229 | -3.02722 | 0.30903 |

| | | | |
|----|----------|----------|----------|
| H | -1.18573 | -2.15118 | 0.71302 |
| H | -2.76226 | -1.35336 | 0.86522 |
| Cl | -2.44016 | 1.24239 | -0.20299 |
| S | -1.00208 | 0.82655 | -3.16346 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.85225 | -0.27979 | 1.22111 |
| C | 0.36695 | -0.21146 | -0.37789 |
| P | -1.28921 | -0.09879 | -0.86570 |
| Cl | 1.27007 | -1.52022 | -3.12529 |
| Si | 1.27005 | 0.31014 | -2.04052 |
| Au | -2.36719 | 0.41508 | -4.19131 |
| Cl | -3.72758 | -0.20641 | -5.87957 |
| C | 2.63978 | -0.43882 | 1.13873 |
| C | 3.34599 | 0.03149 | 2.25277 |
| C | 3.35044 | -0.98484 | 0.06341 |
| C | 4.72895 | -0.00010 | 2.27166 |
| H | 2.80118 | 0.43623 | 3.10016 |
| C | 4.73443 | -1.02235 | 0.09054 |
| H | 2.82161 | -1.42996 | -0.77249 |
| C | 5.42277 | -0.52346 | 1.18811 |
| H | 5.26809 | 0.37814 | 3.13225 |
| H | 5.27716 | -1.44914 | -0.74470 |
| H | 6.50619 | -0.55554 | 1.20533 |
| C | -2.04951 | -1.67929 | -1.21337 |
| C | -3.37615 | -1.72835 | -1.64171 |
| C | -1.30395 | -2.84597 | -1.07485 |
| C | -3.95044 | -2.95082 | -1.93373 |
| H | -3.95620 | -0.81970 | -1.75310 |
| C | -1.89329 | -4.06656 | -1.36521 |
| H | -0.27097 | -2.79890 | -0.75616 |
| C | -3.20958 | -4.11811 | -1.79547 |
| H | -4.97578 | -2.99113 | -2.28019 |
| H | -1.31551 | -4.97730 | -1.26325 |
| H | -3.66339 | -5.07388 | -2.03069 |
| Cl | -2.54553 | 0.78024 | 0.46627 |
| S | -1.02738 | 1.11655 | -2.49466 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.71571 | 0.24598 | 1.25883 |
| C | 0.38582 | -0.18340 | -0.30738 |
| P | -1.06333 | -0.05692 | -1.25537 |
| Au | -1.83996 | 1.49155 | -4.39522 |
| Cl | -3.36242 | 2.23507 | -5.88403 |
| C | 2.52759 | -0.05626 | 1.31607 |
| C | 3.03894 | -1.35898 | 1.45599 |
| C | 3.39855 | 1.04772 | 1.28068 |
| C | 4.41894 | -1.52917 | 1.50600 |
| C | 4.76808 | 0.82498 | 1.33404 |
| C | 5.29915 | -0.45637 | 1.43717 |
| H | 4.81535 | -2.53406 | 1.61621 |
| H | 5.43951 | 1.67810 | 1.30320 |
| C | -1.94944 | -1.63783 | -1.33403 |
| C | -2.53423 | -2.10152 | -0.13079 |
| C | -2.02023 | -2.43459 | -2.50241 |
| C | -3.16530 | -3.33831 | -0.12618 |
| C | -2.67817 | -3.65542 | -2.42220 |
| C | -3.25851 | -4.13066 | -1.25726 |
| H | -3.60151 | -3.68686 | 0.80463 |
| H | -2.72780 | -4.26241 | -3.32007 |
| C | 2.87060 | 2.44863 | 1.17520 |
| H | 2.42502 | 2.64383 | 0.19459 |
| H | 2.09006 | 2.64112 | 1.91778 |
| H | 3.66712 | 3.17750 | 1.32803 |
| C | 2.13963 | -2.55425 | 1.57062 |

| | | | |
|----|----------|----------|----------|
| H | 1.30224 | -2.36219 | 2.24745 |
| H | 1.71563 | -2.83403 | 0.60181 |
| H | 2.69271 | -3.41350 | 1.95155 |
| C | 6.78054 | -0.67369 | 1.46574 |
| H | 7.17487 | -0.78262 | 0.45059 |
| H | 7.29791 | 0.16890 | 1.92768 |
| H | 7.03934 | -1.58044 | 2.01466 |
| C | -2.56572 | -1.35020 | 1.16785 |
| H | -1.65734 | -0.78716 | 1.37847 |
| H | -3.39419 | -0.63857 | 1.18515 |
| H | -2.71338 | -2.05196 | 1.98946 |
| C | -1.44592 | -2.08892 | -3.84203 |
| H | -1.90244 | -1.19230 | -4.26517 |
| H | -0.36975 | -1.92511 | -3.79598 |
| H | -1.62721 | -2.91180 | -4.53291 |
| C | -3.97383 | -5.44384 | -1.23278 |
| H | -4.07905 | -5.82296 | -0.21544 |
| H | -4.97839 | -5.33997 | -1.65423 |
| H | -3.44835 | -6.19198 | -1.82939 |
| S | -0.25854 | 0.79151 | -2.91487 |
| Si | 1.87903 | -0.32707 | -1.53754 |
| Cl | 1.70243 | -2.44842 | -1.17108 |
| Cl | -2.42924 | 1.29469 | -0.57050 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -2.09743 | 1.77458 | 0.43722 |
| C | -1.13484 | 0.42349 | 0.24066 |
| P | 0.61545 | 0.33811 | 0.30741 |
| C | -3.78386 | 1.04855 | 0.38371 |
| C | -4.57682 | 1.25388 | -0.78090 |
| C | -4.25147 | 0.18768 | 1.40014 |
| C | -5.65247 | 0.40760 | -0.98784 |
| C | -5.33655 | -0.64216 | 1.10541 |
| C | -6.01282 | -0.59999 | -0.09652 |
| H | -6.23672 | 0.52113 | -1.88893 |
| H | -5.66683 | -1.33423 | 1.86715 |
| C | -3.82863 | 0.19516 | 2.88495 |
| C | -4.33573 | 2.40049 | -1.78092 |
| C | -7.14468 | -1.55828 | -0.44888 |
| C | -3.03098 | 2.22793 | -2.56023 |
| H | -2.14967 | 2.31079 | -1.91958 |
| H | -2.98665 | 1.25422 | -3.05104 |
| H | -2.94604 | 3.01151 | -3.31902 |
| C | -4.32432 | 3.73704 | -1.02596 |
| H | -5.26838 | 3.89026 | -0.49763 |
| H | -3.51524 | 3.80017 | -0.29550 |
| H | -4.19091 | 4.56151 | -1.73197 |
| C | -5.45463 | 2.49709 | -2.82161 |
| H | -5.48593 | 1.62409 | -3.47760 |
| H | -6.43672 | 2.62445 | -2.36047 |
| H | -5.27015 | 3.37004 | -3.45185 |
| C | -3.46618 | -1.20730 | 3.38455 |
| H | -2.61841 | -1.61781 | 2.83189 |
| H | -3.19776 | -1.16140 | 4.44356 |
| H | -4.29600 | -1.90906 | 3.28826 |
| C | -2.67599 | 1.12682 | 3.24421 |
| H | -1.71224 | 0.74983 | 2.90522 |
| H | -2.82441 | 2.14223 | 2.85829 |
| H | -2.61967 | 1.21554 | 4.33301 |
| C | -5.05067 | 0.70483 | 3.67272 |
| H | -5.31986 | 1.71781 | 3.36234 |
| H | -5.92467 | 0.06839 | 3.53059 |
| H | -4.81790 | 0.72500 | 4.74104 |
| C | -7.38524 | -2.59639 | 0.64368 |
| H | -7.70092 | -2.13569 | 1.58347 |
| H | -8.18029 | -3.27705 | 0.33023 |

| | | | |
|----|----------|----------|----------|
| H | -6.49238 | -3.19659 | 0.83533 |
| C | -6.78100 | -2.29763 | -1.74264 |
| H | -6.64287 | -1.60734 | -2.57716 |
| H | -5.85414 | -2.86313 | -1.62310 |
| H | -7.57840 | -2.99551 | -2.01286 |
| C | -8.44277 | -0.77052 | -0.66075 |
| H | -8.34854 | -0.04053 | -1.46722 |
| H | -9.25670 | -1.45214 | -0.92287 |
| H | -8.72798 | -0.23354 | 0.24743 |
| C | 2.00259 | 1.44524 | -0.08179 |
| C | 2.62959 | 1.24303 | -1.34871 |
| C | 2.75778 | 2.03446 | 0.96815 |
| C | 4.01419 | 1.22903 | -1.37093 |
| C | 4.14206 | 1.98733 | 0.86046 |
| C | 4.79870 | 1.47885 | -0.25063 |
| H | 4.50445 | 1.02028 | -2.31338 |
| H | 4.72758 | 2.37374 | 1.68326 |
| C | 1.92891 | 1.26272 | -2.72235 |
| C | 2.27230 | 0.05466 | -3.59622 |
| C | 2.46671 | 2.53216 | -3.41830 |
| H | 1.87928 | -0.87016 | -3.17582 |
| H | 1.83279 | 0.18949 | -4.58800 |
| H | 3.34934 | -0.06364 | -3.72714 |
| H | 2.25008 | 3.42572 | -2.82755 |
| H | 3.54357 | 2.48953 | -3.58376 |
| H | 1.97961 | 2.64028 | -4.39102 |
| C | 2.19583 | 2.90955 | 2.10583 |
| C | 2.74925 | 4.32323 | 1.82305 |
| C | 2.67208 | 2.48157 | 3.49598 |
| H | 2.44318 | 4.67363 | 0.83442 |
| H | 2.35474 | 5.01894 | 2.56856 |
| H | 3.83789 | 4.35763 | 1.87180 |
| H | 2.28693 | 1.50144 | 3.77409 |
| H | 3.76080 | 2.44613 | 3.56146 |
| H | 2.32275 | 3.20537 | 4.23702 |
| C | 6.30709 | 1.28925 | -0.31069 |
| C | 6.90569 | 2.26971 | -1.32703 |
| C | 6.60506 | -0.14997 | -0.75063 |
| H | 6.70670 | 3.30589 | -1.04141 |
| H | 7.98910 | 2.13357 | -1.38040 |
| H | 6.50191 | 2.11178 | -2.32928 |
| H | 6.17589 | -0.88020 | -0.06090 |
| H | 6.20446 | -0.36149 | -1.74403 |
| H | 7.68625 | -0.30738 | -0.78865 |
| Cl | -2.40777 | -1.48135 | -1.91246 |
| Au | 2.62671 | -2.51453 | -0.03443 |
| Cl | 4.53021 | -3.56046 | 0.59365 |
| C | 0.67922 | 3.05784 | 2.10241 |
| H | 0.30660 | 3.35242 | 1.11878 |
| H | 0.15582 | 2.15964 | 2.42390 |
| H | 0.39753 | 3.84786 | 2.80305 |
| C | 0.41637 | 1.43981 | -2.66377 |
| H | -0.11938 | 0.55019 | -2.33621 |
| H | 0.14233 | 2.27950 | -2.01999 |
| H | 0.04991 | 1.66675 | -3.66798 |
| C | 6.97025 | 1.52660 | 1.04344 |
| H | 6.86368 | 2.56158 | 1.37954 |
| H | 6.56228 | 0.86598 | 1.81218 |
| H | 8.03984 | 1.32033 | 0.96365 |
| Si | -1.58132 | -1.49992 | 0.05765 |
| Cl | 0.99377 | -0.25214 | 2.22829 |
| S | 0.77182 | -1.40902 | -0.75045 |

Coordination through P(sp²) atom
R= H

| | | | |
|----|----------|----------|----------|
| P | 0.47942 | 0.12544 | 1.07803 |
| C | 0.28697 | -0.28316 | -0.49835 |
| P | -1.11822 | -0.25028 | -1.51278 |
| Cl | 1.18298 | -2.74599 | -2.10429 |
| Si | 1.59238 | -0.65395 | -1.95867 |
| H | 1.85957 | -0.06017 | 1.31774 |
| H | -1.72137 | -1.51833 | -1.49207 |
| Cl | -2.65374 | 0.91380 | -0.93690 |
| Au | -0.90522 | 0.81178 | 2.63466 |
| Cl | -2.32013 | 1.50465 | 4.24345 |
| S | -0.28376 | 0.20140 | -3.24904 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.52275 | 0.13529 | 1.02100 |
| C | 0.31462 | -0.23121 | -0.56519 |
| P | -1.13965 | -0.27494 | -1.51213 |
| Cl | 1.49082 | -2.71429 | -1.98725 |
| Si | 1.59065 | -0.57051 | -2.03851 |
| Cl | -2.50143 | 1.15255 | -1.06253 |
| Au | -0.97595 | 0.71761 | 2.52423 |
| Cl | -2.51275 | 1.27341 | 4.08154 |
| C | 2.26098 | -0.08347 | 1.46118 |
| H | 2.37772 | -1.04930 | 1.96015 |
| H | 2.88987 | -0.06121 | 0.56867 |
| H | 2.55701 | 0.70010 | 2.15982 |
| C | -2.03634 | -1.80785 | -1.26688 |
| H | -2.86517 | -1.84904 | -1.97509 |
| H | -1.33727 | -2.62577 | -1.45352 |
| H | -2.41194 | -1.84743 | -0.24282 |
| S | -0.35923 | -0.07210 | -3.33326 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.81540 | 0.07919 | 0.74493 |
| C | 0.55418 | -0.56664 | -0.75224 |
| P | -0.99103 | -0.65528 | -1.56904 |
| Cl | 1.97572 | -3.06895 | -2.13851 |
| Si | 1.72297 | -0.95036 | -2.31544 |
| Au | -0.67962 | 1.01940 | 2.07693 |
| Cl | -2.20695 | 1.97966 | 3.44388 |
| C | 2.60032 | 0.05108 | 1.24105 |
| C | 2.66850 | 0.40493 | 2.72530 |
| C | 3.21782 | -1.32285 | 1.00024 |
| C | 3.31114 | 1.12681 | 0.41258 |
| H | 2.22901 | 1.38251 | 2.93533 |
| H | 2.15845 | -0.33536 | 3.34588 |
| H | 3.71850 | 0.43455 | 3.02983 |
| H | 3.22237 | -1.60307 | -0.05329 |
| H | 4.25651 | -1.30398 | 1.34441 |
| H | 2.69552 | -2.10666 | 1.55345 |
| H | 4.36051 | 1.16846 | 0.72095 |
| H | 3.28253 | 0.90435 | -0.65677 |
| H | 2.87737 | 2.11648 | 0.57578 |
| C | -2.13721 | -2.00170 | -1.01289 |
| C | -1.38708 | -3.32694 | -1.12387 |
| C | -2.57433 | -1.75729 | 0.42733 |
| C | -3.33888 | -1.99529 | -1.95685 |
| H | -1.05793 | -3.52786 | -2.14383 |
| H | -0.51185 | -3.36096 | -0.47383 |
| H | -2.06911 | -4.12576 | -0.81978 |
| H | -3.10589 | -0.81310 | 0.55073 |
| H | -3.25235 | -2.56485 | 0.71743 |
| H | -1.73053 | -1.77433 | 1.11966 |
| H | -3.98454 | -2.83592 | -1.68917 |
| H | -3.92507 | -1.07952 | -1.87025 |
| H | -3.03649 | -2.12513 | -2.99826 |
| Cl | -2.08403 | 1.04287 | -1.34846 |

S -0.36656 -0.86186 -3.45645

R = Ph

P 0.74722 -0.08728 0.96545
C 0.37310 -0.13181 -0.63997
P -1.22778 -0.13956 -1.32609
Cl 1.68976 -1.92976 -2.87170
Si 1.38497 0.12412 -2.31059
Au -0.63619 0.11516 2.67712
Cl -2.07220 0.26264 4.41865
C -2.02679 -1.74481 -1.20950
C -2.65100 -2.13423 -0.02448
C -1.95740 -2.61578 -2.29247
C -3.20732 -3.39758 0.06784
H -2.71114 -1.45704 0.81996
C -2.52043 -3.87813 -2.18865
H -1.46407 -2.30641 -3.20568
C -3.14292 -4.26789 -1.01286
H -3.69591 -3.70049 0.98619
H -2.47006 -4.55720 -3.03139
H -3.58325 -5.25545 -0.93622
C 2.49807 -0.22357 1.24085
C 3.37166 -0.78643 0.30511
C 2.99718 0.27336 2.44946
C 4.72939 -0.82180 0.57087
H 2.99083 -1.23639 -0.60406
C 4.35591 0.23637 2.70339
H 2.31502 0.69261 3.18186
C 5.22147 -0.30657 1.76257
H 5.40455 -1.26273 -0.15276
H 4.74071 0.62796 3.63742
H 6.28588 -0.33943 1.96513
Cl -2.50910 1.12169 -0.39320
S -0.81934 0.44411 -3.18547

R = Mes

P 0.84042 -0.17994 1.38500
C 0.50540 -0.56781 -0.17847
P -0.99400 -0.45776 -1.07293
Cl 1.66376 -2.58462 -2.22608
Si 1.79284 -0.50250 -1.67813
Au -0.53706 0.16100 3.07518
Cl -1.91945 0.46720 4.83948
C -1.98352 -1.93825 -1.37123
C -1.83991 -3.11229 -0.60463
C -2.94317 -1.87701 -2.40551
C -2.62998 -4.20791 -0.92443
C -3.70521 -3.00717 -2.66720
C -3.55846 -4.18676 -1.95417
H -2.51679 -5.11034 -0.33240
H -4.44564 -2.95411 -3.45913
C 2.62422 -0.11522 1.61553
C 3.34441 -1.28746 1.88206
C 3.25599 1.13794 1.59745
C 4.70767 -1.18009 2.12106
C 4.62028 1.18962 1.83947
C 5.36410 0.04414 2.09983
H 5.27209 -2.08243 2.33544
H 5.11655 2.15519 1.82666
C -0.89750 -3.26172 0.54873
H 0.14011 -3.16601 0.22653
H -1.08083 -2.51690 1.32637
H -1.02281 -4.24620 0.99946
C -3.20858 -0.66896 -3.25559
H -3.19915 0.26471 -2.69256
H -2.46469 -0.57662 -4.05029

H -4.18982 -0.76182 -3.72230
C -4.36749 -5.39952 -2.28869
H -5.31797 -5.13011 -2.75165
H -3.82585 -6.03576 -2.99564
H -4.57175 -5.99956 -1.40038
C 6.84087 0.12757 2.33072
H 7.11334 1.05652 2.83470
H 7.19863 -0.70949 2.93210
H 7.37946 0.10243 1.37827
C 2.68402 -2.63194 1.90013
H 1.73043 -2.61120 2.43717
H 2.48187 -2.98094 0.88278
H 3.32192 -3.37130 2.38536
C 2.49304 2.39144 1.29795
H 2.16547 2.40896 0.25367
H 1.59854 2.48299 1.92290
H 3.10965 3.27403 1.46934
S -0.17840 0.34647 -2.72063
Cl -2.29805 0.81756 -0.15408

R = Mes*

P -1.17730 0.65110 0.10483
C -0.39219 -0.77719 0.36850
P 1.29803 -1.23122 0.56265
Cl -1.92970 -2.89930 -1.48406
C 2.91092 -0.51969 0.08869
C 3.46375 -1.03161 -1.12526
C 3.79028 0.03188 1.06123
C 4.81476 -1.33919 -1.12718
C 5.13213 -0.32902 0.97923
C 5.65443 -1.09816 -0.04697
H 5.23335 -1.77329 -2.02629
H 5.79635 0.03249 1.75134
C -2.95322 0.27810 0.15452
C -3.71084 0.15027 -1.04169
C -3.50735 -0.13499 1.39270
C -4.87803 -0.60063 -0.98078
C -4.66463 -0.90443 1.35267
C -5.33626 -1.20525 0.18082
H -5.44174 -0.74456 -1.88729
H -5.06079 -1.27656 2.28872
C -3.37812 0.86406 -2.36570
C -3.05023 0.28658 2.80659
C -6.54699 -2.13117 0.20840
C 3.48157 1.15912 2.07058
C 2.77009 -1.08045 -2.50281
C 7.09823 -1.58160 -0.07207
C -4.25649 0.96222 3.48729
H -3.96732 1.29572 4.48733
H -4.58614 1.83593 2.91965
H -5.10905 0.29236 3.59713
C -1.93061 1.32295 2.85437
H -0.95436 0.90980 2.59961
H -2.13509 2.18600 2.21457
H -1.84277 1.69934 3.87732
C -2.62535 -0.92836 3.63573
H -3.42650 -1.66531 3.71595
H -1.76207 -1.42932 3.19370
H -2.35952 -0.61102 4.64805
C -7.63079 -1.54131 1.11822
H -8.49923 -2.20519 1.14501
H -7.27806 -1.41593 2.14390
H -7.96024 -0.56505 0.75394
C -7.14773 -2.34279 -1.17873
H -7.99187 -3.03265 -1.10685
H -7.52236 -1.41046 -1.60925

| | | | |
|----|----------|----------|----------|
| H | -6.42318 | -2.77753 | -1.87149 |
| C | -6.10653 | -3.49475 | 0.75528 |
| H | -5.32923 | -3.93468 | 0.12631 |
| H | -5.70838 | -3.41475 | 1.76883 |
| H | -6.95775 | -4.18073 | 0.78221 |
| C | -4.40873 | 0.56355 | -3.45866 |
| H | -5.41696 | 0.87496 | -3.17693 |
| H | -4.13421 | 1.12520 | -4.35416 |
| H | -4.42833 | -0.49525 | -3.72780 |
| C | -3.43230 | 2.37765 | -2.11689 |
| H | -4.42453 | 2.67454 | -1.76814 |
| H | -2.70484 | 2.70466 | -1.37075 |
| H | -3.21780 | 2.91891 | -3.04211 |
| C | -2.02211 | 0.46599 | -2.95041 |
| H | -1.17829 | 0.76710 | -2.32691 |
| H | -1.95738 | -0.61160 | -3.10404 |
| H | -1.88099 | 0.96965 | -3.91087 |
| C | 2.05152 | 1.68124 | 2.04252 |
| H | 1.73699 | 1.89720 | 1.01884 |
| H | 1.33105 | 1.01233 | 2.50465 |
| H | 2.00567 | 2.62640 | 2.58798 |
| C | 4.34919 | 2.35113 | 1.60626 |
| H | 4.15921 | 3.20543 | 2.26091 |
| H | 5.41605 | 2.12933 | 1.64155 |
| H | 4.09352 | 2.64751 | 0.58654 |
| C | 3.87943 | 0.80804 | 3.50664 |
| H | 4.93581 | 0.54499 | 3.58749 |
| H | 3.70938 | 1.67585 | 4.14913 |
| H | 3.29382 | -0.02265 | 3.89898 |
| C | 1.32456 | -0.60036 | -2.51796 |
| H | 1.01602 | -0.45774 | -3.55653 |
| H | 0.62735 | -1.31392 | -2.08232 |
| H | 1.21994 | 0.36571 | -2.01626 |
| C | 2.84704 | -2.46026 | -3.16024 |
| H | 2.27967 | -3.19968 | -2.59528 |
| H | 2.42445 | -2.40478 | -4.16684 |
| H | 3.87503 | -2.81529 | -3.25528 |
| C | 3.54974 | -0.07380 | -3.37634 |
| H | 3.51537 | 0.92913 | -2.94417 |
| H | 4.59631 | -0.35313 | -3.50201 |
| H | 3.09089 | -0.03152 | -4.36759 |
| C | 7.84653 | -1.23572 | 1.21241 |
| H | 7.94051 | -0.15601 | 1.35369 |
| H | 7.35638 | -1.65830 | 2.09304 |
| H | 8.85751 | -1.64698 | 1.16619 |
| C | 7.83744 | -0.93876 | -1.25187 |
| H | 7.38242 | -1.20041 | -2.20915 |
| H | 7.84022 | 0.15058 | -1.16681 |
| H | 8.87555 | -1.28116 | -1.27299 |
| C | 7.10266 | -3.10618 | -0.23860 |
| H | 6.59043 | -3.59282 | 0.59477 |
| H | 6.60690 | -3.41401 | -1.16132 |
| H | 8.13091 | -3.47634 | -0.27028 |
| Au | -0.28515 | 2.63797 | -0.35684 |
| Cl | 0.64063 | 4.65413 | -0.84272 |
| Si | -1.13959 | -2.64134 | 0.49817 |
| S | 1.13900 | -3.11493 | -0.08331 |
| Cl | 1.44277 | -1.45281 | 2.60361 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.62478 | 0.20211 | 1.07577 |
| C | 0.32360 | -0.00516 | -0.61658 |
| P | -1.18927 | -0.30757 | -1.43198 |
| Cl | 1.20843 | -2.67972 | -1.89312 |

| | | | |
|----|----------|----------|----------|
| Si | 1.43760 | -0.56971 | -2.18437 |
| H | 2.02641 | -0.07338 | 1.02576 |
| H | -1.58394 | -1.62044 | -1.12916 |
| Cl | -2.82442 | 0.72047 | -0.84345 |
| Au | 0.72122 | 2.09097 | -0.35678 |
| Cl | 1.09077 | 4.28850 | -0.61972 |
| S | -0.64646 | -0.07591 | -3.32050 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.65747 | 0.24799 | 0.96127 |
| C | 0.31385 | 0.01064 | -0.71847 |
| P | -1.22496 | -0.37669 | -1.45442 |
| Cl | 1.55466 | -2.61407 | -1.88312 |
| Si | 1.41916 | -0.50519 | -2.29587 |
| Cl | -2.76420 | 0.87892 | -1.02943 |
| Au | 0.65453 | 2.12736 | -0.50301 |
| Cl | 0.98583 | 4.33901 | -0.73611 |
| C | 2.43888 | -0.16541 | 1.07937 |
| H | 2.88671 | 0.41705 | 1.88640 |
| H | 2.50694 | -1.22556 | 1.34448 |
| H | 2.98875 | -0.00227 | 0.15104 |
| C | -1.82657 | -1.96403 | -0.87420 |
| H | -2.07703 | -1.89081 | 0.18551 |
| H | -2.71152 | -2.23404 | -1.45196 |
| H | -1.03288 | -2.69644 | -1.03500 |
| S | -0.70500 | -0.36784 | -3.37627 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.59284 | 0.29477 | 0.85546 |
| C | 0.35940 | 0.11124 | -0.85804 |
| P | -1.20848 | -0.30187 | -1.56500 |
| Cl | 2.17501 | -1.94761 | -2.55162 |
| Si | 1.41043 | 0.05713 | -2.54838 |
| Au | 0.55266 | 2.24596 | -0.50567 |
| Cl | 0.81228 | 4.48393 | -0.50337 |
| C | 2.39210 | 0.00730 | 1.26868 |
| C | 2.50033 | -1.50828 | 1.47240 |
| C | 3.41440 | 0.48372 | 0.25084 |
| C | 2.60334 | 0.72860 | 2.60215 |
| H | 1.75055 | -1.88463 | 2.17544 |
| H | 2.39858 | -2.04605 | 0.52736 |
| H | 3.48463 | -1.74226 | 1.89085 |
| H | 3.34410 | 1.55880 | 0.07338 |
| H | 4.42111 | 0.27337 | 0.62842 |
| H | 3.32185 | -0.03560 | -0.70536 |
| H | 3.60519 | 0.50477 | 2.98032 |
| H | 2.52099 | 1.81254 | 2.49005 |
| H | 1.88083 | 0.40913 | 3.35817 |
| C | -1.93919 | -1.91181 | -1.00020 |
| C | -3.13634 | -2.20735 | -1.90326 |
| C | -0.87847 | -2.99700 | -1.16684 |
| C | -2.37886 | -1.81375 | 0.45772 |
| H | -3.92314 | -1.45825 | -1.80105 |
| H | -2.84441 | -2.27131 | -2.95318 |
| H | -3.55227 | -3.17502 | -1.60989 |
| H | -0.01088 | -2.82819 | -0.52754 |
| H | -1.32647 | -3.95366 | -0.88397 |
| H | -0.52880 | -3.07515 | -2.19661 |
| H | -2.75876 | -2.79283 | 0.76289 |
| H | -1.55260 | -1.55588 | 1.12329 |
| H | -3.17593 | -1.08350 | 0.59898 |
| Cl | -2.67266 | 1.04881 | -1.13506 |
| S | -0.75076 | -0.27322 | -3.50700 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.65420 | 0.20093 | 1.06346 |
| C | 0.20028 | 0.20575 | -0.60991 |
| P | -1.44178 | -0.00264 | -1.18708 |
| Cl | 1.20626 | -1.83595 | -2.89086 |
| Si | 1.03859 | 0.25744 | -2.42400 |
| Au | 0.58511 | 2.28150 | -0.11246 |
| Cl | 0.94636 | 4.50201 | -0.00417 |
| C | 2.42582 | -0.14724 | 1.11642 |
| C | 3.09593 | 0.30919 | 2.25635 |
| C | 3.12831 | -0.87148 | 0.15175 |
| C | 4.45207 | 0.08123 | 2.40760 |
| H | 2.55149 | 0.85858 | 3.01823 |
| C | 4.48332 | -1.10807 | 0.31544 |
| H | 2.61490 | -1.27903 | -0.71075 |
| C | 5.14668 | -0.62640 | 1.43543 |
| H | 4.96798 | 0.45204 | 3.28549 |
| H | 5.02252 | -1.67258 | -0.43633 |
| H | 6.20810 | -0.81061 | 1.55600 |
| C | -1.98912 | -1.70607 | -1.01936 |
| C | -2.21783 | -2.48187 | -2.14925 |
| C | -2.16975 | -2.24105 | 0.25580 |
| C | -2.63156 | -3.79706 | -2.00159 |
| H | -2.06344 | -2.05883 | -3.13417 |
| C | -2.57784 | -3.55530 | 0.39277 |
| H | -1.99808 | -1.63334 | 1.13773 |
| C | -2.80974 | -4.33218 | -0.73578 |
| H | -2.80962 | -4.40423 | -2.88105 |
| H | -2.71821 | -3.97460 | 1.38198 |
| H | -3.13104 | -5.36144 | -0.62440 |
| Cl | -2.83696 | 1.04495 | -0.14080 |
| S | -1.24551 | 0.61806 | -3.06674 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.61996 | 0.13967 | 1.60858 |
| C | 0.01612 | 0.27490 | -0.01679 |
| P | -1.56650 | 0.06414 | -0.77317 |
| Cl | 1.30835 | -1.13767 | -2.63743 |
| Si | 1.02199 | 0.77305 | -1.67954 |
| Au | 0.06481 | 2.30113 | 0.76730 |
| Cl | -0.04647 | 4.52170 | 1.17234 |
| C | 2.41433 | -0.10067 | 1.37280 |
| C | 3.37417 | 0.84677 | 1.76344 |
| C | 2.81681 | -1.38401 | 0.95313 |
| C | 4.71922 | 0.52503 | 1.62579 |
| C | 4.17250 | -1.65459 | 0.84008 |
| C | 5.14115 | -0.70698 | 1.14663 |
| H | 5.46058 | 1.26374 | 1.91543 |
| H | 4.47956 | -2.64438 | 0.51559 |
| C | -1.99289 | -1.67696 | -1.03923 |
| C | -2.16649 | -2.23788 | -2.32711 |
| C | -2.13112 | -2.49555 | 0.10537 |
| C | -2.37517 | -3.60826 | -2.41983 |
| C | -2.32724 | -3.85955 | -0.06380 |
| C | -2.43115 | -4.44375 | -1.31502 |
| H | -2.50299 | -4.03557 | -3.40905 |
| H | -2.41890 | -4.47900 | 0.82292 |
| C | 3.01097 | 2.18560 | 2.32795 |
| H | 2.73724 | 2.89822 | 1.54430 |
| H | 2.16344 | 2.12767 | 3.01611 |
| H | 3.85475 | 2.60905 | 2.87468 |
| C | 1.82934 | -2.48049 | 0.67961 |
| H | 1.09433 | -2.57163 | 1.48667 |
| H | 1.28128 | -2.31465 | -0.25026 |
| H | 2.34281 | -3.43899 | 0.59488 |
| C | 6.59645 | -1.00972 | 0.96963 |
| H | 7.21385 | -0.40721 | 1.63788 |

| | | | |
|----|----------|----------|----------|
| H | 6.81071 | -2.06352 | 1.15742 |
| H | 6.91155 | -0.79066 | -0.05543 |
| C | -2.17860 | -1.99459 | 1.51820 |
| H | -1.89357 | -2.79143 | 2.20625 |
| H | -1.53520 | -1.14126 | 1.72284 |
| H | -3.19781 | -1.68738 | 1.76884 |
| C | -2.18451 | -1.48192 | -3.62288 |
| H | -2.87160 | -0.63624 | -3.59960 |
| H | -1.19868 | -1.09407 | -3.88017 |
| H | -2.50344 | -2.15356 | -4.42045 |
| C | -2.60162 | -5.92121 | -1.47195 |
| H | -1.63127 | -6.40137 | -1.63258 |
| H | -3.04720 | -6.36928 | -0.58263 |
| H | -3.22848 | -6.16030 | -2.33277 |
| S | -1.21906 | 1.24634 | -2.34899 |
| Cl | -3.16512 | 0.82581 | 0.25742 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.68880 | 0.23202 | 0.99258 |
| C | 0.43514 | 0.13511 | -0.74565 |
| P | -1.13396 | -0.09323 | -1.62948 |
| Cl | 2.78080 | -0.81485 | -3.02666 |
| Au | 0.53459 | 2.28821 | -0.33601 |
| Cl | 0.42489 | 4.55150 | -0.10084 |
| C | 2.52074 | 0.06628 | 1.16768 |
| C | 3.20164 | -1.10285 | 0.72790 |
| C | 3.29828 | 1.16944 | 1.60675 |
| C | 4.53937 | -0.98897 | 0.38428 |
| C | 4.63456 | 1.21630 | 1.20655 |
| C | 5.25845 | 0.19268 | 0.51712 |
| H | 5.04964 | -1.86787 | 0.01140 |
| H | 5.20917 | 2.09197 | 1.47253 |
| C | 2.90202 | 2.23225 | 2.65494 |
| C | 2.66916 | -2.54474 | 0.85189 |
| C | 6.68734 | 0.28736 | -0.00389 |
| C | 3.78035 | 1.92566 | 3.88615 |
| H | 3.58496 | 0.91960 | 4.26677 |
| H | 4.84453 | 1.99774 | 3.65847 |
| H | 3.55437 | 2.64177 | 4.68105 |
| C | 3.20302 | 3.65841 | 2.18594 |
| H | 2.61887 | 3.92774 | 1.30606 |
| H | 2.94533 | 4.36286 | 2.98158 |
| H | 4.25982 | 3.80278 | 1.95568 |
| C | 1.46162 | 2.18151 | 3.15611 |
| H | 1.37156 | 2.84789 | 4.01841 |
| H | 0.73858 | 2.52898 | 2.41788 |
| H | 1.17784 | 1.18043 | 3.49161 |
| C | 2.95813 | -3.38724 | -0.39283 |
| H | 2.51990 | -2.94239 | -1.28447 |
| H | 4.02804 | -3.50439 | -0.57116 |
| H | 2.54228 | -4.39022 | -0.26111 |
| C | 3.42753 | -3.15974 | 2.04424 |
| H | 4.50545 | -3.16160 | 1.87631 |
| H | 3.23204 | -2.60083 | 2.96291 |
| H | 3.10335 | -4.19369 | 2.19618 |
| C | 1.18756 | -2.67388 | 1.18368 |
| H | 0.91544 | -2.11101 | 2.08206 |
| H | 0.54625 | -2.36079 | 0.36131 |
| H | 0.96030 | -3.72411 | 1.38868 |
| C | 7.30248 | 1.66208 | 0.24334 |
| H | 6.71616 | 2.45713 | -0.22366 |
| H | 7.39568 | 1.88293 | 1.30992 |
| H | 8.30667 | 1.69426 | -0.18617 |
| C | 6.67565 | 0.02814 | -1.51525 |
| H | 7.69300 | 0.08052 | -1.91342 |
| H | 6.26966 | -0.95702 | -1.75303 |

| | | | |
|----|----------|----------|----------|
| H | 6.06487 | 0.76955 | -2.03520 |
| C | 7.56468 | -0.76423 | 0.68529 |
| H | 7.58456 | -0.61021 | 1.76715 |
| H | 7.20868 | -1.77894 | 0.49595 |
| H | 8.59090 | -0.69849 | 0.31315 |
| C | -2.36610 | -1.47588 | -1.68097 |
| C | -2.35456 | -2.31940 | -2.83401 |
| C | -3.58471 | -1.35273 | -0.95794 |
| C | -3.57404 | -2.59384 | -3.43360 |
| C | -1.16455 | -3.15623 | -3.34214 |
| C | -4.76352 | -1.69305 | -1.61323 |
| C | -3.73095 | -1.07284 | 0.54926 |
| C | -4.79576 | -2.20608 | -2.89943 |
| H | -3.56384 | -3.17285 | -4.34863 |
| C | -0.80203 | -2.89444 | -4.80534 |
| C | -1.61395 | -4.62955 | -3.22516 |
| C | 0.06428 | -3.04332 | -2.45616 |
| H | -5.69366 | -1.54787 | -1.08227 |
| C | -2.42693 | -0.75183 | 1.25844 |
| C | -4.22785 | -2.40526 | 1.14922 |
| C | -4.75800 | 0.01503 | 0.87375 |
| C | -6.08692 | -2.44399 | -3.67022 |
| H | -0.06723 | -3.63426 | -5.13349 |
| H | -1.67402 | -2.98274 | -5.45727 |
| H | -0.37080 | -1.90519 | -4.94418 |
| H | -2.42087 | -4.87958 | -3.91463 |
| H | -0.76421 | -5.27645 | -3.45903 |
| H | -1.94889 | -4.86131 | -2.21128 |
| H | 0.51200 | -2.05273 | -2.45404 |
| H | -0.17274 | -3.33590 | -1.43124 |
| H | 0.83583 | -3.72373 | -2.82338 |
| H | -1.65260 | -1.48641 | 1.02705 |
| H | -2.05366 | 0.24511 | 1.03296 |
| H | -2.58282 | -0.78066 | 2.33961 |
| H | -4.32586 | -2.29736 | 2.23283 |
| H | -5.19820 | -2.70069 | 0.74841 |
| H | -3.51919 | -3.21283 | 0.94987 |
| H | -5.74762 | -0.21541 | 0.47600 |
| H | -4.85633 | 0.10369 | 1.95874 |
| H | -4.45269 | 0.98581 | 0.48432 |
| C | -7.31225 | -1.93548 | -2.91555 |
| C | -6.26633 | -3.94453 | -3.93071 |
| C | -6.00038 | -1.70223 | -5.00973 |
| H | -7.46925 | -2.47566 | -1.97839 |
| H | -7.23574 | -0.86874 | -2.69112 |
| H | -8.20414 | -2.08221 | -3.52899 |
| H | -5.44692 | -4.35628 | -4.52305 |
| H | -6.31794 | -4.50249 | -2.99256 |
| H | -7.19444 | -4.11907 | -4.48158 |
| H | -5.88389 | -0.62696 | -4.85549 |
| H | -5.15574 | -2.04753 | -5.60920 |
| H | -6.91299 | -1.86708 | -5.58871 |
| Cl | -2.41976 | 1.46133 | -1.23611 |
| Si | 1.53188 | 0.75819 | -2.29431 |
| S | -0.44371 | 0.29573 | -3.47393 |

[R-P=C(Si(II)Cl)-P(S)MeR](AuCl)

Coordination through Si(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.75394 | 0.26943 | 0.84892 |
| C | 0.42809 | -0.15575 | -0.72338 |
| P | -1.15679 | -0.24132 | -1.48835 |
| Cl | 1.60496 | -2.37095 | -2.55308 |
| Si | 1.47617 | -0.30348 | -2.32355 |

| | | | |
|----|----------|----------|----------|
| H | 2.17646 | 0.30539 | 0.72701 |
| H | -1.69274 | -1.53930 | -1.35932 |
| Au | 3.21606 | 1.04096 | -2.75330 |
| Cl | 4.98518 | 2.45186 | -3.11433 |
| C | -2.43698 | 0.83975 | -0.84582 |
| H | -3.34328 | 0.72267 | -1.44298 |
| H | -2.64680 | 0.57218 | 0.19257 |
| H | -2.08989 | 1.87190 | -0.90190 |
| S | -0.55546 | 0.15121 | -3.36741 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.71269 | 0.13905 | 0.83425 |
| C | 0.37516 | -0.15845 | -0.76542 |
| P | -1.24249 | -0.25286 | -1.45573 |
| Cl | 1.70538 | -2.28495 | -2.63123 |
| Si | 1.35038 | -0.23471 | -2.40736 |
| C | -2.40415 | 0.98323 | -0.85725 |
| H | -3.34394 | 0.89898 | -1.40652 |
| H | -2.58758 | 0.82583 | 0.20808 |
| H | -1.97692 | 1.97351 | -1.01448 |
| C | 2.53694 | 0.16553 | 0.91129 |
| H | 2.98236 | 0.55899 | -0.00637 |
| H | 2.85284 | 0.76295 | 1.76774 |
| H | 2.89350 | -0.85827 | 1.06329 |
| C | -2.00235 | -1.86199 | -1.18580 |
| H | -2.21660 | -1.99284 | -0.12262 |
| H | -2.92589 | -1.93459 | -1.76346 |
| H | -1.30223 | -2.62909 | -1.51860 |
| Au | 2.96870 | 1.24088 | -2.91477 |
| Cl | 4.62093 | 2.77889 | -3.33527 |
| S | -0.70877 | 0.03298 | -3.38904 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.71338 | 0.00488 | 0.64588 |
| C | 0.53946 | -0.40414 | -0.95873 |
| P | -1.08102 | -0.48123 | -1.68335 |
| Cl | 2.14366 | -2.55152 | -2.69361 |
| Si | 1.54595 | -0.55347 | -2.58531 |
| C | -2.03553 | 1.01718 | -1.37023 |
| H | -2.98137 | 0.98737 | -1.91271 |
| H | -2.22028 | 1.12631 | -0.30040 |
| H | -1.44439 | 1.86211 | -1.72433 |
| Au | 2.96588 | 1.07578 | -3.22282 |
| Cl | 4.38710 | 2.79524 | -3.78342 |
| C | 2.51703 | 0.15142 | 1.08230 |
| C | 3.44782 | -0.77196 | 0.31281 |
| C | 2.87788 | 1.62168 | 0.83692 |
| C | 2.58792 | -0.15427 | 2.58127 |
| H | 3.14121 | -1.81782 | 0.37906 |
| H | 3.51611 | -0.49596 | -0.74140 |
| H | 4.45806 | -0.68999 | 0.72738 |
| H | 2.20012 | 2.30451 | 1.35850 |
| H | 3.88713 | 1.80824 | 1.21828 |
| H | 2.87113 | 1.86729 | -0.22729 |
| H | 3.60564 | 0.02717 | 2.93902 |
| H | 1.91126 | 0.48007 | 3.16038 |
| H | 2.34049 | -1.19771 | 2.79458 |
| C | -2.10891 | -1.93715 | -1.18838 |
| C | -3.30476 | -2.01590 | -2.13729 |
| C | -1.25712 | -3.19715 | -1.31584 |
| C | -2.57640 | -1.75442 | 0.25481 |
| H | -3.96336 | -1.14873 | -2.05253 |
| H | -2.98826 | -2.11625 | -3.17770 |
| H | -3.89464 | -2.90040 | -1.88166 |
| H | -0.40071 | -3.17944 | -0.64012 |
| H | -1.87524 | -4.06239 | -1.06104 |

| | | | |
|---|----------|----------|----------|
| H | -0.88262 | -3.33288 | -2.33160 |
| H | -3.11417 | -2.65543 | 0.56281 |
| H | -1.73985 | -1.61718 | 0.94435 |
| H | -3.25989 | -0.91034 | 0.36582 |
| S | -0.48940 | -0.57730 | -3.62445 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.86727 | -0.35721 | 0.42567 |
| C | 0.49725 | -0.27810 | -1.19941 |
| P | -1.19745 | -0.36990 | -1.70006 |
| Cl | 2.12119 | -2.15790 | -3.11757 |
| Si | 1.27385 | -0.25724 | -2.94558 |
| C | -2.10420 | 1.14313 | -1.33987 |
| H | -3.09619 | 1.10854 | -1.79343 |
| H | -2.18405 | 1.28784 | -0.26074 |
| H | -1.53781 | 1.96837 | -1.77301 |
| Au | 2.38156 | 1.52008 | -3.77716 |
| Cl | 3.50805 | 3.36695 | -4.55804 |
| C | -2.11733 | -1.74963 | -1.00400 |
| C | -1.65133 | -3.03886 | -1.26433 |
| C | -3.25000 | -1.56395 | -0.21599 |
| C | -2.31631 | -4.13002 | -0.73563 |
| H | -0.77175 | -3.18220 | -1.88356 |
| C | -3.91249 | -2.66341 | 0.30923 |
| H | -3.62377 | -0.56922 | -0.00656 |
| C | -3.44659 | -3.94283 | 0.05040 |
| H | -1.95413 | -5.13061 | -0.93963 |
| H | -4.79484 | -2.51738 | 0.92099 |
| H | -3.96705 | -4.80034 | 0.46108 |
| C | 2.64533 | -0.25343 | 0.63419 |
| C | 3.09457 | -0.61526 | 1.91071 |
| C | 3.57374 | 0.18070 | -0.31725 |
| C | 4.44355 | -0.57528 | 2.21932 |
| H | 2.37597 | -0.93293 | 2.66016 |
| C | 4.91771 | 0.23367 | -0.00044 |
| H | 3.25028 | 0.50458 | -1.30121 |
| C | 5.35424 | -0.15091 | 1.26272 |
| H | 4.78352 | -0.86712 | 3.20602 |
| H | 5.62796 | 0.58014 | -0.74189 |
| H | 6.41070 | -0.11040 | 1.50279 |
| S | -0.86012 | -0.57445 | -3.69075 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.83983 | 0.63401 | 0.28743 |
| C | 0.54026 | -0.49847 | -0.89992 |
| P | -0.96828 | -0.71549 | -1.82393 |
| Cl | 1.58119 | -3.40989 | -1.52984 |
| Si | 1.73209 | -1.39065 | -2.09476 |
| C | -1.92013 | 0.79205 | -2.11404 |
| H | -2.69043 | 0.56676 | -2.85477 |
| H | -2.38985 | 1.15983 | -1.20417 |
| H | -1.23988 | 1.54436 | -2.51406 |
| Au | 3.74558 | -0.60729 | -2.72558 |
| Cl | 5.80204 | 0.26604 | -3.30185 |
| C | -2.10053 | -1.97108 | -1.14049 |
| C | -2.40870 | -3.18915 | -1.79149 |
| C | -2.67386 | -1.69727 | 0.12086 |
| C | -3.24216 | -4.09123 | -1.14142 |
| C | -3.49050 | -2.64839 | 0.71903 |
| C | -3.78251 | -3.85810 | 0.11396 |
| H | -3.47402 | -5.02287 | -1.64735 |
| H | -3.91305 | -2.42366 | 1.69357 |
| C | 2.61580 | 0.48670 | 0.61607 |
| C | 3.12392 | -0.57586 | 1.37789 |
| C | 3.46102 | 1.51063 | 0.15987 |
| C | 4.48987 | -0.61277 | 1.62569 |

| | | | |
|---|----------|----------|----------|
| C | 4.81778 | 1.42443 | 0.42686 |
| C | 5.35489 | 0.36157 | 1.14296 |
| H | 4.89138 | -1.43458 | 2.21113 |
| H | 5.47810 | 2.19247 | 0.03698 |
| C | 2.23998 | -1.65499 | 1.93120 |
| H | 1.33779 | -1.24333 | 2.39457 |
| H | 1.91439 | -2.34973 | 1.15240 |
| H | 2.77020 | -2.23136 | 2.69042 |
| C | 2.93207 | 2.64323 | -0.66592 |
| H | 2.79766 | 2.32935 | -1.70609 |
| H | 1.96274 | 3.00052 | -0.29925 |
| H | 3.62376 | 3.48628 | -0.66417 |
| C | 6.83228 | 0.26210 | 1.35716 |
| H | 7.32709 | -0.01580 | 0.42175 |
| H | 7.25385 | 1.21851 | 1.67472 |
| H | 7.07957 | -0.49053 | 2.10711 |
| C | -2.51339 | -0.40892 | 0.87496 |
| H | -1.56368 | 0.09839 | 0.71109 |
| H | -3.31483 | 0.29021 | 0.61551 |
| H | -2.58960 | -0.59426 | 1.94711 |
| C | -1.92579 | -3.60805 | -3.14981 |
| H | -2.14703 | -2.86963 | -3.92050 |
| H | -0.84843 | -3.77566 | -3.16352 |
| H | -2.41647 | -4.54026 | -3.43052 |
| C | -4.63428 | -4.88422 | 0.79132 |
| H | -5.26077 | -5.41716 | 0.07378 |
| H | -4.00855 | -5.62909 | 1.29258 |
| H | -5.27919 | -4.43336 | 1.54685 |
| S | 0.00675 | -1.14478 | -3.56128 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.39879 | 1.43168 | 1.47185 |
| C | 0.16549 | 0.39367 | 0.28887 |
| P | 1.78787 | -0.33580 | 0.10515 |
| Cl | -1.22012 | 0.84146 | -2.61418 |
| C | 3.48608 | 0.35175 | 0.22170 |
| C | 4.13110 | 0.75887 | -0.98218 |
| C | 4.30126 | -0.02252 | 1.32383 |
| C | 5.45051 | 0.36963 | -1.16320 |
| C | 5.62050 | -0.38023 | 1.06456 |
| C | 6.19180 | -0.29699 | -0.19580 |
| H | 5.92639 | 0.62116 | -2.10286 |
| H | 6.22589 | -0.72042 | 1.89350 |
| C | -2.19596 | 1.49109 | 1.12443 |
| C | -2.73436 | 2.54339 | 0.35071 |
| C | -3.03418 | 0.42966 | 1.55811 |
| C | -3.99215 | 2.35141 | -0.21640 |
| C | -4.26764 | 0.30023 | 0.93468 |
| C | -4.73871 | 1.20249 | -0.01141 |
| H | -4.39459 | 3.12159 | -0.85473 |
| H | -4.88721 | -0.54668 | 1.18828 |
| C | -2.06083 | 3.92402 | 0.21707 |
| C | -2.75581 | -0.42440 | 2.81586 |
| C | -6.04961 | 0.92395 | -0.73786 |
| C | 3.93358 | 0.13831 | 2.81331 |
| C | 3.58480 | 1.77531 | -2.00444 |
| C | 7.59455 | -0.80051 | -0.50945 |
| C | -3.86438 | -1.45188 | 3.06229 |
| H | -3.63881 | -1.99362 | 3.98379 |
| H | -4.83961 | -0.97961 | 3.19737 |
| H | -3.93219 | -2.18519 | 2.25433 |
| C | -2.74656 | 0.54510 | 4.00885 |
| H | -1.93781 | 1.27709 | 3.92760 |
| H | -3.68932 | 1.09312 | 4.07526 |
| H | -2.60611 | -0.00999 | 4.94104 |
| C | -1.43966 | -1.20488 | 2.82295 |

| | | | |
|----|----------|----------|----------|
| H | -1.32122 | -1.80015 | 1.91544 |
| H | -0.56803 | -0.55474 | 2.93346 |
| H | -1.43498 | -1.88168 | 3.68174 |
| C | -7.18656 | 0.75613 | 0.27693 |
| H | -8.12640 | 0.55736 | -0.24547 |
| H | -7.00550 | -0.07805 | 0.95706 |
| H | -7.31516 | 1.66112 | 0.87665 |
| C | -6.42937 | 2.04791 | -1.69818 |
| H | -7.35991 | 1.78926 | -2.20905 |
| H | -6.59262 | 2.99525 | -1.17682 |
| H | -5.66493 | 2.20152 | -2.46393 |
| C | -5.89196 | -0.37130 | -1.54480 |
| H | -5.09684 | -0.27262 | -2.28772 |
| H | -5.64278 | -1.22422 | -0.91050 |
| H | -6.82382 | -0.60103 | -2.06956 |
| C | -2.94329 | 4.91906 | -0.54049 |
| H | -3.91923 | 5.04776 | -0.06768 |
| H | -2.44840 | 5.89307 | -0.54546 |
| H | -3.09630 | 4.62373 | -1.58117 |
| C | -1.85335 | 4.49327 | 1.62818 |
| H | -2.80304 | 4.56210 | 2.16373 |
| H | -1.17604 | 3.87683 | 2.22461 |
| H | -1.41972 | 5.49575 | 1.56804 |
| C | -0.71810 | 3.88907 | -0.51236 |
| H | 0.04947 | 3.35575 | 0.05388 |
| H | -0.80197 | 3.40988 | -1.48827 |
| H | -0.35081 | 4.91024 | -0.65182 |
| C | 2.55486 | 0.74073 | 3.05473 |
| H | 2.42215 | 1.66749 | 2.49301 |
| H | 1.72389 | 0.08047 | 2.81553 |
| H | 2.44853 | 0.98572 | 4.11419 |
| C | 4.92603 | 1.18303 | 3.36825 |
| H | 4.68319 | 1.39003 | 4.41394 |
| H | 5.95911 | 0.83776 | 3.32566 |
| H | 4.85849 | 2.12022 | 2.81113 |
| C | 4.10953 | -1.14808 | 3.62544 |
| H | 5.12939 | -1.53077 | 3.55491 |
| H | 3.90827 | -0.94544 | 4.68048 |
| H | 3.43836 | -1.94513 | 3.30590 |
| C | 2.21486 | 2.33959 | -1.65267 |
| H | 2.00429 | 3.19178 | -2.30337 |
| H | 1.40455 | 1.63015 | -1.80127 |
| H | 2.19022 | 2.70104 | -0.62195 |
| C | 3.57704 | 1.24530 | -3.43981 |
| H | 2.86856 | 0.42683 | -3.55930 |
| H | 3.28544 | 2.04870 | -4.12127 |
| H | 4.56360 | 0.89376 | -3.74932 |
| C | 4.55519 | 2.97453 | -1.93715 |
| H | 4.60848 | 3.38078 | -0.92400 |
| H | 5.56668 | 2.71396 | -2.25051 |
| H | 4.19147 | 3.76340 | -2.60065 |
| C | 8.23030 | -1.51706 | 0.67882 |
| H | 8.38297 | -0.84615 | 1.52813 |
| H | 7.62617 | -2.36478 | 1.01177 |
| H | 9.21035 | -1.90276 | 0.38920 |
| C | 8.49280 | 0.37922 | -0.90042 |
| H | 8.12069 | 0.89887 | -1.78547 |
| H | 8.56277 | 1.10579 | -0.08723 |
| H | 9.50137 | 0.02203 | -1.12495 |
| C | 7.51202 | -1.78645 | -1.68120 |
| H | 6.88828 | -2.64676 | -1.42703 |
| H | 7.09057 | -1.32001 | -2.57377 |
| H | 8.51057 | -2.15286 | -1.93373 |
| Au | -2.09797 | -2.25040 | -0.76565 |
| Cl | -3.61603 | -3.91790 | -0.23800 |
| Si | -0.66055 | -0.55172 | -1.16083 |

| | | | |
|---|---------|----------|----------|
| S | 1.45909 | -1.06813 | -1.78023 |
| C | 1.80225 | -1.86651 | 1.08160 |
| H | 1.79069 | -1.71186 | 2.15541 |
| H | 0.90147 | -2.40794 | 0.78595 |
| H | 2.67876 | -2.44745 | 0.79155 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.61172 | -0.16158 | 1.12559 |
| C | 0.43974 | -0.32679 | -0.51791 |
| P | -0.96904 | 0.08908 | -1.46909 |
| Cl | 0.90659 | -2.58053 | -2.51584 |
| Si | 1.73549 | -0.71057 | -1.94948 |
| H | 1.97889 | -0.58045 | 1.20694 |
| H | -1.62672 | -1.10303 | -1.81135 |
| Au | -1.39606 | 0.33184 | -4.79958 |
| Cl | -2.85174 | -0.10042 | -6.46251 |
| C | -2.23058 | 1.16533 | -0.78383 |
| H | -2.99595 | 1.33385 | -1.54469 |
| H | -2.67897 | 0.68475 | 0.08915 |
| H | -1.78106 | 2.11596 | -0.49615 |
| S | 0.02507 | 0.82824 | -3.08756 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.70767 | 0.09620 | 0.95232 |
| C | 0.45656 | -0.15080 | -0.67239 |
| P | -1.09522 | 0.02739 | -1.46144 |
| Cl | 1.37777 | -2.48362 | -2.49044 |
| Si | 1.66306 | -0.39447 | -2.19848 |
| C | -2.20282 | 1.28861 | -0.81319 |
| H | -3.08691 | 1.34802 | -1.45168 |
| H | -2.50162 | 1.02529 | 0.20420 |
| H | -1.69014 | 2.25032 | -0.80777 |
| C | 2.48342 | -0.29545 | 1.18196 |
| H | 3.07486 | -0.07467 | 0.28933 |
| H | 2.87286 | 0.26291 | 2.03474 |
| H | 2.58013 | -1.36213 | 1.40594 |
| C | -2.00081 | -1.52253 | -1.46444 |
| H | -2.28316 | -1.76075 | -0.43572 |
| H | -2.88890 | -1.42631 | -2.09171 |
| H | -1.35199 | -2.30299 | -1.86258 |
| Au | -1.71255 | -0.51879 | -4.83675 |
| Cl | -3.08971 | -1.49770 | -6.32882 |
| S | -0.37090 | 0.52447 | -3.31827 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.70659 | -0.15837 | 0.61335 |
| C | 0.40685 | -0.31008 | -1.02068 |
| P | -1.26098 | -0.48156 | -1.57153 |
| Cl | 2.06645 | -2.10855 | -2.95572 |
| Si | 1.35618 | -0.09972 | -2.72846 |
| C | -2.31670 | 0.88154 | -1.05096 |
| H | -3.30333 | 0.80367 | -1.50819 |
| H | -2.39629 | 0.86780 | 0.03830 |
| H | -1.84994 | 1.81297 | -1.37182 |
| Au | -1.73505 | 1.49479 | -4.40411 |
| Cl | -2.57998 | 3.42437 | -5.20925 |
| C | 2.55070 | -0.14354 | 0.90511 |
| C | 2.96685 | -1.61034 | 1.05576 |
| C | 3.36408 | 0.53578 | -0.18395 |
| C | 2.74276 | 0.58720 | 2.23638 |
| H | 2.38004 | -2.12549 | 1.82226 |
| H | 2.86107 | -2.15310 | 0.11434 |
| H | 4.01752 | -1.65677 | 1.36240 |

| | | | |
|---|----------|----------|----------|
| H | 3.01710 | 1.55073 | -0.38898 |
| H | 4.41209 | 0.59801 | 0.12953 |
| H | 3.35258 | -0.02869 | -1.12019 |
| H | 3.79498 | 0.53937 | 2.53218 |
| H | 2.46348 | 1.64161 | 2.16306 |
| H | 2.14869 | 0.13670 | 3.03611 |
| C | -2.08385 | -2.07744 | -1.11518 |
| C | -3.38014 | -2.18847 | -1.91847 |
| C | -1.14646 | -3.22983 | -1.46632 |
| C | -2.38559 | -2.07537 | 0.38238 |
| H | -4.09608 | -1.40352 | -1.66625 |
| H | -3.19639 | -2.16176 | -2.99411 |
| H | -3.84937 | -3.14751 | -1.68264 |
| H | -0.21166 | -3.18073 | -0.90631 |
| H | -1.64642 | -4.17000 | -1.21769 |
| H | -0.90178 | -3.24823 | -2.52959 |
| H | -2.80448 | -3.04953 | 0.64971 |
| H | -1.48715 | -1.92410 | 0.98514 |
| H | -3.12039 | -1.31560 | 0.65587 |
| S | -0.92045 | -0.48927 | -3.61436 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.84288 | -0.25088 | 1.09478 |
| C | 0.40494 | -0.20947 | -0.51674 |
| P | -1.26707 | -0.05443 | -1.00761 |
| Cl | 1.34870 | -1.65127 | -3.15591 |
| Si | 1.36779 | 0.23525 | -2.16243 |
| C | -2.35213 | 0.85099 | 0.11014 |
| H | -3.33577 | 0.95986 | -0.35022 |
| H | -2.44851 | 0.29939 | 1.04768 |
| H | -1.92609 | 1.83709 | 0.29580 |
| Au | -2.34221 | 0.35630 | -4.35090 |
| Cl | -3.81288 | -0.25690 | -5.95132 |
| C | 2.63401 | -0.42175 | 1.08218 |
| C | 3.31229 | 0.07588 | 2.20049 |
| C | 3.36859 | -1.00757 | 0.04562 |
| C | 4.69401 | 0.03038 | 2.26110 |
| H | 2.74795 | 0.51224 | 3.01896 |
| C | 4.75110 | -1.05771 | 0.11371 |
| H | 2.85835 | -1.47157 | -0.79181 |
| C | 5.41338 | -0.53284 | 1.21497 |
| H | 5.21210 | 0.42932 | 3.12538 |
| H | 5.31252 | -1.51444 | -0.69289 |
| H | 6.49545 | -0.57507 | 1.26463 |
| C | -2.03612 | -1.65134 | -1.29631 |
| C | -3.35430 | -1.70863 | -1.75056 |
| C | -1.32474 | -2.82418 | -1.06332 |
| C | -3.95352 | -2.93619 | -1.96612 |
| H | -3.90952 | -0.80243 | -1.96514 |
| C | -1.93513 | -4.05030 | -1.27735 |
| H | -0.29641 | -2.77731 | -0.72928 |
| C | -3.24457 | -4.10633 | -1.72794 |
| H | -4.97075 | -2.97757 | -2.33590 |
| H | -1.37868 | -4.96323 | -1.10170 |
| H | -3.71523 | -5.06660 | -1.90448 |
| S | -0.92046 | 1.05199 | -2.71369 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.89034 | -0.70491 | 1.04260 |
| C | 0.37810 | -0.89952 | -0.53171 |
| P | -1.32117 | -0.87710 | -0.99310 |
| Cl | 1.30544 | -2.21964 | -3.20246 |
| Si | 1.33153 | -0.33670 | -2.15055 |
| C | -2.35374 | -0.08950 | 0.25888 |
| H | -3.36786 | 0.05809 | -0.10730 |
| H | -2.37420 | -0.75081 | 1.12941 |

| | | | |
|----|----------|----------|----------|
| H | -1.91438 | 0.87121 | 0.52877 |
| Au | -0.92406 | 2.39295 | -1.79154 |
| Cl | -0.81279 | 4.46366 | -0.89521 |
| C | 2.67391 | -0.36803 | 0.87963 |
| C | 3.10767 | 0.95094 | 1.09211 |
| C | 3.60219 | -1.39642 | 0.66457 |
| C | 4.46833 | 1.22003 | 1.05465 |
| C | 4.95411 | -1.07839 | 0.64196 |
| C | 5.40756 | 0.22192 | 0.82498 |
| H | 4.80304 | 2.24132 | 1.21102 |
| H | 5.67535 | -1.87463 | 0.48212 |
| C | -2.15115 | -2.42066 | -1.46565 |
| C | -3.39560 | -2.32395 | -2.12603 |
| C | -1.61102 | -3.69204 | -1.17385 |
| C | -4.03288 | -3.49169 | -2.52712 |
| C | -2.30473 | -4.81912 | -1.59195 |
| C | -3.50507 | -4.74845 | -2.28386 |
| H | -4.98199 | -3.40541 | -3.04712 |
| H | -1.88138 | -5.79275 | -1.36696 |
| C | 2.12890 | 2.06266 | 1.31818 |
| H | 1.62247 | 2.34810 | 0.39072 |
| H | 1.34850 | 1.77885 | 2.03336 |
| H | 2.62588 | 2.95255 | 1.70579 |
| C | 6.86863 | 0.54390 | 0.75942 |
| H | 7.14869 | 0.85575 | -0.25166 |
| H | 7.12723 | 1.36146 | 1.43491 |
| H | 7.48043 | -0.32243 | 1.01643 |
| C | 3.17487 | -2.81919 | 0.45845 |
| H | 2.36505 | -3.10491 | 1.13639 |
| H | 2.81553 | -2.98116 | -0.56228 |
| H | 4.00906 | -3.50159 | 0.62723 |
| C | -0.33829 | -3.91944 | -0.41757 |
| H | 0.51652 | -3.48449 | -0.93495 |
| H | -0.37460 | -3.48556 | 0.58365 |
| H | -0.16202 | -4.98998 | -0.31121 |
| C | -4.13862 | -1.04474 | -2.39372 |
| H | -3.50030 | -0.17358 | -2.52734 |
| H | -4.73644 | -1.14769 | -3.30005 |
| H | -4.83513 | -0.83283 | -1.57604 |
| C | -4.19346 | -5.98693 | -2.76321 |
| H | -3.77322 | -6.31022 | -3.72059 |
| H | -4.06683 | -6.81063 | -2.05833 |
| H | -5.26097 | -5.81899 | -2.91230 |
| S | -1.02581 | 0.29022 | -2.69829 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -2.06030 | 1.75853 | 0.57315 |
| C | -1.09406 | 0.42897 | 0.29009 |
| P | 0.67314 | 0.33056 | 0.39738 |
| C | -3.75441 | 1.04291 | 0.47188 |
| C | -4.54078 | 1.31130 | -0.68466 |
| C | -4.23532 | 0.13407 | 1.43888 |
| C | -5.61718 | 0.48013 | -0.94392 |
| C | -5.31976 | -0.67724 | 1.09271 |
| C | -5.98620 | -0.57228 | -0.11046 |
| H | -6.19501 | 0.64344 | -1.84150 |
| H | -5.65702 | -1.40829 | 1.81391 |
| C | -3.82323 | 0.04925 | 2.92525 |
| C | -4.29647 | 2.51100 | -1.62076 |
| C | -7.11653 | -1.50891 | -0.52140 |
| C | -3.00129 | 2.37081 | -2.42240 |
| H | -2.11400 | 2.40556 | -1.78760 |
| H | -2.97397 | 1.42675 | -2.96948 |
| H | -2.91725 | 3.19557 | -3.13646 |
| C | -4.26580 | 3.80361 | -0.79328 |
| H | -5.20317 | 3.93514 | -0.24729 |

| | | | |
|----|----------|----------|----------|
| H | -3.44860 | 3.82015 | -0.06952 |
| H | -4.13283 | 4.66445 | -1.45463 |
| C | -5.42478 | 2.67747 | -2.64265 |
| H | -5.46769 | 1.84699 | -3.35111 |
| H | -6.40184 | 2.78166 | -2.16516 |
| H | -5.24034 | 3.58628 | -3.22008 |
| C | -3.45030 | -1.38063 | 3.33082 |
| H | -2.60472 | -1.74923 | 2.74564 |
| H | -3.17767 | -1.40454 | 4.38971 |
| H | -4.27608 | -2.07964 | 3.19059 |
| C | -2.68410 | 0.96632 | 3.35914 |
| H | -1.71605 | 0.62450 | 2.99710 |
| H | -2.83672 | 2.00254 | 3.03861 |
| H | -2.63781 | 0.97758 | 4.45193 |
| C | -5.05360 | 0.49403 | 3.73904 |
| H | -5.32843 | 1.52399 | 3.49716 |
| H | -5.92225 | -0.13668 | 3.54844 |
| H | -4.82741 | 0.44235 | 4.80780 |
| C | -7.36718 | -2.60246 | 0.51336 |
| H | -7.68957 | -2.19097 | 1.47351 |
| H | -8.16067 | -3.26441 | 0.15849 |
| H | -6.47654 | -3.21332 | 0.68020 |
| C | -6.74411 | -2.18034 | -1.84917 |
| H | -6.59796 | -1.44738 | -2.64505 |
| H | -5.81913 | -2.75318 | -1.75216 |
| H | -7.54054 | -2.86138 | -2.16208 |
| C | -8.41206 | -0.70922 | -0.70177 |
| H | -8.31027 | 0.06200 | -1.46792 |
| H | -9.22491 | -1.37467 | -1.00572 |
| H | -8.70359 | -0.22002 | 0.23109 |
| C | 2.04820 | 1.46762 | 0.00627 |
| C | 2.66563 | 1.34157 | -1.27192 |
| C | 2.82118 | 1.98590 | 1.07994 |
| C | 4.05135 | 1.32421 | -1.31067 |
| C | 4.20528 | 1.93903 | 0.96090 |
| C | 4.84931 | 1.49996 | -0.18671 |
| H | 4.52972 | 1.16752 | -2.26928 |
| H | 4.80007 | 2.27055 | 1.80114 |
| C | 1.95036 | 1.43708 | -2.63339 |
| C | 2.29340 | 0.28640 | -3.58209 |
| C | 2.47041 | 2.74972 | -3.25847 |
| H | 1.92521 | -0.66724 | -3.20623 |
| H | 1.82919 | 0.46971 | -4.55468 |
| H | 3.36903 | 0.19566 | -3.74422 |
| H | 2.25028 | 3.60540 | -2.61521 |
| H | 3.54649 | 2.72708 | -3.43417 |
| H | 1.97437 | 2.90954 | -4.21952 |
| C | 2.26936 | 2.78582 | 2.27717 |
| C | 2.87342 | 4.19952 | 2.13632 |
| C | 2.70556 | 2.22748 | 3.63482 |
| H | 2.61368 | 4.64090 | 1.17147 |
| H | 2.47327 | 4.84279 | 2.92477 |
| H | 3.95987 | 4.19561 | 2.22497 |
| H | 2.30598 | 1.23290 | 3.83131 |
| H | 3.79246 | 2.16351 | 3.71094 |
| H | 2.35922 | 2.89049 | 4.43198 |
| C | 6.35540 | 1.29899 | -0.27209 |
| C | 6.95454 | 2.29649 | -1.27081 |
| C | 6.62933 | -0.13273 | -0.75116 |
| H | 6.77033 | 3.32748 | -0.95789 |
| H | 8.03572 | 2.14987 | -1.33939 |
| H | 6.53921 | 2.16820 | -2.27242 |
| H | 6.20382 | -0.87308 | -0.06980 |
| H | 6.20656 | -0.31520 | -1.74110 |
| H | 7.70754 | -0.30300 | -0.81253 |
| Cl | -2.37101 | -1.37097 | -1.96906 |

| | | | |
|----|----------|----------|----------|
| Au | 2.57597 | -2.57140 | -0.06295 |
| Cl | 4.40491 | -3.70749 | 0.63074 |
| C | 0.75939 | 2.99762 | 2.24366 |
| H | 0.43913 | 3.42323 | 1.29058 |
| H | 0.16985 | 2.10048 | 2.42247 |
| H | 0.47937 | 3.70477 | 3.02834 |
| C | 0.43802 | 1.59579 | -2.54388 |
| H | -0.08298 | 0.68367 | -2.25717 |
| H | 0.16638 | 2.39399 | -1.84872 |
| H | 0.05381 | 1.87459 | -3.52815 |
| C | 7.03961 | 1.49497 | 1.07809 |
| H | 6.93912 | 2.51981 | 1.44585 |
| H | 6.64301 | 0.81253 | 1.83373 |
| H | 8.10754 | 1.28963 | 0.97634 |
| Si | -1.51734 | -1.47568 | -0.01788 |
| S | 0.81238 | -1.34430 | -0.81943 |
| C | 1.01524 | -0.35953 | 2.04147 |
| H | 2.06891 | -0.63305 | 2.10450 |
| H | 0.74473 | 0.31901 | 2.84529 |
| H | 0.40805 | -1.26452 | 2.11683 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.49306 | 0.10708 | 1.03936 |
| C | 0.31685 | -0.28225 | -0.54193 |
| P | -1.11039 | -0.20030 | -1.55446 |
| Cl | 1.20250 | -2.76520 | -2.05920 |
| Si | 1.64254 | -0.67043 | -1.97413 |
| H | 1.86872 | -0.06836 | 1.31235 |
| H | -1.72236 | -1.46801 | -1.50395 |
| Au | -0.95631 | 0.77862 | 2.55398 |
| Cl | -2.49119 | 1.46545 | 4.05678 |
| C | -2.40931 | 0.95117 | -1.09730 |
| H | -2.81950 | 0.68016 | -0.12141 |
| H | -1.99998 | 1.96105 | -1.06029 |
| H | -3.19684 | 0.90394 | -1.85282 |
| S | -0.21995 | 0.14492 | -3.30733 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.79305 | 0.03053 | 0.86530 |
| C | 0.38921 | -0.20940 | -0.70450 |
| P | -1.21205 | -0.22648 | -1.42145 |
| Cl | 1.51496 | -2.57681 | -2.30030 |
| Si | 1.46124 | -0.42694 | -2.34691 |
| C | -2.31682 | 1.09074 | -0.89083 |
| H | -3.23800 | 1.03288 | -1.47506 |
| H | -2.54777 | 0.98337 | 0.17169 |
| H | -1.83654 | 2.05267 | -1.06953 |
| C | 2.57839 | -0.14655 | 1.08175 |
| H | 3.08897 | -0.04177 | 0.12218 |
| H | 2.93478 | 0.60253 | 1.79003 |
| H | 2.78700 | -1.13706 | 1.49432 |
| C | -2.03039 | -1.78287 | -1.04347 |
| H | -2.25071 | -1.83228 | 0.02550 |
| H | -2.95528 | -1.85143 | -1.61966 |
| H | -1.35989 | -2.59511 | -1.32678 |
| Au | -0.56224 | 0.44059 | 2.56067 |
| Cl | -2.01295 | 0.84544 | 4.24706 |
| S | -0.67817 | -0.07784 | -3.35289 |

R = t-Bu

| | | | |
|---|----------|----------|----------|
| P | 0.79867 | 0.08241 | 0.73968 |
| C | 0.52525 | -0.48270 | -0.78626 |
| P | -1.06151 | -0.56082 | -1.56353 |

| | | | |
|----|----------|----------|----------|
| Cl | 2.06547 | -2.85740 | -2.25613 |
| Si | 1.65429 | -0.75640 | -2.39338 |
| C | -2.02569 | 0.95350 | -1.38102 |
| H | -2.89403 | 0.90814 | -2.04005 |
| H | -2.34526 | 1.09998 | -0.34783 |
| H | -1.39264 | 1.78700 | -1.68623 |
| Au | -0.71871 | 0.95559 | 2.10525 |
| Cl | -2.31486 | 1.87052 | 3.42995 |
| C | 2.58342 | 0.03355 | 1.24221 |
| C | 2.66191 | 0.48975 | 2.69727 |
| C | 3.12067 | -1.38995 | 1.10879 |
| C | 3.36021 | 1.00200 | 0.34777 |
| H | 2.27793 | 1.50358 | 2.83126 |
| H | 2.10616 | -0.17309 | 3.36452 |
| H | 3.70971 | 0.48199 | 3.01081 |
| H | 3.07681 | -1.75886 | 0.08387 |
| H | 4.16719 | -1.40048 | 1.42932 |
| H | 2.57076 | -2.08903 | 1.74368 |
| H | 4.41145 | 0.99494 | 0.65255 |
| H | 3.31496 | 0.71858 | -0.70692 |
| H | 2.99126 | 2.02583 | 0.44617 |
| C | -2.11215 | -1.98478 | -1.00714 |
| C | -1.31340 | -3.27559 | -1.15583 |
| C | -2.53887 | -1.79498 | 0.44543 |
| C | -3.33765 | -2.02103 | -1.92229 |
| H | -0.99026 | -3.43745 | -2.18478 |
| H | -0.42577 | -3.28209 | -0.52162 |
| H | -1.95171 | -4.11263 | -0.85920 |
| H | -3.12644 | -0.88888 | 0.60374 |
| H | -3.16463 | -2.64477 | 0.73320 |
| H | -1.68479 | -1.77472 | 1.12470 |
| H | -3.92380 | -2.91077 | -1.67689 |
| H | -3.98649 | -1.15385 | -1.78347 |
| H | -3.05555 | -2.08854 | -2.97543 |
| S | -0.45106 | -0.78797 | -3.47475 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77923 | -0.16379 | 0.87286 |
| C | 0.40685 | -0.13949 | -0.73132 |
| P | -1.23761 | -0.12531 | -1.36905 |
| Cl | 1.82974 | -1.85524 | -2.95145 |
| Si | 1.38653 | 0.18155 | -2.40226 |
| C | -2.32287 | 1.09874 | -0.61638 |
| H | -3.27619 | 1.09028 | -1.14856 |
| H | -2.48695 | 0.89067 | 0.44245 |
| H | -1.85183 | 2.07603 | -0.72465 |
| Au | -0.66435 | -0.05733 | 2.55257 |
| Cl | -2.23475 | 0.03110 | 4.18381 |
| C | -2.03241 | -1.73310 | -1.19466 |
| C | -2.76860 | -2.03564 | -0.04873 |
| C | -1.86646 | -2.69063 | -2.19157 |
| C | -3.33912 | -3.29010 | 0.09005 |
| H | -2.89803 | -1.30824 | 0.74438 |
| C | -2.43995 | -3.94310 | -2.04351 |
| H | -1.28826 | -2.45078 | -3.07611 |
| C | -3.17589 | -4.24228 | -0.90633 |
| H | -3.91109 | -3.52122 | 0.98081 |
| H | -2.30985 | -4.68700 | -2.82058 |
| H | -3.62446 | -5.22275 | -0.79428 |
| C | 2.52812 | -0.25754 | 1.18376 |
| C | 3.44327 | -0.71311 | 0.23029 |
| C | 2.98015 | 0.16391 | 2.43825 |
| C | 4.79498 | -0.71876 | 0.52768 |
| H | 3.10091 | -1.10109 | -0.72157 |
| C | 4.33319 | 0.15646 | 2.72423 |
| H | 2.26599 | 0.50157 | 3.18235 |

| | | | |
|---|----------|----------|----------|
| C | 5.24023 | -0.28042 | 1.76758 |
| H | 5.50274 | -1.07619 | -0.21078 |
| H | 4.68104 | 0.48859 | 3.69513 |
| H | 6.30027 | -0.29003 | 1.99422 |
| S | -0.81916 | 0.33762 | -3.28112 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.85623 | -0.21373 | 1.36826 |
| C | 0.51656 | -0.55655 | -0.20312 |
| P | -1.01877 | -0.42720 | -1.07192 |
| Cl | 1.70914 | -2.53303 | -2.22995 |
| Si | 1.81014 | -0.43965 | -1.69088 |
| C | -2.14796 | 0.71344 | -0.24251 |
| H | -3.05460 | 0.85020 | -0.83100 |
| H | -2.41850 | 0.29389 | 0.72998 |
| H | -1.64687 | 1.67142 | -0.10179 |
| Au | -0.53979 | 0.07428 | 3.06290 |
| Cl | -1.98971 | 0.35244 | 4.78044 |
| C | -1.98624 | -1.93632 | -1.37825 |
| C | -1.85835 | -3.10377 | -0.59910 |
| C | -2.93941 | -1.88955 | -2.41808 |
| C | -2.67114 | -4.19122 | -0.89008 |
| C | -3.72726 | -3.00989 | -2.65343 |
| C | -3.60724 | -4.17401 | -1.91280 |
| H | -2.56695 | -5.08507 | -0.28326 |
| H | -4.46131 | -2.96245 | -3.45184 |
| C | 2.63803 | -0.12178 | 1.61194 |
| C | 3.37211 | -1.29121 | 1.85319 |
| C | 3.25480 | 1.13849 | 1.62851 |
| C | 4.73265 | -1.17289 | 2.10258 |
| C | 4.61679 | 1.20163 | 1.88071 |
| C | 5.37362 | 0.05948 | 2.11655 |
| H | 5.30752 | -2.07346 | 2.29564 |
| H | 5.10114 | 2.17325 | 1.89404 |
| C | -0.89552 | -3.25815 | 0.53731 |
| H | 0.13539 | -3.15940 | 0.19495 |
| H | -1.06115 | -2.51809 | 1.32379 |
| H | -1.01138 | -4.24460 | 0.98653 |
| C | -3.16032 | -0.71847 | -3.33317 |
| H | -3.10270 | 0.25224 | -2.84156 |
| H | -2.41438 | -0.70532 | -4.13133 |
| H | -4.14664 | -0.79524 | -3.79248 |
| C | -4.44370 | -5.37735 | -2.21450 |
| H | -5.36265 | -5.10452 | -2.73536 |
| H | -3.89497 | -6.07383 | -2.85600 |
| H | -4.70936 | -5.91570 | -1.30286 |
| C | 6.84817 | 0.15517 | 2.35702 |
| H | 7.10807 | 1.07911 | 2.87661 |
| H | 7.21160 | -0.68722 | 2.94757 |
| H | 7.39217 | 0.14997 | 1.40732 |
| C | 2.72971 | -2.64430 | 1.83097 |
| H | 1.78177 | -2.65462 | 2.37826 |
| H | 2.52054 | -2.95946 | 0.80402 |
| H | 3.38263 | -3.39126 | 2.28351 |
| C | 2.48000 | 2.39002 | 1.35248 |
| H | 2.16067 | 2.42541 | 0.30604 |
| H | 1.58088 | 2.45723 | 1.97387 |
| H | 3.08583 | 3.27520 | 1.54755 |
| S | -0.17439 | 0.35263 | -2.73999 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.15529 | 0.63875 | 0.08184 |
| C | -0.35542 | -0.74806 | 0.47896 |
| P | 1.34718 | -1.15834 | 0.79731 |
| Cl | -1.87650 | -3.08404 | -1.13439 |
| C | 2.95917 | -0.52369 | 0.18642 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 3.50747 | -1.15811 | -0.96692 | H | 4.82526 | 0.69494 | 3.64858 |
| C | 3.85194 | 0.10982 | 1.09480 | H | 3.68661 | 1.97753 | 4.05198 |
| C | 4.85922 | -1.46826 | -0.94731 | H | 3.12954 | 0.31110 | 3.91684 |
| C | 5.19215 | -0.26384 | 1.04954 | C | 1.35580 | -0.89324 | -2.37018 |
| C | 5.70754 | -1.12807 | 0.09783 | H | 1.02742 | -0.87674 | -3.41224 |
| H | 5.26898 | -1.99445 | -1.80009 | H | 0.67496 | -1.55554 | -1.83830 |
| H | 5.86048 | 0.16491 | 1.78312 | H | 1.25295 | 0.12366 | -1.98215 |
| C | -2.93376 | 0.26238 | 0.13528 | C | 2.87984 | -2.80584 | -2.82288 |
| C | -3.66359 | 0.00326 | -1.05679 | H | 2.32604 | -3.47865 | -2.16847 |
| C | -3.51948 | -0.01391 | 1.39650 | H | 2.44136 | -2.86575 | -3.82249 |
| C | -4.83058 | -0.74208 | -0.94424 | H | 3.90884 | -3.16380 | -2.89483 |
| C | -4.67505 | -0.78758 | 1.41179 | C | 3.56805 | -0.45568 | -3.31226 |
| C | -5.31639 | -1.21880 | 0.26435 | H | 3.53292 | 0.58930 | -2.99479 |
| H | -5.37095 | -0.98643 | -1.84345 | H | 4.61496 | -0.74272 | -3.41809 |
| H | -5.09438 | -1.05782 | 2.37237 | H | 3.09844 | -0.52651 | -4.29688 |
| C | -3.30362 | 0.57567 | -2.44147 | C | 7.90975 | -1.14533 | 1.34756 |
| C | -3.10153 | 0.55250 | 2.77239 | H | 8.00438 | -0.05694 | 1.38016 |
| C | -6.52473 | -2.14317 | 0.36346 | H | 7.42766 | -1.47832 | 2.27020 |
| C | 3.53931 | 1.31931 | 2.00236 | H | 8.92043 | -1.55975 | 1.33389 |
| C | 2.80334 | -1.36099 | -2.32318 | C | 7.88236 | -1.09697 | -1.13319 |
| C | 7.15033 | -1.61622 | 0.11016 | H | 7.41857 | -1.45058 | -2.05604 |
| C | -4.32214 | 1.30087 | 3.34256 | H | 7.88924 | -0.00459 | -1.15691 |
| H | -4.06477 | 1.72596 | 4.31633 | H | 8.91922 | -1.44391 | -1.12844 |
| H | -4.61994 | 2.11925 | 2.68249 | C | 7.15133 | -3.14972 | 0.09685 |
| H | -5.18662 | 0.65261 | 3.48331 | H | 6.64586 | -3.54974 | 0.97910 |
| C | -1.97549 | 1.58340 | 2.75563 | H | 6.64633 | -3.54674 | -0.78585 |
| H | -0.99502 | 1.14308 | 2.57491 | H | 8.17856 | -3.52414 | 0.09319 |
| H | -2.14756 | 2.37625 | 2.02285 | Au | -0.29111 | 2.60613 | -0.50676 |
| H | -1.92400 | 2.06187 | 3.73760 | Cl | 0.60840 | 4.60656 | -1.10591 |
| C | -2.71358 | -0.57404 | 3.73416 | C | 1.44143 | -1.22833 | 2.61246 |
| H | -3.53326 | -1.27794 | 3.88858 | H | 2.39468 | -1.68190 | 2.88613 |
| H | -1.86523 | -1.14488 | 3.35109 | H | 1.31107 | -0.27586 | 3.11588 |
| H | -2.44462 | -0.15563 | 4.70835 | H | 0.63516 | -1.90455 | 2.90615 |
| C | -7.63247 | -1.46479 | 1.17760 | Si | -1.07669 | -2.59124 | 0.79456 |
| H | -8.49930 | -2.12680 | 1.25556 | S | 1.18791 | -3.12487 | 0.32472 |
| H | -7.30519 | -1.22691 | 2.19177 | | | | |
| H | -7.95588 | -0.53556 | 0.70191 | | | | |
| C | -7.09050 | -2.50749 | -1.00654 | | | | |
| H | -7.93428 | -3.19008 | -0.88065 | | | | |
| H | -7.45668 | -1.62935 | -1.54474 | | | | |
| H | -6.34767 | -3.01075 | -1.63008 | | | | |
| C | -6.09371 | -3.43699 | 1.06542 | | | | |
| H | -5.29952 | -3.93765 | 0.50696 | | | | |
| H | -5.72088 | -3.24487 | 2.07356 | | | | |
| H | -6.94308 | -4.12111 | 1.14619 | | | | |
| C | -4.30285 | 0.14762 | -3.52088 | | | | |
| H | -5.32107 | 0.47468 | -3.29924 | | | | |
| H | -4.01088 | 0.61398 | -4.46427 | | | | |
| H | -4.30510 | -0.93409 | -3.67554 | | | | |
| C | -3.37762 | 2.10637 | -2.35663 | | | | |
| H | -4.38043 | 2.42805 | -2.06469 | | | | |
| H | -2.67073 | 2.51748 | -1.63261 | | | | |
| H | -3.14513 | 2.54853 | -3.32906 | | | | |
| C | -1.92849 | 0.13703 | -2.94639 | | | | |
| H | -1.10530 | 0.53559 | -2.35122 | | | | |
| H | -1.83818 | -0.94961 | -2.96012 | | | | |
| H | -1.77820 | 0.51738 | -3.96078 | | | | |
| C | 2.15307 | 1.91316 | 1.78268 | | | | |
| H | 2.04227 | 2.24281 | 0.74820 | | | | |
| H | 1.32116 | 1.25086 | 2.00986 | | | | |
| H | 2.03066 | 2.79636 | 2.41395 | | | | |
| C | 4.50473 | 2.44290 | 1.56302 | | | | |
| H | 4.24796 | 3.36112 | 2.09753 | | | | |
| H | 5.54686 | 2.21044 | 1.78289 | | | | |
| H | 4.41438 | 2.64090 | 0.49320 | | | | |
| C | 3.80499 | 1.04922 | 3.48710 | | | | |

Coordination through $\pi(\text{C}=\text{P})$ bond**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.62132 | 0.19639 | 1.02280 |
| C | 0.33040 | -0.02028 | -0.66668 |
| P | -1.20925 | -0.29468 | -1.48439 |
| Cl | 1.24811 | -2.70890 | -1.77816 |
| Si | 1.48243 | -0.61229 | -2.18398 |
| H | 2.02842 | -0.05778 | 0.99057 |
| H | -1.61649 | -1.59014 | -1.11035 |
| Au | 0.69914 | 2.09130 | -0.40997 |
| Cl | 0.97292 | 4.29482 | -0.76333 |
| C | -2.61807 | 0.74585 | -1.07739 |
| H | -3.47972 | 0.41266 | -1.66022 |
| H | -2.84071 | 0.65649 | -0.01133 |
| H | -2.38962 | 1.78317 | -1.32424 |
| S | -0.59472 | -0.22027 | -3.38021 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.62994 | 0.10033 | 1.04431 |
| C | 0.28386 | 0.15215 | -0.64737 |
| P | -1.28342 | -0.13799 | -1.41506 |
| Cl | 1.65928 | -2.21549 | -2.08788 |
| Si | 1.40378 | -0.07866 | -2.26966 |
| C | -2.63586 | 0.96700 | -0.97173 |
| H | -3.52531 | 0.67849 | -1.53673 |
| H | -2.84158 | 0.88994 | 0.09839 |
| H | -2.36641 | 1.99327 | -1.22132 |
| C | 2.42987 | -0.24122 | 1.09923 |
| H | 2.96691 | 0.11377 | 0.21801 |
| H | 2.85219 | 0.20610 | 2.00070 |
| H | 2.55026 | -1.32732 | 1.16506 |
| C | -1.83431 | -1.79931 | -0.99536 |
| H | -2.08472 | -1.84897 | 0.06688 |
| H | -2.71022 | -2.04787 | -1.59763 |
| H | -1.02481 | -2.49398 | -1.22301 |
| Au | 0.52998 | 2.21723 | -0.05647 |
| Cl | 0.68582 | 4.46343 | 0.02018 |
| S | -0.72796 | 0.02126 | -3.33743 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.60044 | 0.24471 | 0.80602 |
| C | 0.37444 | 0.09833 | -0.90896 |
| P | -1.22705 | -0.27560 | -1.61386 |
| Cl | 2.24632 | -1.92492 | -2.56235 |
| Si | 1.41939 | 0.05951 | -2.59000 |
| C | -2.48537 | 0.98957 | -1.32603 |
| H | -3.42777 | 0.67995 | -1.78140 |
| H | -2.62627 | 1.15254 | -0.25647 |
| H | -2.15366 | 1.91653 | -1.79398 |
| Au | 0.55399 | 2.23291 | -0.50900 |
| Cl | 0.72754 | 4.48292 | -0.55325 |
| C | 2.39942 | -0.02651 | 1.23548 |
| C | 2.53593 | -1.54385 | 1.40242 |
| C | 3.42082 | 0.49574 | 0.23896 |
| C | 2.58518 | 0.66457 | 2.58835 |
| H | 1.78704 | -1.95133 | 2.08900 |
| H | 2.45266 | -2.05926 | 0.44340 |
| H | 3.52081 | -1.76942 | 1.82442 |
| H | 3.33613 | 1.57506 | 0.09559 |
| H | 4.42848 | 0.28805 | 0.61575 |
| H | 3.33975 | 0.00689 | -0.73385 |
| H | 3.58827 | 0.45148 | 2.96963 |
| H | 2.48182 | 1.74929 | 2.50354 |
| H | 1.86307 | 0.31137 | 3.32966 |

| | | | |
|---|----------|----------|----------|
| C | -1.93728 | -1.88095 | -1.00999 |
| C | -3.05870 | -2.27815 | -1.97135 |
| C | -0.84994 | -2.95029 | -1.02445 |
| C | -2.49328 | -1.70242 | 0.40216 |
| H | -3.87852 | -1.55638 | -1.98130 |
| H | -2.68967 | -2.40207 | -2.99091 |
| H | -3.47121 | -3.23581 | -1.64182 |
| H | -0.04796 | -2.72872 | -0.31886 |
| H | -1.29830 | -3.90549 | -0.73672 |
| H | -0.40466 | -3.06502 | -2.01360 |
| H | -2.83882 | -2.67536 | 0.76313 |
| H | -1.73766 | -1.33946 | 1.10277 |
| H | -3.34634 | -1.02168 | 0.42813 |
| S | -0.70424 | -0.36628 | -3.55758 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77923 | -0.16379 | 0.87286 |
| C | 0.40685 | -0.13949 | -0.73132 |
| P | -1.23761 | -0.12531 | -1.36905 |
| Cl | 1.82974 | -1.85524 | -2.95145 |
| Si | 1.38653 | 0.18155 | -2.40226 |
| C | -2.32287 | 1.09874 | -0.61638 |
| H | -3.27619 | 1.09028 | -1.14856 |
| H | -2.48695 | 0.89067 | 0.44245 |
| H | -1.85183 | 2.07603 | -0.72465 |
| Au | -0.66435 | -0.05733 | 2.55257 |
| Cl | -2.23475 | 0.03110 | 4.18381 |
| C | -2.03241 | -1.73310 | -1.19466 |
| C | -2.76860 | -2.03564 | -0.04873 |
| C | -1.86646 | -2.69063 | -2.19157 |
| C | -3.33912 | -3.29010 | 0.09005 |
| H | -2.89803 | -1.30824 | 0.74438 |
| C | -2.43995 | -3.94310 | -2.04351 |
| H | -1.28826 | -2.45078 | -3.07611 |
| C | -3.17589 | -4.24228 | -0.90633 |
| H | -3.91109 | -3.52122 | 0.98081 |
| H | -2.30985 | -4.68700 | -2.82058 |
| H | -3.62446 | -5.22275 | -0.79428 |
| C | 2.52812 | -0.25754 | 1.18376 |
| C | 3.44327 | -0.71311 | 0.23029 |
| C | 2.98015 | 0.16391 | 2.43825 |
| C | 4.79498 | -0.71876 | 0.52768 |
| H | 3.10091 | -1.10109 | -0.72157 |
| C | 4.33319 | 0.15646 | 2.72423 |
| H | 2.26599 | 0.50157 | 3.18235 |
| C | 5.24023 | -0.28042 | 1.76758 |
| H | 5.50274 | -1.07619 | -0.21078 |
| H | 4.68104 | 0.48859 | 3.69513 |
| H | 6.30027 | -0.29003 | 1.99422 |
| S | -0.81916 | 0.33762 | -3.28112 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.64723 | 0.02295 | 1.13559 |
| C | -0.00722 | 0.37778 | -0.45758 |
| P | -1.72726 | 0.01203 | -0.78076 |
| Cl | 1.52628 | 0.76761 | -3.45157 |
| Si | 0.22700 | 1.53392 | -1.99213 |
| C | -2.90719 | 0.90017 | 0.26733 |
| H | -3.92164 | 0.54468 | 0.07882 |
| H | -2.66481 | 0.82152 | 1.32371 |
| H | -2.83118 | 1.94283 | -0.04332 |
| Au | 0.29859 | 2.35544 | 0.37255 |
| Cl | 0.72891 | 4.34701 | 1.40808 |
| C | 2.44865 | -0.18932 | 0.97009 |
| C | 3.27169 | 0.47042 | 1.90339 |
| C | 3.01382 | -1.10699 | 0.06451 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| C | 4.64463 | 0.26442 | 1.85264 | H | 1.33635 | 2.71001 | 4.06140 |
| C | 4.39086 | -1.28095 | 0.06137 | H | 0.70251 | 2.40989 | 2.45642 |
| C | 5.22822 | -0.59065 | 0.92906 | H | 1.18145 | 1.04996 | 3.49639 |
| H | 5.27444 | 0.78581 | 2.56743 | C | 3.00449 | -3.37706 | -0.48891 |
| H | 4.82207 | -1.99433 | -0.63517 | H | 2.52511 | -2.90890 | -1.34646 |
| C | -2.05308 | -1.78001 | -0.76448 | H | 4.06998 | -3.45813 | -0.70955 |
| C | -1.74633 | -2.57764 | -1.89105 | H | 2.61726 | -4.39451 | -0.38206 |
| C | -2.61008 | -2.39292 | 0.38379 | C | 3.54523 | -3.24014 | 1.93999 |
| C | -2.11668 | -3.91760 | -1.88063 | H | 4.61725 | -3.22893 | 1.73876 |
| C | -2.95173 | -3.73758 | 0.32625 | H | 3.37576 | -2.71665 | 2.88432 |
| C | -2.74848 | -4.51473 | -0.80324 | H | 3.23295 | -4.28142 | 2.06429 |
| H | -1.87887 | -4.51775 | -2.75321 | C | 1.27557 | -2.74694 | 1.17430 |
| H | -3.37550 | -4.19623 | 1.21409 | H | 1.03514 | -2.22907 | 2.10741 |
| C | 2.71825 | 1.39170 | 2.94755 | H | 0.60104 | -2.39866 | 0.39304 |
| H | 2.42699 | 2.35886 | 2.52636 | H | 1.06193 | -3.80805 | 1.33307 |
| H | 1.82410 | 0.97907 | 3.42395 | C | 7.28925 | 1.72404 | 0.26192 |
| H | 3.46121 | 1.57331 | 3.72546 | H | 6.68550 | 2.50753 | -0.20241 |
| C | 2.18741 | -1.94236 | -0.86699 | H | 7.37331 | 1.94062 | 1.33014 |
| H | 1.28646 | -2.32500 | -0.38031 | C | 8.29392 | 1.78288 | -0.16371 |
| H | 1.86801 | -1.36908 | -1.73904 | C | 6.71000 | 0.08593 | -1.50868 |
| H | 2.76829 | -2.79495 | -1.22238 | H | 7.72750 | 0.16675 | -1.90181 |
| C | 6.71390 | -0.76669 | 0.86884 | H | 6.33069 | -0.90802 | -1.75382 |
| H | 7.17815 | -0.57371 | 1.83757 | H | 6.08207 | 0.81373 | -2.02731 |
| H | 6.98394 | -1.77590 | 0.55181 | C | 7.60667 | -0.69793 | 0.69162 |
| H | 7.15588 | -0.06981 | 0.14956 | H | 7.61920 | -0.54844 | 1.77424 |
| C | -2.81213 | -1.72633 | 1.71662 | H | 7.27371 | -1.71939 | 0.49664 |
| H | -2.91771 | -2.49317 | 2.48399 | H | 8.63252 | -0.60769 | 0.32341 |
| H | -1.96215 | -1.10384 | 2.00165 | C | -2.37551 | -1.46087 | -1.68143 |
| H | -3.71772 | -1.11774 | 1.74781 | C | -2.36836 | -2.34272 | -2.80254 |
| C | -0.99917 | -2.11722 | -3.10850 | C | -3.60305 | -1.29410 | -0.98131 |
| H | -1.65685 | -1.63188 | -3.83125 | C | -3.58754 | -2.63394 | -3.39944 |
| H | -0.20213 | -1.41311 | -2.87935 | C | -1.18047 | -3.19460 | -3.28986 |
| H | -0.54789 | -2.98347 | -3.59455 | C | -4.78235 | -1.64444 | -1.63166 |
| C | -3.17481 | -5.94756 | -0.84631 | C | -3.76045 | -0.95140 | 0.51307 |
| H | -2.55662 | -6.52739 | -1.53330 | C | -4.81007 | -2.21597 | -2.89343 |
| H | -3.12336 | -6.40922 | 0.14121 | H | -3.57487 | -3.24551 | -4.29302 |
| H | -4.21075 | -6.02701 | -1.19057 | C | -0.84910 | -2.99772 | -4.77076 |
| S | -1.90078 | 0.88781 | -2.61537 | C | -1.62073 | -4.66214 | -3.09326 |
| | | | | C | 0.06943 | -3.03505 | -2.44129 |
| | | | | H | -5.71563 | -1.46796 | -1.11522 |
| | | | | C | -2.45264 | -0.65714 | 1.22818 |
| | | | | C | -4.30920 | -2.23864 | 1.16403 |
| | | | | C | -4.76132 | 0.17675 | 0.78138 |
| | | | | C | -6.09801 | -2.48346 | -3.66104 |
| | | | | H | -0.09505 | -3.72951 | -5.07230 |
| | | | | H | -1.72571 | -3.14793 | -5.40489 |
| | | | | H | -0.45249 | -2.00300 | -4.96457 |
| | | | | H | -2.45295 | -4.94258 | -3.73982 |
| | | | | H | -0.77882 | -5.31816 | -3.32991 |
| | | | | H | -1.91695 | -4.84964 | -2.05823 |
| | | | | H | 0.52570 | -2.05159 | -2.51952 |
| | | | | H | -0.14643 | -3.25361 | -1.39375 |
| | | | | H | 0.82174 | -3.75233 | -2.77690 |
| | | | | H | -1.71347 | -1.43894 | 1.04430 |
| | | | | H | -2.00901 | 0.30313 | 0.97044 |
| | | | | H | -2.62432 | -0.62297 | 2.30666 |
| | | | | H | -4.41376 | -2.08323 | 2.24129 |
| | | | | H | -5.28512 | -2.51752 | 0.76529 |
| | | | | H | -3.62669 | -3.07680 | 1.00517 |
| | | | | H | -5.75543 | -0.05566 | 0.39613 |
| | | | | H | -4.85723 | 0.32686 | 1.85970 |
| | | | | H | -4.45151 | 1.12552 | 0.34193 |
| | | | | C | -7.32488 | -1.92900 | -2.94201 |
| | | | | C | -6.28610 | -3.99432 | -3.84417 |
| | | | | C | -5.99951 | -1.81375 | -5.03696 |
| | | | | H | -7.49195 | -2.41962 | -1.97968 |
| R = Mes* | | | | | | | |
| P | 0.70412 | 0.14367 | 0.96509 | | | | |
| C | 0.45160 | 0.12109 | -0.77629 | | | | |
| P | -1.15583 | -0.05873 | -1.65541 | | | | |
| Cl | 2.86008 | -0.72001 | -3.01614 | | | | |
| Au | 0.53569 | 2.25375 | -0.28609 | | | | |
| Cl | 0.31369 | 4.51416 | -0.03763 | | | | |
| C | 2.54089 | 0.01309 | 1.15384 | | | | |
| C | 3.24964 | -1.13542 | 0.70769 | | | | |
| C | 3.29372 | 1.12701 | 1.60960 | | | | |
| C | 4.58691 | -0.98999 | 0.37213 | | | | |
| C | 4.62985 | 1.20800 | 1.21502 | | | | |
| C | 5.27934 | 0.20523 | 0.51804 | | | | |
| H | 5.11640 | -1.85414 | -0.00906 | | | | |
| H | 5.18465 | 2.09243 | 1.49425 | | | | |
| C | 2.87408 | 2.16323 | 2.67634 | | | | |
| C | 2.74353 | -2.58885 | 0.79640 | | | | |
| C | 6.70799 | 0.33653 | 0.00412 | | | | |
| C | 3.76494 | 1.86073 | 3.89966 | | | | |
| H | 3.59865 | 0.84327 | 4.26337 | | | | |
| H | 4.82596 | 1.96589 | 3.67035 | | | | |
| H | 3.52202 | 2.55663 | 4.70749 | | | | |
| C | 3.13581 | 3.60420 | 2.23011 | | | | |
| H | 2.53748 | 3.87535 | 1.36025 | | | | |
| H | 2.86899 | 4.28882 | 3.04001 | | | | |
| H | 4.18645 | 3.77767 | 1.99184 | | | | |
| C | 1.43800 | 2.06564 | 3.18370 | | | | |

| | | | |
|----|----------|----------|----------|
| H | -7.24288 | -0.85262 | -2.77141 |
| H | -8.21381 | -2.10077 | -3.55326 |
| H | -5.46416 | -4.44136 | -4.40664 |
| H | -6.34867 | -4.50174 | -2.87841 |
| H | -7.21079 | -4.19226 | -4.39298 |
| H | -5.88016 | -0.73206 | -4.93897 |
| H | -5.15215 | -2.19278 | -5.61161 |
| H | -6.90861 | -2.00504 | -5.61333 |
| Si | 1.50835 | 0.77480 | -2.31340 |
| S | -0.40203 | 0.22919 | -3.52138 |
| C | -2.26746 | 1.37022 | -1.45765 |
| H | -2.62817 | 1.51125 | -0.44360 |
| H | -1.71751 | 2.25669 | -1.77425 |
| H | -3.10960 | 1.21400 | -2.13423 |

| | | | |
|----|----------|----------|----------|
| C | 2.13092 | 2.43163 | 1.04761 |
| C | 2.59496 | 0.04831 | 1.66285 |
| H | 3.27545 | -0.11756 | -1.01817 |
| H | 2.97715 | 1.58774 | -1.42912 |
| H | 4.20801 | 1.16339 | -0.24902 |
| H | 1.39861 | 2.53316 | 1.85354 |
| H | 3.10773 | 2.72037 | 1.44801 |
| H | 1.87150 | 3.13883 | 0.25634 |
| H | 3.56925 | 0.34605 | 2.06275 |
| H | 1.87404 | 0.08356 | 2.48451 |
| H | 2.67573 | -0.98649 | 1.32101 |
| C | -2.01299 | -1.79915 | -1.87551 |
| C | -3.07656 | -2.07920 | -2.93897 |
| C | -0.99165 | -2.93955 | -1.83684 |
| C | -2.64504 | -1.59564 | -0.50140 |
| H | -3.83316 | -1.29404 | -2.97688 |
| H | -2.63490 | -2.18868 | -3.93107 |
| H | -3.57660 | -3.01764 | -2.68468 |
| H | -0.21451 | -2.76899 | -1.09001 |
| H | -1.52032 | -3.85909 | -1.57219 |
| H | -0.50897 | -3.08902 | -2.80337 |
| H | -3.13327 | -2.52773 | -0.20464 |
| H | -1.90050 | -1.35351 | 0.26093 |
| H | -3.39981 | -0.80811 | -0.51107 |
| Cl | -2.45763 | 1.19144 | -2.36947 |

PCPX-E(II)-AuCl model systems

E = Ge(II)

[R-P=C(Ge(II)Cl)-P(O)ClR](AuCl)

Coordination through Ge(II) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.49593 | 0.37629 | 0.47512 |
| C | 0.10649 | 0.28291 | -1.13263 |
| P | -1.43497 | -0.00849 | -1.90287 |
| Ge | 0.89471 | 0.67379 | -2.96703 |
| Cl | 1.52944 | -1.31599 | -3.55201 |
| O | -1.08636 | 0.42819 | -3.32311 |
| Au | 1.90229 | 2.65137 | -3.65924 |
| Cl | 2.88750 | 4.60344 | -4.26329 |
| H | 1.87506 | 0.70748 | 0.30856 |
| H | -1.88686 | -1.33664 | -1.84821 |
| Cl | -2.98868 | 0.97375 | -1.14308 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.54375 | 0.37472 | 0.45453 |
| C | 0.12537 | 0.26610 | -1.14339 |
| P | -1.42167 | -0.06077 | -1.88376 |
| Ge | 0.86004 | 0.67209 | -2.98343 |
| Cl | 1.55327 | -1.30268 | -3.60086 |
| O | -1.08533 | 0.38798 | -3.31469 |
| C | -1.98499 | -1.75093 | -1.82496 |
| H | -2.21006 | -2.03541 | -0.79639 |
| H | -2.87718 | -1.85246 | -2.44529 |
| H | -1.18134 | -2.37374 | -2.22406 |
| C | 2.32440 | 0.78963 | 0.40819 |
| H | 2.89420 | -0.14519 | 0.38639 |
| H | 2.59436 | 1.38776 | -0.46403 |
| H | 2.59427 | 1.32185 | 1.32177 |
| Au | 1.87845 | 2.64754 | -3.67856 |
| Cl | 2.89271 | 4.59647 | -4.25876 |
| Cl | -2.94005 | 1.01039 | -1.13490 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.45371 | 0.54781 | 0.09602 |
| C | 0.36071 | 0.16846 | -1.51495 |
| P | -1.10133 | -0.29805 | -2.37643 |
| Ge | 1.35454 | 0.11046 | -3.28660 |
| Cl | 2.28296 | -1.86353 | -3.26017 |
| O | -0.48989 | -0.43697 | -3.78223 |
| Au | 2.27711 | 1.90667 | -4.45464 |
| Cl | 3.16188 | 3.70776 | -5.52806 |
| C | 2.21043 | 0.99396 | 0.51922 |
| C | 3.21153 | 0.89626 | -0.61568 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.66627 | 0.40142 | 0.27965 |
| C | 0.22445 | 0.18329 | -1.30685 |
| P | -1.37382 | -0.14504 | -1.93219 |
| Ge | 0.83790 | 0.55903 | -3.19097 |
| Cl | 1.58312 | -1.38479 | -3.86669 |
| O | -1.10693 | 0.18538 | -3.40962 |
| Au | 1.72748 | 2.54565 | -4.02355 |
| Cl | 2.62382 | 4.49566 | -4.77989 |
| C | 2.42372 | 0.76740 | 0.25647 |
| C | 2.90165 | 1.47586 | 1.36452 |
| C | 3.31625 | 0.39694 | -0.75455 |
| C | 4.23249 | 1.85089 | 1.43565 |
| H | 2.21869 | 1.74584 | 2.16411 |
| C | 4.64679 | 0.76260 | -0.67348 |
| H | 2.97986 | -0.20978 | -1.58781 |
| C | 5.10286 | 1.49755 | 0.41481 |
| H | 4.59157 | 2.41630 | 2.28740 |
| H | 5.33276 | 0.47491 | -1.46127 |
| H | 6.14583 | 1.78755 | 0.46938 |
| C | -2.02604 | -1.79119 | -1.73628 |
| C | -1.85321 | -2.68943 | -2.78759 |
| C | -2.63264 | -2.19696 | -0.54820 |
| C | -2.29808 | -3.99447 | -2.64599 |
| H | -1.37674 | -2.36547 | -3.70458 |
| C | -3.06657 | -3.50352 | -0.41669 |
| H | -2.77248 | -1.49491 | 0.26579 |
| C | -2.90050 | -4.40020 | -1.46504 |
| H | -2.17207 | -4.69454 | -3.46317 |
| H | -3.54088 | -3.82306 | 0.50351 |
| H | -3.24623 | -5.42204 | -1.35899 |
| Cl | -2.77032 | 1.07030 | -1.15379 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.75031 | 0.19211 | 0.74825 |
| C | 0.19021 | 0.05019 | -0.80791 |
| P | -1.39146 | -0.18457 | -1.53829 |
| Ge | 0.86291 | 0.77259 | -2.55927 |
| Cl | 1.54326 | -1.02246 | -3.61042 |
| O | -1.08770 | 0.53488 | -2.86495 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| Au | 1.82508 | 2.86284 | -2.94561 | C | -2.03889 | 4.01711 | -0.20955 |
| Cl | 2.78704 | 4.91458 | -3.19906 | C | -2.83060 | 0.00194 | 2.88538 |
| C | 2.46602 | 0.73515 | 0.48764 | C | -5.92601 | 0.83805 | -0.99393 |
| C | 2.77492 | 2.08637 | 0.70574 | C | 4.00055 | 0.89436 | 2.63521 |
| C | 3.46709 | -0.18402 | 0.14265 | C | 3.40030 | 1.11282 | -2.47159 |
| C | 4.08437 | 2.50700 | 0.52788 | C | 7.54841 | -0.84402 | -0.47279 |
| C | 4.76506 | 0.28461 | -0.01505 | C | -3.91395 | -1.04133 | 3.17305 |
| C | 5.09177 | 1.62455 | 0.15654 | H | -3.72453 | -1.47984 | 4.15531 |
| H | 4.31989 | 3.55737 | 0.66908 | H | -4.91238 | -0.60024 | 3.20451 |
| H | 5.54610 | -0.42183 | -0.27996 | H | -3.90802 | -1.85403 | 2.44204 |
| C | -2.01075 | -1.84871 | -1.74611 | C | -2.93083 | 1.08841 | 3.96803 |
| C | -2.41028 | -2.32066 | -3.01713 | H | -2.14603 | 1.84231 | 3.85731 |
| C | -2.09021 | -2.68567 | -0.61418 | H | -3.89538 | 1.59940 | 3.92243 |
| C | -2.84508 | -3.63635 | -3.10964 | H | -2.82676 | 0.63916 | 4.95986 |
| C | -2.53615 | -3.98844 | -0.77745 | C | -1.48905 | -0.71520 | 3.04656 |
| C | -2.90679 | -4.48954 | -2.01663 | H | -1.29306 | -1.40935 | 2.22704 |
| H | -3.15825 | -4.00293 | -4.08190 | H | -0.64291 | -0.02593 | 3.12271 |
| H | -2.60088 | -4.62751 | 0.09751 | H | -1.50304 | -1.28551 | 3.97922 |
| C | -2.41548 | -1.50631 | -4.27750 | C | -7.12016 | 0.78407 | -0.03372 |
| H | -2.93872 | -0.55738 | -4.15941 | H | -8.02522 | 0.50403 | -0.57962 |
| H | -1.40160 | -1.26869 | -4.60337 | H | -6.97309 | 0.04811 | 0.75878 |
| H | -2.90587 | -2.07177 | -5.06982 | H | -7.29230 | 1.75675 | 0.43461 |
| C | -1.70430 | -2.24857 | 0.76586 | C | -6.25786 | 1.82160 | -2.11289 |
| H | -0.62110 | -2.30378 | 0.90620 | H | -7.15361 | 1.48311 | -2.63891 |
| H | -2.01044 | -1.22714 | 0.99670 | H | -6.46129 | 2.82534 | -1.72964 |
| H | -2.16346 | -2.90262 | 1.50765 | H | -5.45070 | 1.88792 | -2.84666 |
| C | -3.35087 | -5.90905 | -2.17434 | C | -5.70960 | -0.54755 | -1.61567 |
| H | -2.50096 | -6.54630 | -2.43809 | H | -4.87551 | -0.53246 | -2.32139 |
| H | -3.77873 | -6.29913 | -1.24969 | H | -5.49020 | -1.30740 | -0.86311 |
| H | -4.09134 | -6.00887 | -2.96960 | H | -6.60769 | -0.85933 | -2.15640 |
| C | 3.17138 | -1.64268 | -0.04844 | C | -2.90022 | 4.89022 | -1.12593 |
| H | 2.54523 | -2.03783 | 0.75831 | H | -3.89843 | 5.05809 | -0.71593 |
| H | 2.64407 | -1.82673 | -0.98862 | H | -2.41922 | 5.86506 | -1.23395 |
| H | 4.09447 | -2.22329 | -0.06537 | H | -3.00116 | 4.46307 | -2.12635 |
| C | 1.71040 | 3.07683 | 1.06845 | C | -1.88427 | 4.78042 | 1.11330 |
| H | 1.15808 | 3.39731 | 0.17924 | H | -2.85308 | 4.91985 | 1.59848 |
| H | 0.98342 | 2.65808 | 1.77396 | H | -1.22852 | 4.26224 | 1.81788 |
| H | 2.14249 | 3.96882 | 1.52314 | H | -1.44843 | 5.76616 | 0.92718 |
| C | 6.48747 | 2.11556 | -0.07065 | C | -0.67146 | 3.89347 | -0.88713 |
| H | 6.55137 | 2.65248 | -1.02176 | H | 0.09148 | 3.47828 | -0.22445 |
| H | 6.79689 | 2.81017 | 0.71328 | H | -0.72017 | 3.25985 | -1.77388 |
| H | 7.20152 | 1.29155 | -0.10287 | H | -0.32240 | 4.88658 | -1.18474 |
| Cl | -2.84859 | 0.84840 | -0.59201 | C | 2.59314 | 1.44810 | 2.80424 |
| | | | | H | 2.34800 | 2.17105 | 2.02227 |
| | | | | H | 1.82914 | 0.67247 | 2.83005 |
| | | | | H | 2.52448 | 1.97637 | 3.75806 |
| | | | | C | 4.95004 | 2.08863 | 2.86478 |
| | | | | H | 4.74982 | 2.52374 | 3.84752 |
| | | | | H | 5.99974 | 1.79547 | 2.83453 |
| | | | | H | 4.79357 | 2.86396 | 2.11090 |
| | | | | C | 4.26764 | -0.15251 | 3.71993 |
| | | | | H | 5.29778 | -0.51202 | 3.69728 |
| | | | | H | 4.09756 | 0.29236 | 4.70389 |
| | | | | H | 3.60685 | -1.01317 | 3.61951 |
| | | | | C | 2.23273 | 2.03078 | -2.11955 |
| | | | | H | 1.87487 | 2.52548 | -3.02534 |
| | | | | H | 1.36976 | 1.51480 | -1.70789 |
| | | | | H | 2.54721 | 2.80555 | -1.41520 |
| | | | | C | 2.99802 | 0.06569 | -3.51418 |
| | | | | H | 2.21284 | -0.59174 | -3.15092 |
| | | | | H | 2.63916 | 0.56792 | -4.41644 |
| | | | | H | 3.85866 | -0.54767 | -3.79349 |
| | | | | C | 4.44920 | 2.03686 | -3.12342 |
| | | | | H | 4.85895 | 2.75013 | -2.40437 |
| | | | | H | 5.27757 | 1.49047 | -3.57533 |
| | | | | H | 3.96463 | 2.60159 | -3.92356 |

| R = Mes* | | | |
|----------|----------|----------|----------|
| P | -0.44970 | 1.78621 | 1.50716 |
| C | 0.17918 | 0.65416 | 0.46076 |
| P | 1.74594 | -0.12584 | 0.20883 |
| Cl | -0.97977 | 0.54918 | -2.72339 |
| O | 1.34806 | -0.87819 | -1.07950 |
| C | 3.46082 | 0.44993 | 0.08846 |
| C | 4.04003 | 0.48963 | -1.21581 |
| C | 4.31935 | 0.38506 | 1.21690 |
| C | 5.35375 | 0.06443 | -1.33497 |
| C | 5.63438 | -0.01323 | 1.00618 |
| C | 6.14941 | -0.28482 | -0.25077 |
| H | 5.78257 | 0.02388 | -2.32738 |
| H | 6.27878 | -0.10756 | 1.86885 |
| C | -2.21860 | 1.73702 | 1.03111 |
| C | -2.71155 | 2.65987 | 0.08261 |
| C | -3.05722 | 0.70617 | 1.53008 |
| C | -3.92232 | 2.36058 | -0.53923 |
| C | -4.24190 | 0.46561 | 0.84709 |
| C | -4.66517 | 1.23221 | -0.23234 |
| H | -4.28931 | 3.02751 | -1.30279 |
| H | -4.86256 | -0.35903 | 1.16412 |

| | | | |
|----|----------|----------|----------|
| C | 8.25126 | -1.18099 | 0.83948 |
| H | 8.42255 | -0.29236 | 1.45245 |
| H | 7.68311 | -1.90438 | 1.42955 |
| H | 9.22760 | -1.62186 | 0.62607 |
| C | 8.40063 | 0.18209 | -1.22944 |
| H | 7.97731 | 0.42249 | -2.20653 |
| H | 8.49001 | 1.11227 | -0.66295 |
| H | 9.40618 | -0.21524 | -1.39129 |
| C | 7.43778 | -2.12710 | -1.30560 |
| H | 6.84294 | -2.88191 | -0.78599 |
| H | 6.97089 | -1.94222 | -2.27496 |
| H | 8.43280 | -2.54219 | -1.48653 |
| Ge | -0.61327 | -0.59861 | -0.90441 |
| Au | -2.01248 | -2.41514 | -0.44789 |
| Cl | -3.47523 | -4.08183 | 0.11750 |
| Cl | 1.87201 | -1.60622 | 1.60276 |

Coordination through O atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.51603 | 0.18548 | 0.69503 |
| C | 0.28631 | 0.28298 | -0.94351 |
| P | -1.21534 | 0.36274 | -1.80128 |
| Ge | 1.43002 | 0.67859 | -2.64760 |
| Cl | 1.31938 | -1.39576 | -3.41232 |
| O | -0.76372 | 1.09048 | -3.07636 |
| Au | -2.00204 | 1.37387 | -4.76627 |
| Cl | -3.31568 | 1.66448 | -6.53186 |
| H | -1.76368 | -0.89376 | -2.09474 |
| H | 1.94713 | 0.21213 | 0.68662 |
| Cl | -2.72826 | 1.28323 | -0.89235 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.53705 | 0.13118 | 0.68073 |
| C | 0.28486 | 0.28691 | -0.94799 |
| P | -1.23693 | 0.31848 | -1.77141 |
| Ge | 1.35673 | 0.80889 | -2.66094 |
| Cl | 1.51287 | -1.26447 | -3.45942 |
| O | -0.78853 | 1.00893 | -3.08332 |
| C | -1.97736 | -1.27147 | -2.08044 |
| H | -2.28162 | -1.72300 | -1.13507 |
| H | -2.84233 | -1.14189 | -2.73407 |
| H | -1.22293 | -1.88896 | -2.57334 |
| C | 2.36407 | 0.13447 | 0.84262 |
| H | 2.71575 | -0.90016 | 0.77664 |
| H | 2.85867 | 0.72106 | 0.06660 |
| H | 2.64042 | 0.51632 | 1.82695 |
| Au | -2.00841 | 1.27863 | -4.78313 |
| Cl | -3.31114 | 1.55154 | -6.56163 |
| Cl | -2.67272 | 1.40004 | -0.88255 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.69040 | -0.35016 | 0.45049 |
| C | 0.24924 | 0.30937 | -1.00637 |
| P | -1.36248 | 0.19794 | -1.66835 |
| Ge | 0.92407 | 1.62430 | -2.49424 |
| Cl | 1.79223 | 0.07317 | -3.84086 |
| O | -1.17962 | 1.12463 | -2.89530 |
| Au | -2.56330 | 1.91781 | -4.27225 |
| Cl | -4.00761 | 2.76178 | -5.73548 |
| C | -2.02315 | -1.45037 | -2.11654 |
| C | -3.40413 | -1.29648 | -2.75488 |
| C | -1.04032 | -2.06151 | -3.11867 |
| C | -2.11160 | -2.30971 | -0.85666 |
| H | -4.13472 | -0.88249 | -2.05886 |

| | | | |
|----|----------|----------|----------|
| H | -3.38043 | -0.66675 | -3.64708 |
| H | -3.74822 | -2.29010 | -3.05487 |
| H | -0.03785 | -2.17049 | -2.70183 |
| H | -1.40830 | -3.05508 | -3.38797 |
| H | -0.96580 | -1.46763 | -4.03039 |
| H | -2.47356 | -3.29975 | -1.14639 |
| H | -1.14057 | -2.43843 | -0.37388 |
| H | -2.81069 | -1.89721 | -0.12723 |
| C | 2.50034 | 0.00348 | 0.73477 |
| C | 3.19186 | -1.36174 | 0.64564 |
| C | 3.13476 | 0.98495 | -0.23234 |
| C | 2.58954 | 0.53089 | 2.17028 |
| H | 2.73430 | -2.09607 | 1.31472 |
| H | 3.16545 | -1.75958 | -0.37150 |
| H | 4.24107 | -1.25594 | 0.94029 |
| H | 2.63724 | 1.95854 | -0.20841 |
| H | 4.18200 | 1.15294 | 0.04092 |
| H | 3.13375 | 0.59988 | -1.25603 |
| H | 3.64075 | 0.63539 | 2.45620 |
| H | 2.11573 | 1.51063 | 2.27164 |
| H | 2.11605 | -0.14934 | 2.88334 |
| Cl | -2.73425 | 1.01677 | -0.43752 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.51662 | -0.26952 | 0.76271 |
| C | 0.22802 | 0.10184 | -0.83089 |
| P | -1.31794 | 0.13871 | -1.60938 |
| Ge | 1.18031 | 1.21276 | -2.30276 |
| Cl | 1.72860 | -0.45334 | -3.68439 |
| O | -0.98779 | 1.10696 | -2.76719 |
| Au | -2.27785 | 1.83990 | -4.26547 |
| Cl | -3.62225 | 2.61638 | -5.85618 |
| C | -1.95383 | -1.41557 | -2.20368 |
| C | -2.63892 | -2.27785 | -1.34802 |
| C | -1.70090 | -1.78060 | -3.52452 |
| C | -3.07261 | -3.50329 | -1.81934 |
| H | -2.84152 | -1.98974 | -0.32294 |
| C | -2.14687 | -3.00841 | -3.98683 |
| H | -1.16323 | -1.11191 | -4.18474 |
| C | -2.82860 | -3.86647 | -3.13801 |
| H | -3.60972 | -4.17397 | -1.15943 |
| H | -1.96217 | -3.28990 | -5.01642 |
| H | -3.17712 | -4.82473 | -3.50570 |
| C | 2.30380 | -0.10270 | 0.94012 |
| C | 3.22298 | -0.28319 | -0.09877 |
| C | 2.77411 | 0.21051 | 2.21906 |
| C | 4.57726 | -0.11440 | 0.13283 |
| H | 2.88195 | -0.60529 | -1.07753 |
| C | 4.12887 | 0.38975 | 2.44407 |
| H | 2.06915 | 0.32658 | 3.03655 |
| C | 5.02967 | 0.23094 | 1.40026 |
| H | 5.28380 | -0.26213 | -0.67565 |
| H | 4.48373 | 0.64795 | 3.43498 |
| H | 6.09096 | 0.36255 | 1.57733 |
| Cl | -2.77604 | 0.90325 | -0.45504 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.33031 | 0.20765 | 0.82469 |
| C | 0.17456 | 0.04963 | -0.81730 |
| P | -1.17402 | 0.04909 | -1.91868 |
| Ge | 1.60692 | 0.47503 | -2.24285 |
| Cl | 2.00495 | -1.63150 | -2.87631 |
| O | -0.43545 | 0.59942 | -3.16058 |
| Au | -1.06091 | 1.92730 | -4.68474 |
| Cl | -1.67507 | 3.33328 | -6.29431 |
| C | -2.00161 | -1.51637 | -2.18657 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | -2.67723 | -2.10014 | -1.09134 | H | 6.25381 | 2.20508 | 2.85106 |
| C | -1.95987 | -2.18138 | -3.43468 | H | 5.08749 | 2.83689 | 4.01262 |
| C | -3.26008 | -3.34747 | -1.25270 | C | 3.14538 | -0.37677 | -3.49296 |
| C | -2.57506 | -3.42402 | -3.52639 | H | 2.18156 | -0.65471 | -3.06115 |
| C | -3.21664 | -4.03204 | -2.45808 | H | 2.98761 | -0.16817 | -4.55479 |
| H | -3.77285 | -3.79164 | -0.40543 | H | 3.80556 | -1.24263 | -3.41901 |
| H | -2.54645 | -3.93519 | -4.48303 | C | 2.77839 | 2.02742 | -3.01889 |
| C | 2.14513 | 0.31191 | 1.01613 | H | 1.75138 | 1.79367 | -2.73646 |
| C | 2.73703 | 1.57213 | 1.18954 | H | 3.10354 | 2.92809 | -2.48852 |
| C | 2.91858 | -0.85697 | 1.08936 | H | 2.75873 | 2.27683 | -4.08366 |
| C | 4.10788 | 1.64331 | 1.39900 | C | 5.04088 | 1.24842 | -3.51946 |
| C | 4.28516 | -0.73447 | 1.30432 | H | 5.49060 | 2.12935 | -3.05457 |
| C | 4.90044 | 0.50324 | 1.45256 | H | 5.78044 | 0.44772 | -3.50415 |
| H | 4.56796 | 2.61844 | 1.52925 | H | 4.82797 | 1.48549 | -4.56530 |
| H | 4.88646 | -1.63676 | 1.36553 | C | 6.99753 | -2.53591 | -0.93711 |
| C | 1.91939 | 2.82774 | 1.12852 | H | 7.38000 | -1.95779 | -1.78244 |
| H | 1.62540 | 3.06294 | 0.10068 | H | 7.73205 | -3.31329 | -0.71424 |
| H | 0.99673 | 2.74059 | 1.71234 | H | 6.07470 | -3.03288 | -1.24665 |
| H | 2.48001 | 3.67958 | 1.51494 | C | 6.32530 | -2.57285 | 1.44942 |
| C | 2.30095 | -2.21578 | 0.94685 | H | 6.20324 | -2.01509 | 2.37991 |
| H | 1.40407 | -2.31828 | 1.56646 | H | 5.36739 | -3.04447 | 1.21893 |
| H | 2.00396 | -2.40899 | -0.08783 | H | 7.06343 | -3.36036 | 1.62486 |
| H | 3.00390 | -2.99399 | 1.24620 | C | 8.12436 | -1.01815 | 0.66882 |
| C | 6.38150 | 0.60509 | 1.64932 | H | 8.04776 | -0.41760 | 1.57744 |
| H | 6.89594 | 0.64951 | 0.68428 | H | 8.88021 | -1.78908 | 0.84239 |
| H | 6.64925 | 1.50580 | 2.20416 | H | 8.47941 | -0.36834 | -0.13503 |
| H | 6.77259 | -0.26031 | 2.18717 | C | -2.15503 | 1.32820 | 0.30318 |
| C | -2.85298 | -1.43098 | 0.23843 | C | -2.76476 | 0.72260 | 1.44297 |
| H | -1.95930 | -0.91325 | 0.59069 | C | -2.94446 | 2.15741 | -0.53607 |
| H | -3.65642 | -0.69125 | 0.19774 | C | -4.14661 | 0.63054 | 1.44511 |
| H | -3.11865 | -2.16976 | 0.99494 | C | -4.32465 | 2.02254 | -0.45406 |
| C | -1.31836 | -1.65390 | -4.68258 | C | -4.94939 | 1.17648 | 0.45061 |
| H | -1.74818 | -0.69891 | -4.99385 | H | -4.61837 | 0.10780 | 2.26722 |
| H | -0.24643 | -1.50164 | -4.55698 | H | -4.93303 | 2.61091 | -1.12695 |
| H | -1.46737 | -2.36561 | -5.49411 | C | -2.04194 | 0.32575 | 2.74425 |
| C | -3.82609 | -5.39063 | -2.59789 | C | -2.11836 | -1.17234 | 3.04482 |
| H | -4.65658 | -5.52924 | -1.90401 | C | -2.75641 | 1.08288 | 3.88276 |
| H | -4.18849 | -5.56161 | -3.61275 | H | -1.52631 | -1.75570 | 2.34083 |
| H | -3.08360 | -6.16507 | -2.38109 | H | -1.72969 | -1.36222 | 4.04900 |
| Cl | -2.59930 | 1.39796 | -1.43513 | H | -3.14659 | -1.53798 | 3.00738 |
| | | | | H | -2.77182 | 2.15926 | 3.69473 |
| | | | | H | -3.78356 | 0.74961 | 4.03212 |
| | | | | H | -2.21509 | 0.90777 | 4.81594 |
| | | | | C | -2.42729 | 3.33757 | -1.38081 |
| | | | | C | -3.03965 | 4.59599 | -0.73001 |
| | | | | C | -2.88612 | 3.28106 | -2.83997 |
| | | | | H | -2.74266 | 4.67870 | 0.31825 |
| | | | | H | -2.68168 | 5.48457 | -1.25707 |
| | | | | H | -4.12905 | 4.59446 | -0.77304 |
| | | | | H | -2.46395 | 2.42423 | -3.36392 |
| | | | | H | -3.97281 | 3.22460 | -2.92311 |
| | | | | H | -2.56406 | 4.18835 | -3.35802 |
| | | | | C | -6.44803 | 0.91227 | 0.44390 |
| | | | | C | -7.07592 | 1.48446 | 1.72080 |
| | | | | C | -6.67800 | -0.60361 | 0.39530 |
| | | | | H | -6.92430 | 2.56505 | 1.78550 |
| | | | | H | -8.15191 | 1.29084 | 1.72469 |
| | | | | H | -6.65386 | 1.02984 | 2.61925 |
| | | | | H | -6.22610 | -1.05041 | -0.49264 |
| | | | | H | -6.25117 | -1.10893 | 1.26341 |
| | | | | H | -7.75070 | -0.81444 | 0.38004 |
| | | | | Cl | 2.03397 | -1.61644 | 1.85455 |
| | | | | O | -0.74010 | -1.00142 | 0.09712 |
| | | | | Cl | -1.04386 | 0.36400 | -2.35715 |
| | | | | Au | -2.35214 | -2.29693 | -0.36537 |
| | | | | Cl | -4.04829 | -3.66430 | -0.84461 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.99096 | 2.07364 | -0.19543 |
| C | 1.03069 | 0.71910 | -0.22922 |
| P | -0.69381 | 0.48678 | -0.34685 |
| C | 3.65221 | 1.28112 | -0.20149 |
| C | 4.39584 | 1.23219 | 1.00825 |
| C | 4.10752 | 0.57093 | -1.33169 |
| C | 5.40512 | 0.28846 | 1.10678 |
| C | 5.11267 | -0.38232 | -1.14243 |
| C | 5.73609 | -0.58481 | 0.07330 |
| H | 5.95260 | 0.20880 | 2.03442 |
| H | 5.42476 | -0.96924 | -1.99532 |
| C | 3.73419 | 0.85651 | -2.80285 |
| C | 4.17032 | 2.21102 | 2.17565 |
| C | 6.78538 | -1.66756 | 0.29999 |
| C | 2.82407 | 1.99239 | 2.87126 |
| H | 1.97500 | 2.24696 | 2.23128 |
| H | 2.70057 | 0.95313 | 3.17998 |
| H | 2.75784 | 2.63435 | 3.75460 |
| C | 4.25989 | 3.65065 | 1.65109 |
| H | 5.23161 | 3.83416 | 1.18627 |
| H | 3.48584 | 3.87671 | 0.91460 |
| H | 4.13854 | 4.35582 | 2.47805 |
| C | 5.24755 | 2.06768 | 3.25377 |
| H | 5.20103 | 1.09971 | 3.75806 |

| | | | |
|----|----------|----------|----------|
| C | -0.91791 | 3.54132 | -1.32503 |
| H | -0.55177 | 3.55696 | -0.29565 |
| H | -0.36119 | 2.79428 | -1.88796 |
| H | -0.67085 | 4.50927 | -1.76792 |
| C | -0.59234 | 0.79298 | 2.78877 |
| H | 0.06601 | 0.23252 | 2.12846 |
| H | -0.51143 | 1.85891 | 2.55944 |
| H | -0.19789 | 0.63920 | 3.79612 |
| C | -7.13878 | 1.54498 | -0.76116 |
| H | -7.07537 | 2.63645 | -0.74678 |
| H | -6.71720 | 1.18424 | -1.70254 |
| H | -8.19865 | 1.28113 | -0.75073 |
| Ge | 1.46236 | -1.32571 | -0.28189 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.42616 | 0.27709 | 0.53146 |
| C | 0.16492 | 0.17232 | -1.07919 |
| P | -1.31066 | 0.05384 | -1.98209 |
| Ge | 1.18971 | 0.46642 | -2.92832 |
| Cl | 1.34354 | -1.71807 | -3.35094 |
| O | -0.86635 | 0.57640 | -3.33655 |
| Au | -0.90489 | 0.26896 | 2.27645 |
| Cl | -2.27101 | 0.25672 | 4.06726 |
| H | 1.82650 | 0.38822 | 0.67613 |
| H | -1.79337 | -1.26257 | -2.02964 |
| Cl | -2.88576 | 1.03861 | -1.25472 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.51440 | 0.33559 | 0.49676 |
| C | 0.18542 | 0.22799 | -1.09940 |
| P | -1.33172 | 0.00906 | -1.91836 |
| Ge | 1.11190 | 0.45592 | -2.99496 |
| Cl | 1.48243 | -1.74291 | -3.25624 |
| O | -0.92001 | 0.36423 | -3.34451 |
| C | -2.01322 | -1.63095 | -1.77464 |
| H | -2.29777 | -1.82712 | -0.73984 |
| H | -2.88639 | -1.70991 | -2.42469 |
| H | -1.23946 | -2.33008 | -2.09964 |
| C | 2.29184 | 0.51333 | 0.77078 |
| H | 2.65102 | -0.37434 | 1.29817 |
| H | 2.82875 | 0.62514 | -0.17042 |
| H | 2.46774 | 1.37633 | 1.41655 |
| Au | -0.86339 | 0.22975 | 2.21257 |
| Cl | -2.27906 | 0.08358 | 3.96635 |
| Cl | -2.79375 | 1.23027 | -1.27883 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.73327 | -0.34646 | 0.50134 |
| C | 0.17880 | 0.23589 | -0.92681 |
| P | -1.43192 | 0.14234 | -1.60317 |
| Ge | 0.67571 | 1.66382 | -2.42813 |
| Cl | 1.61721 | 0.23933 | -3.88232 |
| O | -1.28580 | 1.13328 | -2.75887 |
| C | -2.06972 | -1.47571 | -2.17393 |
| C | -3.37721 | -1.20016 | -2.92137 |
| C | -1.02890 | -2.05565 | -3.13432 |
| C | -2.30097 | -2.42266 | -1.00199 |
| H | -4.15522 | -0.82077 | -2.25712 |
| H | -3.23357 | -0.48986 | -3.73737 |
| H | -3.72913 | -2.14301 | -3.34863 |
| H | -0.07421 | -2.24381 | -2.64035 |
| H | -1.41042 | -3.00913 | -3.50955 |
| H | -0.84471 | -1.39968 | -3.98537 |

| | | | |
|----|----------|----------|----------|
| H | -2.68105 | -3.36939 | -1.39547 |
| H | -1.37786 | -2.64053 | -0.46075 |
| H | -3.03299 | -2.03642 | -0.29169 |
| C | 2.52777 | -0.01611 | 0.79646 |
| C | 3.20964 | -1.38825 | 0.83849 |
| C | 3.14371 | 0.85568 | -0.28532 |
| C | 2.63515 | 0.65836 | 2.16668 |
| H | 2.75929 | -2.04424 | 1.58756 |
| H | 3.16944 | -1.88894 | -0.13146 |
| H | 4.26185 | -1.24932 | 1.10459 |
| H | 2.67894 | 1.84411 | -0.32413 |
| H | 4.20437 | 1.00427 | -0.06126 |
| H | 3.07718 | 0.39234 | -1.27209 |
| H | 3.69283 | 0.78673 | 2.41460 |
| H | 2.16459 | 1.64431 | 2.17182 |
| H | 2.17641 | 0.05562 | 2.95411 |
| Cl | -2.80785 | 0.82868 | -0.29066 |
| Au | -0.37617 | -1.45734 | 2.06157 |
| Cl | -1.50569 | -2.59349 | 3.66161 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.54464 | 0.49087 | 0.15773 |
| C | 0.40952 | -0.02371 | -1.39205 |
| P | -1.02931 | -0.38713 | -2.29854 |
| Ge | 1.52631 | -0.15031 | -3.17791 |
| Cl | 2.07823 | -2.32241 | -2.99370 |
| O | -0.44342 | -0.46886 | -3.70576 |
| Au | -1.07833 | 0.98074 | 1.57498 |
| Cl | -2.77562 | 1.43100 | 3.00182 |
| Cl | -2.40255 | 1.08004 | -2.17879 |
| C | 2.24951 | 0.63575 | 0.65429 |
| C | 3.27669 | -0.05011 | -0.00033 |
| C | 2.54385 | 1.45866 | 1.74405 |
| C | 4.58426 | 0.11206 | 0.42018 |
| H | 3.04859 | -0.73849 | -0.80653 |
| C | 3.85630 | 1.62098 | 2.15247 |
| H | 1.74134 | 1.97227 | 2.26351 |
| C | 4.87492 | 0.95112 | 1.48914 |
| H | 5.37949 | -0.42637 | -0.08161 |
| H | 4.08391 | 2.26674 | 2.99214 |
| H | 5.90178 | 1.07342 | 1.81422 |
| C | -1.88985 | -1.87546 | -1.83167 |
| C | -1.59579 | -3.04263 | -2.53421 |
| C | -2.78381 | -1.89519 | -0.76146 |
| C | -2.20795 | -4.22962 | -2.16433 |
| H | -0.89310 | -3.01631 | -3.35785 |
| C | -3.38321 | -3.08780 | -0.39825 |
| H | -3.01664 | -0.98667 | -0.21743 |
| C | -3.09657 | -4.25211 | -1.09991 |
| H | -1.98675 | -5.13902 | -2.71021 |
| H | -4.07847 | -3.10690 | 0.43239 |
| H | -3.57177 | -5.18342 | -0.81353 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.45446 | 0.51661 | 0.84531 |
| C | 0.16398 | -0.04834 | -0.66332 |
| P | -1.21762 | -0.26970 | -1.70340 |
| Ge | 1.38645 | 0.18371 | -2.36238 |
| Cl | 1.76153 | -2.00868 | -2.71766 |
| O | -0.57370 | 0.18547 | -3.01328 |
| Au | -0.91554 | 1.04186 | 2.49759 |
| Cl | -2.29489 | 1.58523 | 4.20778 |
| C | 2.23182 | 0.72173 | 1.04316 |
| C | 3.05344 | -0.40371 | 1.21311 |
| C | 2.76568 | 2.02053 | 1.06330 |
| C | 4.41542 | -0.19815 | 1.39003 |

| | | | |
|----|----------|----------|----------|
| C | 4.13375 | 2.16786 | 1.23761 |
| C | 4.97473 | 1.07357 | 1.40476 |
| H | 5.05865 | -1.06245 | 1.52373 |
| H | 4.55471 | 3.16864 | 1.24186 |
| C | -1.93953 | -1.90741 | -1.77908 |
| C | -2.34062 | -2.54131 | -0.58543 |
| C | -2.11930 | -2.55103 | -3.02452 |
| C | -2.87944 | -3.81713 | -0.65338 |
| C | -2.66565 | -3.82826 | -3.02068 |
| C | -3.04042 | -4.48539 | -1.85794 |
| H | -3.19026 | -4.29697 | 0.26926 |
| H | -2.81019 | -4.32371 | -3.97538 |
| C | 1.89770 | 3.22794 | 0.87605 |
| H | 1.42914 | 3.23437 | -0.11281 |
| H | 1.09217 | 3.26415 | 1.61654 |
| H | 2.48061 | 4.14399 | 0.97306 |
| C | 2.50571 | -1.79937 | 1.21508 |
| H | 1.63171 | -1.88787 | 1.86784 |
| H | 2.19873 | -2.11031 | 0.21256 |
| H | 3.25736 | -2.50457 | 1.57070 |
| C | 6.44301 | 1.26351 | 1.62688 |
| H | 6.65506 | 1.40863 | 2.69081 |
| H | 7.01206 | 0.39391 | 1.29472 |
| H | 6.81511 | 2.14245 | 1.09770 |
| C | -2.20939 | -1.91397 | 0.76768 |
| H | -1.18173 | -1.98206 | 1.13394 |
| H | -2.49318 | -0.86044 | 0.78049 |
| H | -2.84683 | -2.42910 | 1.48638 |
| C | -1.77815 | -1.96185 | -4.36195 |
| H | -2.20485 | -0.96907 | -4.50359 |
| H | -0.69861 | -1.86403 | -4.48595 |
| H | -2.15671 | -2.61434 | -5.14900 |
| C | -3.59208 | -5.87510 | -1.90213 |
| H | -4.12345 | -6.06375 | -2.83629 |
| H | -2.78251 | -6.60842 | -1.83216 |
| H | -4.27395 | -6.06044 | -1.07067 |
| Cl | -2.74320 | 0.99286 | -1.27392 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.15269 | 0.84528 | 0.02807 |
| C | -0.25918 | -0.47827 | 0.40047 |
| P | 1.39945 | -0.99411 | 0.62444 |
| Cl | -1.42391 | -3.08392 | -1.40180 |
| O | 1.20085 | -2.48157 | 0.32460 |
| C | 3.03432 | -0.48868 | 0.02415 |
| C | 3.57763 | -1.30524 | -1.01125 |
| C | 3.91685 | 0.27939 | 0.82824 |
| C | 4.92719 | -1.61146 | -0.93519 |
| C | 5.26067 | -0.07881 | 0.82777 |
| C | 5.77682 | -1.08739 | 0.03077 |
| H | 5.33527 | -2.28450 | -1.67804 |
| H | 5.92844 | 0.47093 | 1.47591 |
| C | -2.88214 | 0.28852 | 0.10343 |
| C | -3.58474 | -0.04009 | -1.08654 |
| C | -3.41913 | -0.05901 | 1.36775 |
| C | -4.67505 | -0.89443 | -0.96922 |
| C | -4.49829 | -0.93646 | 1.38712 |
| C | -5.11045 | -1.41366 | 0.24099 |
| H | -5.19245 | -1.18951 | -1.86659 |
| H | -4.88039 | -1.25321 | 2.34910 |
| C | -3.27937 | 0.55815 | -2.47381 |
| C | -3.01735 | 0.51596 | 2.74425 |
| C | -6.23831 | -2.43491 | 0.34363 |
| C | 3.58493 | 1.59695 | 1.55407 |
| C | 2.84579 | -1.75582 | -2.28942 |
| C | 7.22407 | -1.55481 | 0.11593 |

| | | | |
|---|----------|----------|----------|
| C | -4.28838 | 1.11023 | 3.38087 |
| H | -4.03583 | 1.55294 | 4.34776 |
| H | -4.71084 | 1.89457 | 2.74821 |
| H | -5.06402 | 0.36457 | 3.55390 |
| C | -2.01031 | 1.66295 | 2.71231 |
| H | -0.99522 | 1.33697 | 2.48103 |
| H | -2.30231 | 2.45296 | 2.01531 |
| H | -1.96240 | 2.11642 | 3.70616 |
| C | -2.46950 | -0.58423 | 3.65791 |
| H | -3.17659 | -1.40796 | 3.77202 |
| H | -1.53675 | -0.99612 | 3.26740 |
| H | -2.26746 | -0.17536 | 4.65194 |
| C | -7.39291 | -1.84855 | 1.16434 |
| H | -8.20349 | -2.57796 | 1.24526 |
| H | -7.08074 | -1.58612 | 2.17722 |
| H | -7.79199 | -0.94773 | 0.69160 |
| C | -6.77977 | -2.84111 | -1.02445 |
| H | -7.56519 | -3.58959 | -0.89589 |
| H | -7.21856 | -1.99432 | -1.55845 |
| H | -6.00246 | -3.28177 | -1.65335 |
| C | -5.70332 | -3.69185 | 1.04081 |
| H | -4.87803 | -4.13061 | 0.47508 |
| H | -5.34068 | -3.47349 | 2.04742 |
| H | -6.49633 | -4.43991 | 1.12617 |
| C | -4.21654 | 0.01063 | -3.55507 |
| H | -5.26601 | 0.22955 | -3.34647 |
| H | -3.96821 | 0.49316 | -4.50270 |
| H | -4.10057 | -1.06707 | -3.69332 |
| C | -3.52313 | 2.07185 | -2.40351 |
| H | -4.55790 | 2.28308 | -2.12261 |
| H | -2.87270 | 2.56536 | -1.67800 |
| H | -3.33268 | 2.52844 | -3.37839 |
| C | -1.85982 | 0.26936 | -2.96854 |
| H | -1.08645 | 0.78026 | -2.39057 |
| H | -1.64453 | -0.79945 | -2.95371 |
| H | -1.75506 | 0.63641 | -3.99334 |
| C | 2.14183 | 2.05437 | 1.39754 |
| H | 1.83918 | 2.02954 | 0.34779 |
| H | 1.43378 | 1.47684 | 1.98835 |
| H | 2.05273 | 3.09285 | 1.72336 |
| C | 4.43300 | 2.67673 | 0.84776 |
| H | 4.21204 | 3.65157 | 1.28960 |
| H | 5.50355 | 2.49520 | 0.94741 |
| H | 4.19330 | 2.72857 | -0.21666 |
| C | 3.96752 | 1.57865 | 3.03617 |
| H | 5.02607 | 1.35501 | 3.18185 |
| H | 3.77806 | 2.56374 | 3.47045 |
| H | 3.38709 | 0.84513 | 3.59495 |
| C | 1.49878 | -1.06752 | -2.48954 |
| H | 1.14424 | -1.26840 | -3.50336 |
| H | 0.72001 | -1.43942 | -1.82855 |
| H | 1.58472 | 0.01723 | -2.38033 |
| C | 2.68058 | -3.27632 | -2.35445 |
| H | 2.04259 | -3.63937 | -1.55096 |
| H | 2.22635 | -3.55565 | -3.30884 |
| H | 3.64773 | -3.78049 | -2.28492 |
| C | 3.71300 | -1.30713 | -3.48328 |
| H | 3.89278 | -0.22955 | -3.45971 |
| H | 4.67843 | -1.81188 | -3.52359 |
| H | 3.18341 | -1.54230 | -4.40979 |
| C | 7.98553 | -0.87631 | 1.25144 |
| H | 8.07086 | 0.20272 | 1.09987 |
| H | 7.51087 | -1.05291 | 2.21986 |
| H | 8.99969 | -1.27932 | 1.30085 |
| C | 7.94400 | -1.24582 | -1.20232 |
| H | 7.47793 | -1.75286 | -2.04934 |

| | | | |
|----|----------|----------|----------|
| H | 7.94020 | -0.17286 | -1.40898 |
| H | 8.98418 | -1.57807 | -1.14672 |
| C | 7.23898 | -3.06855 | 0.36126 |
| H | 6.74092 | -3.31792 | 1.30120 |
| H | 6.73492 | -3.61369 | -0.43911 |
| H | 8.26979 | -3.42896 | 0.41513 |
| Cl | 1.60912 | -0.95509 | 2.66557 |
| Au | -0.52857 | 2.91235 | -0.50564 |
| Cl | 0.10022 | 5.03194 | -1.02227 |
| Ge | -0.84125 | -2.52312 | 0.69473 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.43623 | -0.14722 | 0.66482 |
| C | 0.13781 | 0.54961 | -0.88573 |
| P | -1.29828 | 0.45412 | -1.87599 |
| Ge | 1.19090 | 1.06622 | -2.69026 |
| Cl | 1.38634 | -1.07733 | -3.31623 |
| O | -0.85617 | 1.19045 | -3.12818 |
| Au | 0.17742 | 2.20616 | 0.47716 |
| Cl | 0.16734 | 4.24408 | 1.41643 |
| H | 1.86350 | -0.11760 | 0.60806 |
| H | -1.65090 | -0.88200 | -2.12069 |
| Cl | -3.00420 | 1.19000 | -1.13565 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.46687 | -0.01079 | 0.65209 |
| C | 0.10008 | 0.70276 | -0.87326 |
| P | -1.34777 | 0.49603 | -1.84037 |
| Ge | 1.11778 | 1.20593 | -2.69074 |
| Cl | 1.61047 | -0.94523 | -3.17058 |
| O | -0.88589 | 1.08613 | -3.16955 |
| C | -1.87187 | -1.20325 | -1.98548 |
| H | -2.20966 | -1.57569 | -1.01747 |
| H | -2.68367 | -1.25960 | -2.71256 |
| H | -1.01301 | -1.77697 | -2.34094 |
| C | 2.29762 | -0.09706 | 0.66556 |
| H | 2.56781 | -1.09411 | 0.30141 |
| H | 2.77947 | 0.64973 | 0.03558 |
| H | 2.65253 | -0.00420 | 1.69368 |
| Au | 0.07460 | 2.33598 | 0.51831 |
| Cl | 0.00271 | 4.32576 | 1.56449 |
| Cl | -2.98265 | 1.46977 | -1.18147 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.64836 | -0.11054 | 0.45758 |
| C | 0.05982 | 0.71629 | -0.94194 |
| P | -1.45929 | 0.36517 | -1.78265 |
| Ge | 0.74818 | 1.65039 | -2.75800 |
| Cl | 1.81546 | -0.14868 | -3.59975 |
| O | -1.14353 | 0.94535 | -3.15968 |
| Au | -0.14250 | 2.12026 | 0.68401 |
| Cl | -0.43518 | 3.88688 | 2.05244 |
| C | -2.05461 | -1.36465 | -1.88289 |
| C | -3.20792 | -1.38791 | -2.88900 |
| C | -0.89710 | -2.22173 | -2.40030 |
| C | -2.51408 | -1.85472 | -0.51221 |
| H | -4.06122 | -0.80018 | -2.54679 |
| H | -2.89590 | -1.01618 | -3.86631 |
| H | -3.53758 | -2.42382 | -3.00671 |
| H | -0.06429 | -2.25653 | -1.69592 |
| H | -1.26572 | -3.24249 | -2.53367 |
| H | -0.51640 | -1.86562 | -3.35803 |
| H | -2.81557 | -2.90178 | -0.60484 |
| H | -1.71500 | -1.80480 | 0.23120 |

| | | | |
|----|----------|----------|----------|
| H | -3.36991 | -1.28945 | -0.14138 |
| C | 2.50490 | 0.07272 | 0.54866 |
| C | 3.03324 | -1.26305 | 0.00923 |
| C | 3.11744 | 1.23344 | -0.21495 |
| C | 2.82068 | 0.18953 | 2.04188 |
| H | 2.59821 | -2.11793 | 0.53561 |
| H | 2.83631 | -1.36983 | -1.05981 |
| H | 4.11677 | -1.30338 | 0.15970 |
| H | 2.70924 | 2.19516 | 0.10412 |
| H | 4.19712 | 1.25537 | -0.03246 |
| H | 2.98408 | 1.12544 | -1.29312 |
| H | 3.90374 | 0.13451 | 2.18713 |
| H | 2.47241 | 1.13942 | 2.45467 |
| H | 2.36564 | -0.61979 | 2.61984 |
| Cl | -3.01255 | 1.39628 | -0.98824 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.33247 | 0.47169 | 0.48810 |
| C | 0.17461 | 0.67976 | -1.21684 |
| P | -1.27291 | 0.40031 | -2.16674 |
| Ge | 1.21828 | 0.93927 | -3.08291 |
| Cl | 1.70162 | -1.22113 | -3.51074 |
| O | -0.78479 | 0.79151 | -3.55858 |
| Au | 0.26584 | 2.68612 | -0.40739 |
| Cl | 0.38812 | 4.90381 | -0.03783 |
| C | -1.87807 | -1.27722 | -2.10609 |
| C | -2.44831 | -1.78567 | -0.93974 |
| C | -1.75619 | -2.07324 | -3.24092 |
| C | -2.89404 | -3.09440 | -0.91303 |
| H | -2.54784 | -1.16143 | -0.05823 |
| C | -2.21243 | -3.38215 | -3.20535 |
| H | -1.30152 | -1.66915 | -4.13631 |
| C | -2.77700 | -3.89070 | -2.04617 |
| H | -3.33679 | -3.49480 | -0.00881 |
| H | -2.12043 | -4.00574 | -4.08656 |
| H | -3.12951 | -4.91553 | -2.02208 |
| C | 2.09839 | 0.26321 | 0.81834 |
| C | 3.01628 | -0.26271 | -0.09200 |
| C | 2.52085 | 0.59117 | 2.10989 |
| C | 4.33981 | -0.42919 | 0.27933 |
| H | 2.69157 | -0.57335 | -1.07831 |
| C | 3.84867 | 0.43880 | 2.47002 |
| H | 1.80644 | 0.98064 | 2.82869 |
| C | 4.75870 | -0.07054 | 1.55389 |
| H | 5.04708 | -0.84374 | -0.42967 |
| H | 4.17344 | 0.71227 | 3.46709 |
| H | 5.79720 | -0.19801 | 1.83742 |
| Cl | -2.86033 | 1.52688 | -1.63522 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.31520 | 0.36389 | 1.04217 |
| C | -0.04966 | 0.67088 | -0.61929 |
| P | -1.44180 | 0.42953 | -1.67975 |
| Ge | 1.00455 | 1.47992 | -2.29976 |
| Cl | 1.80869 | -0.40043 | -3.25348 |
| O | -0.95021 | 1.22660 | -2.88731 |
| Au | -0.28236 | 2.58175 | 0.39048 |
| Cl | -0.61914 | 4.74303 | 0.94995 |
| C | -1.86110 | -1.27651 | -2.04191 |
| C | -2.24953 | -2.12497 | -0.98344 |
| C | -1.80316 | -1.77196 | -3.36556 |
| C | -2.46443 | -3.46957 | -1.24722 |
| C | -2.04481 | -3.12634 | -3.56097 |
| C | -2.34727 | -3.99718 | -2.52452 |
| H | -2.75062 | -4.11893 | -0.42575 |
| H | -1.99745 | -3.51060 | -4.57480 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| C | 2.13758 | 0.28147 | 1.10012 | H | 2.61617 | -3.07370 | -1.21988 |
| C | 2.72786 | -0.88837 | 0.58433 | H | 4.11860 | -3.60455 | -0.46936 |
| C | 2.91829 | 1.22073 | 1.79145 | H | 2.63931 | -4.49845 | -0.16334 |
| C | 4.10315 | -1.03980 | 0.68334 | C | 3.49478 | -3.19586 | 2.12056 |
| C | 4.29284 | 1.02349 | 1.85635 | H | 4.57299 | -3.16251 | 1.95615 |
| C | 4.90853 | -0.08446 | 1.29156 | H | 3.27524 | -2.62653 | 3.02736 |
| H | 4.55623 | -1.94277 | 0.28497 | H | 3.20601 | -4.23747 | 2.29077 |
| H | 4.89790 | 1.75771 | 2.38000 | C | 1.24423 | -2.79702 | 1.23299 |
| C | 2.33097 | 2.42062 | 2.47025 | H | 0.95231 | -2.25003 | 2.13524 |
| H | 2.13826 | 3.23712 | 1.76811 | H | 0.59870 | -2.49933 | 0.40736 |
| H | 1.38108 | 2.19205 | 2.96155 | H | 1.04145 | -3.85336 | 1.43219 |
| H | 3.01476 | 2.79949 | 3.23130 | C | 7.21447 | 1.69696 | 0.07667 |
| C | 1.91128 | -1.99518 | -0.01528 | H | 6.58631 | 2.47848 | -0.35782 |
| H | 1.04364 | -2.24082 | 0.60690 | H | 7.35554 | 1.91780 | 1.13801 |
| H | 1.54258 | -1.73547 | -1.00970 | H | 8.19466 | 1.75533 | -0.40258 |
| H | 2.51272 | -2.90012 | -0.10998 | C | 6.53999 | 0.05199 | -1.65408 |
| C | 6.39535 | -0.25202 | 1.34206 | H | 7.53505 | 0.12461 | -2.10222 |
| H | 6.83120 | 0.29873 | 2.17715 | H | 6.13955 | -0.93902 | -1.87563 |
| H | 6.67535 | -1.30285 | 1.43767 | H | 5.89094 | 0.78331 | -2.14100 |
| H | 6.85573 | 0.12491 | 0.42337 | C | 7.55995 | -0.72270 | 0.49504 |
| C | -2.53864 | -1.64598 | 0.40706 | H | 7.63022 | -0.57200 | 1.57527 |
| H | -2.47106 | -2.47346 | 1.11417 | H | 7.22158 | -1.74568 | 0.31874 |
| H | -1.86901 | -0.86139 | 0.75890 | H | 8.56406 | -0.62874 | 0.07215 |
| H | -3.55414 | -1.24332 | 0.46043 | C | -2.36613 | -1.45447 | -1.66726 |
| C | -1.54014 | -0.94639 | -4.59080 | C | -2.33016 | -2.33583 | -2.79146 |
| H | -2.17316 | -0.06056 | -4.63412 | C | -3.60266 | -1.27145 | -0.99121 |
| H | -0.50618 | -0.60271 | -4.62892 | C | -3.53992 | -2.65097 | -3.39108 |
| H | -1.73269 | -1.55147 | -5.47705 | C | -1.10146 | -3.10215 | -3.31657 |
| C | -2.54347 | -5.45815 | -2.77850 | C | -4.76743 | -1.66246 | -1.64205 |
| H | -2.95159 | -5.63819 | -3.77437 | C | -3.79808 | -0.82725 | 0.46950 |
| H | -1.58701 | -5.98682 | -2.71721 | C | -4.77360 | -2.25794 | -2.89137 |
| H | -3.21294 | -5.90573 | -2.04226 | H | -3.51290 | -3.25734 | -4.28648 |
| Cl | -3.17207 | 1.29033 | -1.05547 | C | -0.60022 | -2.57668 | -4.66494 |
| R = Mes* | | | | C | -1.51051 | -4.57555 | -3.52335 |
| P | 0.68315 | 0.06050 | 1.14967 | C | 0.01116 | -3.15218 | -2.27764 |
| C | 0.37669 | 0.14554 | -0.56719 | H | -5.70840 | -1.48394 | -1.14158 |
| P | -1.08247 | -0.14747 | -1.60295 | C | -2.51062 | -0.47359 | 1.19157 |
| O | -0.37151 | -0.05615 | -2.95396 | C | -4.37455 | -2.05498 | 1.20332 |
| Cl | 2.68454 | -1.03794 | -3.00785 | C | -4.78479 | 0.33532 | 0.61329 |
| Au | 0.26123 | 2.20288 | 0.11787 | C | -6.05044 | -2.56554 | -3.66226 |
| Cl | -0.03897 | 4.44752 | 0.29433 | H | 0.20428 | -3.22051 | -5.03022 |
| C | 2.53088 | -0.02589 | 1.24131 | H | -1.40528 | -2.59485 | -5.40449 |
| C | 3.21687 | -1.17659 | 0.76272 | H | -0.22158 | -1.56148 | -4.59305 |
| C | 3.29869 | 1.09459 | 1.64313 | H | -2.17744 | -4.71924 | -4.37410 |
| C | 4.53288 | -1.02639 | 0.35423 | H | -0.60887 | -5.15972 | -3.72350 |
| C | 4.60929 | 1.18238 | 1.17035 | H | -1.99251 | -4.98860 | -2.63408 |
| C | 5.22466 | 0.17543 | 0.44917 | H | 0.43443 | -2.18069 | -2.03466 |
| H | 5.04678 | -1.89058 | -0.04597 | H | -0.34680 | -3.62725 | -1.36082 |
| H | 5.17157 | 2.07501 | 1.40625 | H | 0.84131 | -3.74735 | -2.66296 |
| C | 2.92565 | 2.13757 | 2.71852 | H | -1.76460 | -1.26455 | 1.09045 |
| C | 2.72458 | -2.63041 | 0.91170 | H | -2.08416 | 0.47245 | 0.85818 |
| C | 6.62209 | 0.30790 | -0.14446 | H | -2.70926 | -0.35656 | 2.25939 |
| C | 3.92451 | 1.90893 | 3.87268 | H | -4.50737 | -1.81321 | 2.26128 |
| H | 3.84123 | 0.89297 | 4.26739 | H | -5.34216 | -2.35977 | 0.80325 |
| H | 4.95764 | 2.06405 | 3.56056 | H | -3.69544 | -2.90807 | 1.13138 |
| H | 3.70839 | 2.60965 | 4.68374 | H | -5.76495 | 0.10059 | 0.19512 |
| C | 3.08422 | 3.57555 | 2.21903 | H | -4.92670 | 0.55947 | 1.67374 |
| H | 2.39829 | 3.80194 | 1.40253 | H | -4.41464 | 1.23709 | 0.12583 |
| H | 2.86721 | 4.27233 | 3.03330 | C | -7.29422 | -2.02976 | -2.95837 |
| H | 4.10079 | 3.77837 | 1.87756 | C | -6.20130 | -4.08294 | -3.82481 |
| C | 1.54389 | 1.97696 | 3.34606 | C | -5.95910 | -1.91223 | -5.04667 |
| H | 1.47848 | 2.62945 | 4.22088 | H | -7.45382 | -2.50808 | -1.98862 |
| H | 0.72970 | 2.27441 | 2.68355 | H | -7.23970 | -0.94898 | -2.80599 |
| H | 1.36670 | 0.95400 | 3.68869 | H | -8.17529 | -2.23405 | -3.57102 |
| C | 3.04486 | -3.49373 | -0.31147 | H | -5.36335 | -4.51895 | -4.37209 |
| | | | | H | -6.26180 | -4.57739 | -2.85217 |

| | | | |
|----|----------|----------|----------|
| H | -7.11585 | -4.31015 | -4.37924 |
| H | -5.86048 | -0.82744 | -4.96216 |
| H | -5.10302 | -2.28268 | -5.61392 |
| H | -6.86241 | -2.12893 | -5.62317 |
| Ge | 1.43861 | 0.71240 | -2.35503 |
| Cl | -2.29407 | 1.50514 | -1.59320 |

[R-P=C(Ge(II)Cl)-P(O)MeR](AuCl)

Coordination through Ge(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.53608 | 0.35901 | 0.47014 |
| C | 0.11408 | 0.28943 | -1.12944 |
| P | -1.44949 | 0.02918 | -1.89357 |
| Ge | 0.89018 | 0.66444 | -2.97085 |
| Cl | 1.53924 | -1.33059 | -3.53882 |
| O | -1.05723 | 0.44394 | -3.32625 |
| C | -2.83411 | 0.95281 | -1.25070 |
| H | -2.58389 | 2.01458 | -1.24744 |
| H | -3.70794 | 0.78347 | -1.88326 |
| H | -3.05089 | 0.62081 | -0.23252 |
| Au | 1.91521 | 2.63497 | -3.66708 |
| Cl | 2.89046 | 4.59657 | -4.27329 |
| H | 1.91255 | 0.69659 | 0.29396 |
| H | -1.84301 | -1.32292 | -1.83820 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.54552 | 0.34860 | 0.44967 |
| C | 0.11370 | 0.26877 | -1.14451 |
| P | -1.45412 | -0.02789 | -1.88436 |
| Ge | 0.84722 | 0.66221 | -2.98658 |
| Cl | 1.57508 | -1.30944 | -3.58705 |
| O | -1.06939 | 0.39078 | -3.32910 |
| C | -2.79883 | 0.97210 | -1.25637 |
| H | -2.51105 | 2.02256 | -1.31019 |
| H | -3.69215 | 0.80900 | -1.86294 |
| H | -3.00828 | 0.70456 | -0.21853 |
| C | -1.96126 | -1.74305 | -1.82050 |
| H | -2.18254 | -2.03242 | -0.79125 |
| H | -2.84752 | -1.88669 | -2.44233 |
| H | -1.14348 | -2.35355 | -2.20648 |
| C | 2.32865 | 0.76199 | 0.41098 |
| H | 2.89835 | -0.17277 | 0.42206 |
| H | 2.60719 | 1.33619 | -0.47422 |
| H | 2.58996 | 1.31930 | 1.31229 |
| Au | 1.85932 | 2.64410 | -3.68158 |
| Cl | 2.84054 | 4.61518 | -4.26074 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.45708 | 0.48299 | 0.20271 |
| C | 0.28404 | 0.16420 | -1.41281 |
| P | -1.23204 | -0.24835 | -2.23122 |
| Ge | 1.17831 | 0.20543 | -3.23621 |
| Cl | 2.17840 | -1.73052 | -3.37595 |
| O | -0.65321 | -0.33154 | -3.67367 |
| C | -2.43186 | 1.08283 | -2.12275 |
| H | -1.94555 | 1.99235 | -2.47916 |
| H | -3.29723 | 0.87128 | -2.75249 |
| H | -2.74935 | 1.22835 | -1.08929 |
| Au | 1.97763 | 2.11428 | -4.32026 |
| Cl | 2.70465 | 4.03728 | -5.30559 |
| C | 2.22947 | 0.93261 | 0.56543 |
| C | 3.17697 | 0.87428 | -0.61733 |
| C | 2.16937 | 2.35285 | 1.13928 |
| C | 2.67322 | -0.04332 | 1.66050 |

| | | | |
|---|----------|----------|----------|
| H | 3.22257 | -0.12545 | -1.05552 |
| H | 2.90272 | 1.58971 | -1.39689 |
| H | 4.18907 | 1.13322 | -0.28919 |
| H | 1.47276 | 2.42658 | 1.97932 |
| H | 3.16145 | 2.63596 | 1.50490 |
| H | 1.87230 | 3.08144 | 0.38128 |
| H | 3.66407 | 0.24766 | 2.02323 |
| H | 1.99125 | -0.03740 | 2.51553 |
| H | 2.74207 | -1.06703 | 1.28428 |
| C | -2.03088 | -1.82461 | -1.75616 |
| C | -3.11460 | -2.12749 | -2.79465 |
| C | -0.97186 | -2.92648 | -1.77701 |
| C | -2.63618 | -1.69264 | -0.35951 |
| H | -3.92528 | -1.39592 | -2.77495 |
| H | -2.70282 | -2.16629 | -3.80495 |
| H | -3.55037 | -3.10491 | -2.56988 |
| H | -0.18476 | -2.74784 | -1.04268 |
| H | -1.45383 | -3.87763 | -1.53467 |
| H | -0.50367 | -3.02092 | -2.75772 |
| H | -3.04902 | -2.66061 | -0.06247 |
| H | -1.88880 | -1.40983 | 0.38650 |
| H | -3.45033 | -0.96544 | -0.32793 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.62761 | 0.41303 | 0.27365 |
| C | 0.19429 | 0.19365 | -1.31228 |
| P | -1.42039 | -0.11123 | -1.94425 |
| Ge | 0.81788 | 0.52369 | -3.20235 |
| Cl | 1.57788 | -1.43137 | -3.83251 |
| O | -1.10581 | 0.18352 | -3.43540 |
| C | -2.67855 | 0.99518 | -1.31140 |
| H | -2.34176 | 2.02205 | -1.46005 |
| H | -3.61277 | 0.82803 | -1.85055 |
| H | -2.83639 | 0.81827 | -0.24580 |
| Au | 1.71134 | 2.50403 | -4.05217 |
| Cl | 2.57899 | 4.46548 | -4.82306 |
| C | 2.38957 | 0.77498 | 0.27422 |
| C | 2.86074 | 1.48800 | 1.38120 |
| C | 3.28976 | 0.38950 | -0.72320 |
| C | 4.19434 | 1.85129 | 1.46564 |
| H | 2.17118 | 1.77016 | 2.17095 |
| C | 4.62294 | 0.74429 | -0.62972 |
| H | 2.95641 | -0.21809 | -1.55703 |
| C | 5.07374 | 1.48257 | 0.45811 |
| H | 4.54841 | 2.41975 | 2.31758 |
| H | 5.31475 | 0.44491 | -1.40809 |
| H | 6.11867 | 1.76337 | 0.52289 |
| C | -2.01174 | -1.78864 | -1.74483 |
| C | -1.96046 | -2.65540 | -2.83318 |
| C | -2.49306 | -2.23517 | -0.51424 |
| C | -2.40085 | -3.96228 | -2.68945 |
| H | -1.57455 | -2.30319 | -3.78209 |
| C | -2.92678 | -3.54220 | -0.37845 |
| H | -2.52136 | -1.57175 | 0.34390 |
| C | -2.88263 | -4.40422 | -1.46685 |
| H | -2.36293 | -4.63703 | -3.53640 |
| H | -3.29912 | -3.89052 | 0.57769 |
| H | -3.22366 | -5.42734 | -1.35790 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.75342 | 0.17090 | 0.74379 |
| C | 0.16766 | 0.07072 | -0.80476 |
| P | -1.43794 | -0.14558 | -1.52489 |
| Ge | 0.82947 | 0.79053 | -2.56032 |
| Cl | 1.55273 | -0.99910 | -3.59963 |
| O | -1.09211 | 0.55572 | -2.86953 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| C | -2.75611 | 0.79317 | -0.74327 | C | -2.74180 | 2.71264 | -0.20378 |
| H | -2.40912 | 1.81598 | -0.58960 | C | -3.01448 | 1.01689 | 1.54584 |
| H | -3.61192 | 0.79785 | -1.42211 | C | -3.97201 | 2.31676 | -0.72228 |
| H | -3.06000 | 0.35709 | 0.20776 | C | -4.22398 | 0.66857 | 0.95917 |
| Au | 1.76111 | 2.89733 | -2.94533 | C | -4.69325 | 1.24771 | -0.21271 |
| Cl | 2.65864 | 4.98247 | -3.19561 | H | -4.37589 | 2.85564 | -1.56441 |
| C | 2.46709 | 0.72891 | 0.48513 | H | -4.83257 | -0.08481 | 1.43936 |
| C | 2.77674 | 2.08087 | 0.69535 | C | -2.09124 | 4.00919 | -0.72687 |
| C | 3.47020 | -0.19190 | 0.15173 | C | -2.70831 | 0.46825 | 2.95820 |
| C | 4.08788 | 2.49928 | 0.52350 | C | -5.97929 | 0.73555 | -0.85223 |
| C | 4.76994 | 0.27395 | -0.00207 | C | 3.97196 | 1.09721 | 2.62350 |
| C | 5.09718 | 1.61398 | 0.16422 | C | 3.37940 | 0.92711 | -2.48678 |
| H | 4.32357 | 3.55022 | 0.66048 | C | 7.54197 | -0.83099 | -0.34513 |
| H | 5.55112 | -0.43486 | -0.26040 | C | -4.01922 | 0.19309 | 3.71068 |
| C | -2.00383 | -1.84263 | -1.74679 | H | -3.78703 | -0.03239 | 4.75429 |
| C | -2.39818 | -2.32434 | -3.01554 | H | -4.68864 | 1.05618 | 3.68906 |
| C | -2.08288 | -2.68215 | -0.61964 | H | -4.55366 | -0.67106 | 3.31353 |
| C | -2.84030 | -3.63787 | -3.10679 | C | -1.95490 | 1.50395 | 3.79583 |
| C | -2.53830 | -3.98453 | -0.77620 | H | -0.93495 | 1.69036 | 3.43659 |
| C | -2.91262 | -4.48787 | -2.01162 | H | -2.47866 | 2.46252 | 3.81824 |
| H | -3.14822 | -4.00663 | -4.08016 | H | -1.85136 | 1.14176 | 4.82218 |
| H | -2.60101 | -4.62140 | 0.10088 | C | -1.91650 | -0.84141 | 2.94270 |
| C | -2.38192 | -1.52050 | -4.28398 | H | -2.42947 | -1.61098 | 2.36231 |
| H | -2.89745 | -0.56508 | -4.18513 | H | -0.92250 | -0.70512 | 2.51800 |
| H | -1.36191 | -1.29267 | -4.59700 | H | -1.80044 | -1.21266 | 3.96550 |
| H | -2.86583 | -2.08911 | -5.07829 | C | -7.14070 | 0.85705 | 0.14125 |
| C | -1.66729 | -2.26575 | 0.76016 | H | -8.06318 | 0.48782 | -0.31522 |
| H | -0.60126 | -2.45286 | 0.91595 | H | -6.96483 | 0.27406 | 1.04726 |
| H | -1.83280 | -1.21081 | 0.97959 | H | -7.29905 | 1.89810 | 0.43477 |
| H | -2.21387 | -2.84214 | 1.50783 | C | -6.34697 | 1.51144 | -2.11422 |
| C | -3.36755 | -5.90475 | -2.16761 | H | -7.25723 | 1.08946 | -2.54671 |
| H | -2.54363 | -6.53452 | -2.51712 | H | -6.54145 | 2.56685 | -1.90474 |
| H | -3.72016 | -6.31810 | -1.22168 | H | -5.56175 | 1.44758 | -2.87154 |
| H | -4.17099 | -5.98579 | -2.90213 | C | -5.78435 | -0.73791 | -1.23142 |
| C | 3.17283 | -1.65024 | -0.03818 | H | -4.96839 | -0.85252 | -1.94880 |
| H | 2.54296 | -2.04280 | 0.76709 | H | -5.54860 | -1.35746 | -0.36416 |
| H | 2.64720 | -1.83274 | -0.97968 | H | -6.69710 | -1.13227 | -1.68672 |
| H | 4.09474 | -2.23293 | -0.05204 | C | -2.99015 | 4.72832 | -1.73576 |
| C | 1.71341 | 3.07606 | 1.04895 | H | -3.97280 | 4.96074 | -1.31940 |
| H | 1.15274 | 3.37707 | 0.15798 | H | -2.51778 | 5.67300 | -2.01489 |
| H | 0.99592 | 2.66932 | 1.77054 | H | -3.12739 | 4.14862 | -2.65150 |
| H | 2.14842 | 3.97829 | 1.48004 | C | -1.89542 | 4.96704 | 0.45722 |
| C | 6.49517 | 2.10214 | -0.05649 | H | -2.84788 | 5.17512 | 0.95047 |
| H | 6.56934 | 2.62496 | -1.01470 | H | -1.20989 | 4.56433 | 1.20651 |
| H | 6.79720 | 2.80792 | 0.72034 | H | -1.47785 | 5.91478 | 0.10545 |
| H | 7.20941 | 1.27766 | -0.06963 | C | -0.74867 | 3.78272 | -1.42525 |
| | | | | H | 0.02893 | 3.43386 | -0.74046 |
| | | | | H | -0.83418 | 3.04999 | -2.22829 |
| | | | | H | -0.39342 | 4.72740 | -1.84764 |
| | | | | C | 2.56583 | 1.66854 | 2.74785 |
| | | | | H | 2.33897 | 2.35203 | 1.92710 |
| | | | | H | 1.77940 | 0.91662 | 2.79810 |
| | | | | H | 2.49169 | 2.24431 | 3.67349 |
| | | | | C | 4.91641 | 2.30840 | 2.77136 |
| | | | | H | 4.71269 | 2.81371 | 3.71933 |
| | | | | H | 5.96689 | 2.01691 | 2.76421 |
| | | | | H | 4.75906 | 3.02549 | 1.96241 |
| | | | | C | 4.24915 | 0.13680 | 3.78419 |
| | | | | H | 5.28885 | -0.19435 | 3.79802 |
| | | | | H | 4.05437 | 0.64307 | 4.73318 |
| | | | | H | 3.62300 | -0.75561 | 3.74846 |
| | | | | C | 2.18072 | 1.83247 | -2.22167 |
| | | | | H | 1.83593 | 2.26118 | -3.16542 |
| | | | | H | 1.32536 | 1.31453 | -1.79957 |
| | | | | H | 2.45641 | 2.65784 | -1.55965 |
| | | | | C | 3.01737 | -0.20872 | -3.44798 |
| R = Mes* | | | | | | | |
| P | -0.40276 | 2.04360 | 1.20992 | | | | |
| C | 0.14869 | 0.66014 | 0.46998 | | | | |
| P | 1.73012 | -0.15255 | 0.31009 | | | | |
| Cl | -1.06856 | 0.26967 | -2.66951 | | | | |
| O | 1.32666 | -0.96564 | -0.96363 | | | | |
| C | 1.85038 | -1.42500 | 1.58635 | | | | |
| H | 2.67398 | -2.08649 | 1.31094 | | | | |
| H | 2.00139 | -1.05057 | 2.59316 | | | | |
| H | 0.91615 | -1.99087 | 1.54515 | | | | |
| C | 3.43360 | 0.47080 | 0.11550 | | | | |
| C | 4.02030 | 0.41602 | -1.18248 | | | | |
| C | 4.29497 | 0.48638 | 1.24475 | | | | |
| C | 5.33845 | -0.00903 | -1.27006 | | | | |
| C | 5.61425 | 0.08233 | 1.06877 | | | | |
| C | 6.13615 | -0.27250 | -0.16466 | | | | |
| H | 5.76666 | -0.12355 | -2.25710 | | | | |
| H | 6.25825 | 0.05683 | 1.93678 | | | | |
| C | -2.20077 | 1.95018 | 0.85582 | | | | |

| | | | |
|----|----------|----------|----------|
| H | 2.25112 | -0.85923 | -3.03417 |
| H | 2.64632 | 0.21053 | -4.38705 |
| H | 3.89791 | -0.81433 | -3.67844 |
| C | 4.41279 | 1.82811 | -3.19328 |
| H | 4.78476 | 2.61021 | -2.52696 |
| H | 5.26786 | 1.27516 | -3.58330 |
| H | 3.92801 | 2.31085 | -4.04532 |
| C | 8.24751 | -1.06370 | 0.98817 |
| H | 8.40718 | -0.13103 | 1.53538 |
| H | 7.68770 | -1.74945 | 1.62919 |
| H | 9.22944 | -1.50699 | 0.80775 |
| C | 8.38362 | 0.14721 | -1.17356 |
| H | 7.95779 | 0.31209 | -2.16510 |
| H | 8.46166 | 1.11672 | -0.67549 |
| H | 9.39387 | -0.24896 | -1.30687 |
| C | 7.44879 | -2.17211 | -1.08290 |
| H | 6.86517 | -2.89589 | -0.50897 |
| H | 6.97813 | -2.06418 | -2.06199 |
| H | 8.44899 | -2.58616 | -1.23570 |
| Au | -1.86015 | -2.64298 | -0.25873 |
| Cl | -3.10660 | -4.46897 | 0.33356 |
| Ge | -0.61005 | -0.73479 | -0.78550 |

Coordination through O atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.53475 | 0.19662 | 0.68169 |
| C | 0.29462 | 0.30392 | -0.95361 |
| P | -1.21545 | 0.39364 | -1.82151 |
| Ge | 1.45099 | 0.64563 | -2.65831 |
| Cl | 1.35346 | -1.47055 | -3.32404 |
| O | -0.68463 | 1.03087 | -3.13510 |
| C | -2.55364 | 1.31998 | -1.08988 |
| H | -2.22277 | 2.34179 | -0.89975 |
| H | -3.40697 | 1.32970 | -1.77122 |
| H | -2.83899 | 0.84389 | -0.14803 |
| Au | -1.97784 | 1.37990 | -4.75638 |
| Cl | -3.39242 | 1.75637 | -6.42717 |
| H | -1.72753 | -0.89230 | -2.07131 |
| H | 1.96549 | 0.24746 | 0.68071 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.52263 | 0.10077 | 0.65034 |
| C | 0.28136 | 0.28298 | -0.97553 |
| P | -1.25171 | 0.32322 | -1.80710 |
| Ge | 1.36892 | 0.77785 | -2.68421 |
| Cl | 1.57790 | -1.32707 | -3.40137 |
| O | -0.73630 | 0.93358 | -3.15329 |
| C | -2.51558 | 1.36364 | -1.08401 |
| H | -2.12167 | 2.37362 | -0.96656 |
| H | -3.39125 | 1.38767 | -1.73631 |
| H | -2.79498 | 0.96672 | -0.10523 |
| C | -1.95091 | -1.29972 | -2.07454 |
| H | -2.27089 | -1.72351 | -1.12025 |
| H | -2.80388 | -1.22174 | -2.75262 |
| H | -1.18136 | -1.93159 | -2.52065 |
| C | 2.34743 | 0.14200 | 0.84793 |
| H | 2.71772 | -0.88781 | 0.82805 |
| H | 2.84643 | 0.70886 | 0.06055 |
| H | 2.59835 | 0.56399 | 1.82295 |
| Au | -2.01891 | 1.30818 | -4.77156 |
| Cl | -3.42593 | 1.70731 | -6.44561 |

R = t-Bu

| | | | |
|---|---------|---------|---------|
| P | 0.62925 | 0.02623 | 0.35813 |
|---|---------|---------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.40201 | 0.07879 | -1.28241 |
| P | -1.17812 | 0.01789 | -2.04950 |
| Ge | 1.40237 | 0.49369 | -3.07767 |
| Cl | 2.01487 | -1.60591 | -3.53652 |
| O | -0.69824 | 0.23594 | -3.52688 |
| C | -2.23190 | 1.38381 | -1.55109 |
| H | -1.67867 | 2.30920 | -1.71785 |
| H | -3.14482 | 1.40409 | -2.14813 |
| H | -2.47518 | 1.29984 | -0.49058 |
| Au | -1.86238 | 0.92942 | -5.12991 |
| Cl | -3.10679 | 1.67894 | -6.81390 |
| C | -2.10786 | -1.55357 | -1.88017 |
| C | -3.34895 | -1.50220 | -2.77468 |
| C | -1.19951 | -2.70212 | -2.31704 |
| C | -2.51852 | -1.72733 | -0.41755 |
| H | -4.05150 | -0.72365 | -2.47102 |
| H | -3.09487 | -1.34585 | -3.82502 |
| H | -3.86837 | -2.46143 | -2.69550 |
| H | -0.30321 | -2.77368 | -1.69915 |
| H | -1.75673 | -3.63826 | -2.22299 |
| H | -0.88279 | -2.59631 | -3.35523 |
| H | -3.01472 | -2.69584 | -0.31124 |
| H | -1.65961 | -1.71953 | 0.25782 |
| H | -3.22438 | -0.96050 | -0.09103 |
| C | 2.45794 | 0.15307 | 0.72048 |
| C | 3.32863 | 0.52401 | -0.46508 |
| C | 2.58481 | 1.20234 | 1.82845 |
| C | 2.85649 | -1.22168 | 1.26789 |
| H | 3.29818 | -0.24413 | -1.24281 |
| H | 3.04089 | 1.48680 | -0.89609 |
| H | 4.37315 | 0.61185 | -0.14698 |
| H | 1.94390 | 0.96963 | 2.68324 |
| H | 3.61879 | 1.23537 | 2.18584 |
| H | 2.32211 | 2.20140 | 1.47095 |
| H | 3.88976 | -1.18403 | 1.62850 |
| H | 2.22485 | -1.52533 | 2.10763 |
| H | 2.79617 | -1.99275 | 0.49630 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.48052 | 0.41728 | 0.44060 |
| C | 0.37166 | 0.15189 | -1.19373 |
| P | -1.10678 | 0.14905 | -2.12225 |
| Ge | 1.60501 | 0.31884 | -2.85383 |
| Cl | 1.84459 | -1.86188 | -3.29095 |
| O | -0.47243 | 0.40111 | -3.52678 |
| C | -2.26724 | 1.44764 | -1.70209 |
| H | -1.75653 | 2.40796 | -1.78541 |
| H | -3.11518 | 1.41767 | -2.38887 |
| H | -2.61767 | 1.31640 | -0.67625 |
| Au | -1.54926 | 0.86142 | -5.26875 |
| Cl | -2.70532 | 1.36062 | -7.10148 |
| C | -1.98928 | -1.40687 | -2.09731 |
| C | -2.79871 | -1.73145 | -1.00851 |
| C | -1.84578 | -2.30153 | -3.15424 |
| C | -3.46657 | -2.94294 | -0.98419 |
| H | -2.90527 | -1.04762 | -0.17301 |
| C | -2.52275 | -3.51078 | -3.12401 |
| H | -1.20776 | -2.05297 | -3.99299 |
| C | -3.33055 | -3.83055 | -2.04377 |
| H | -4.09569 | -3.19502 | -0.13875 |
| H | -2.41614 | -4.20371 | -3.94994 |
| H | -3.85781 | -4.77742 | -2.02465 |
| C | 2.24903 | 0.35403 | 0.80372 |
| C | 2.69000 | 1.08842 | 1.90789 |
| C | 3.17444 | -0.39308 | 0.06890 |
| C | 4.03419 | 1.11621 | 2.24136 |

| | | | |
|---|---------|----------|----------|
| H | 1.97368 | 1.65020 | 2.49966 |
| C | 4.51569 | -0.37168 | 0.41174 |
| H | 2.83766 | -1.02864 | -0.74390 |
| C | 4.94747 | 0.38899 | 1.49103 |
| H | 4.36965 | 1.70069 | 3.09022 |
| H | 5.22603 | -0.95795 | -0.15962 |
| H | 5.99851 | 0.40321 | 1.75597 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.35943 | 0.09013 | 0.80258 |
| C | 0.18950 | 0.05515 | -0.84422 |
| P | -1.18726 | 0.08340 | -1.93503 |
| Ge | 1.59580 | 0.53234 | -2.27744 |
| Cl | 2.07316 | -1.57113 | -2.88438 |
| O | -0.40062 | 0.57825 | -3.19505 |
| C | -2.41727 | 1.33356 | -1.54111 |
| H | -1.90956 | 2.29934 | -1.51352 |
| H | -3.17648 | 1.35081 | -2.32564 |
| H | -2.88501 | 1.14137 | -0.57715 |
| Au | -1.09234 | 1.89902 | -4.67903 |
| Cl | -1.81710 | 3.31154 | -6.23715 |
| C | -2.00033 | -1.50775 | -2.19564 |
| C | -2.70631 | -2.06663 | -1.11007 |
| C | -1.94314 | -2.20095 | -3.42712 |
| C | -3.31847 | -3.30263 | -1.26205 |
| C | -2.58642 | -3.43007 | -3.51515 |
| C | -3.26935 | -4.00614 | -2.45471 |
| H | -3.85256 | -3.72354 | -0.41567 |
| H | -2.54383 | -3.95861 | -4.46202 |
| C | 2.16934 | 0.26153 | 1.00758 |
| C | 2.72662 | 1.53484 | 1.19585 |
| C | 2.97410 | -0.88559 | 1.07911 |
| C | 4.09306 | 1.64069 | 1.42034 |
| C | 4.33524 | -0.72969 | 1.30735 |
| C | 4.91577 | 0.52217 | 1.47235 |
| H | 4.52562 | 2.62663 | 1.56350 |
| H | 4.95988 | -1.61638 | 1.36378 |
| C | 1.87962 | 2.77133 | 1.14036 |
| H | 1.58072 | 3.00260 | 0.11303 |
| H | 0.96015 | 2.66011 | 1.72460 |
| H | 2.42143 | 3.63416 | 1.52940 |
| C | 2.39408 | -2.25763 | 0.91043 |
| H | 1.49464 | -2.39301 | 1.52027 |
| H | 2.11050 | -2.43935 | -0.13023 |
| H | 3.11435 | -3.02266 | 1.20277 |
| C | 6.39187 | 0.66249 | 1.68369 |
| H | 6.91330 | 0.73701 | 0.72425 |
| H | 6.62941 | 1.56131 | 2.25528 |
| H | 6.80273 | -0.20001 | 2.21144 |
| C | -2.88114 | -1.39081 | 0.21985 |
| H | -2.02770 | -0.78465 | 0.52616 |
| H | -3.76703 | -0.74836 | 0.21646 |
| H | -3.03218 | -2.13765 | 1.00010 |
| C | -1.25035 | -1.71750 | -4.66674 |
| H | -1.65024 | -0.76316 | -5.01710 |
| H | -0.18084 | -1.58136 | -4.50806 |
| H | -1.38663 | -2.44726 | -5.46462 |
| C | -3.90872 | -5.35196 | -2.59015 |
| H | -4.70749 | -5.49052 | -1.86011 |
| H | -4.32376 | -5.49535 | -3.58937 |
| H | -3.17124 | -6.14408 | -2.42756 |

R = Mes*

| | | | |
|---|----------|---------|----------|
| P | 1.97406 | 2.05802 | -0.37323 |
| C | 1.00231 | 0.71467 | -0.31627 |
| P | -0.73661 | 0.48297 | -0.47657 |

| | | | |
|---|----------|----------|----------|
| C | 3.64317 | 1.27638 | -0.30576 |
| C | 4.36043 | 1.29392 | 0.92138 |
| C | 4.13441 | 0.51769 | -1.38753 |
| C | 5.37202 | 0.36303 | 1.09183 |
| C | 5.14003 | -0.41818 | -1.12714 |
| C | 5.73239 | -0.55889 | 0.11213 |
| H | 5.89790 | 0.33440 | 2.03484 |
| H | 5.47461 | -1.04646 | -1.94107 |
| C | 3.78711 | 0.71273 | -2.87979 |
| C | 4.10994 | 2.33359 | 2.03045 |
| C | 6.77745 | -1.62589 | 0.41902 |
| C | 2.75676 | 2.14280 | 2.72067 |
| H | 1.91462 | 2.35994 | 2.05949 |
| H | 2.63525 | 1.11930 | 3.07909 |
| H | 2.67850 | 2.82671 | 3.57102 |
| C | 4.19611 | 3.74328 | 1.42952 |
| H | 5.17307 | 3.90952 | 0.96903 |
| H | 3.43084 | 3.92221 | 0.67129 |
| H | 4.05761 | 4.49111 | 2.21539 |
| C | 5.17407 | 2.25985 | 3.12871 |
| H | 5.12584 | 1.32290 | 3.68842 |
| H | 6.18489 | 2.37934 | 2.73168 |
| H | 4.99955 | 3.07106 | 3.83913 |
| C | 3.18542 | -0.55585 | -3.48988 |
| H | 2.22649 | -0.80244 | -3.02881 |
| H | 3.02043 | -0.41426 | -4.56182 |
| H | 3.84048 | -1.41976 | -3.36461 |
| C | 2.85666 | 1.88408 | -3.18670 |
| H | 1.82339 | 1.69105 | -2.89755 |
| H | 3.18992 | 2.81008 | -2.70885 |
| H | 2.85433 | 2.06189 | -4.26590 |
| C | 5.10559 | 1.03437 | -3.60944 |
| H | 5.56532 | 1.93762 | -3.20075 |
| H | 5.83268 | 0.22599 | -3.53446 |
| H | 4.90516 | 1.20361 | -4.67088 |
| C | 7.02239 | -2.55413 | -0.76748 |
| H | 7.42566 | -2.01770 | -1.63048 |
| H | 7.75181 | -3.31786 | -0.48759 |
| H | 6.10818 | -3.06784 | -1.07529 |
| C | 6.28895 | -2.47415 | 1.59973 |
| H | 6.14231 | -1.87082 | 2.49764 |
| H | 5.33741 | -2.95815 | 1.36846 |
| H | 7.02283 | -3.25057 | 1.83326 |
| C | 8.10579 | -0.95592 | 0.78931 |
| H | 8.00491 | -0.31100 | 1.66454 |
| H | 8.85798 | -1.71529 | 1.02056 |
| H | 8.48058 | -0.34594 | -0.03652 |
| C | -2.17944 | 1.34852 | 0.21681 |
| C | -2.78080 | 0.78557 | 1.37945 |
| C | -2.98590 | 2.14171 | -0.64102 |
| C | -4.16388 | 0.68601 | 1.39788 |
| C | -4.36583 | 2.00705 | -0.54576 |
| C | -4.97990 | 1.19205 | 0.39443 |
| H | -4.62436 | 0.18773 | 2.24141 |
| H | -4.98234 | 2.57082 | -1.23266 |
| C | -2.04562 | 0.43456 | 2.68601 |
| C | -2.09506 | -1.05612 | 3.02726 |
| C | -2.76349 | 1.20762 | 3.81149 |
| H | -1.49504 | -1.64737 | 2.33753 |
| H | -1.69992 | -1.21211 | 4.03477 |
| H | -3.11786 | -1.43863 | 3.00444 |
| H | -2.80730 | 2.27748 | 3.59303 |
| H | -3.78014 | 0.85447 | 3.98616 |
| H | -2.20542 | 1.07273 | 4.74149 |
| C | -2.47599 | 3.29007 | -1.53404 |
| C | -3.12425 | 4.57263 | -0.97203 |

| | | | |
|----|----------|----------|----------|
| C | -2.90417 | 3.15109 | -2.99769 |
| H | -2.86376 | 4.71252 | 0.07955 |
| H | -2.75958 | 5.43804 | -1.53220 |
| H | -4.21133 | 4.55515 | -1.05102 |
| H | -2.47573 | 2.27148 | -3.47830 |
| H | -3.98915 | 3.07970 | -3.09249 |
| H | -2.58209 | 4.03106 | -3.56087 |
| C | -6.47792 | 0.92221 | 0.41224 |
| C | -7.09524 | 1.52928 | 1.67794 |
| C | -6.70285 | -0.59511 | 0.41088 |
| H | -6.94745 | 2.61189 | 1.70882 |
| H | -8.17032 | 1.33152 | 1.69981 |
| H | -6.66104 | 1.10370 | 2.58475 |
| H | -6.25949 | -1.06592 | -0.46908 |
| H | -6.26338 | -1.07232 | 1.28858 |
| H | -7.77466 | -0.81119 | 0.41449 |
| Cl | 1.95984 | -1.53380 | 1.92001 |
| O | -0.75640 | -0.99162 | 0.08722 |
| Au | -2.33950 | -2.30612 | -0.36900 |
| Cl | -4.02233 | -3.68260 | -0.86980 |
| C | -0.97300 | 3.53106 | -1.44100 |
| H | -0.65004 | 3.63827 | -0.40329 |
| H | -0.36270 | 2.75792 | -1.90446 |
| H | -0.72443 | 4.46131 | -1.95758 |
| C | -0.60577 | 0.93041 | 2.70220 |
| H | 0.04918 | 0.38038 | 2.03115 |
| H | -0.55261 | 1.99545 | 2.46111 |
| H | -0.18958 | 0.79300 | 3.70308 |
| C | -7.18454 | 1.51645 | -0.80321 |
| H | -7.12266 | 2.60794 | -0.82306 |
| H | -6.77400 | 1.12775 | -1.73845 |
| H | -8.24381 | 1.25167 | -0.77215 |
| Ge | 1.38789 | -1.33528 | -0.22810 |
| C | -1.07431 | 0.25547 | -2.23998 |
| H | -2.11627 | -0.04051 | -2.37152 |
| H | -0.84964 | 1.12580 | -2.84887 |
| H | -0.43446 | -0.57249 | -2.55545 |

Coordination through P(sp²) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.48645 | 0.28047 | 0.52064 |
| C | 0.19575 | 0.19747 | -1.08372 |
| P | -1.31608 | 0.12388 | -1.96194 |
| Ge | 1.19014 | 0.43490 | -2.95798 |
| Cl | 1.28520 | -1.77261 | -3.30929 |
| O | -0.83114 | 0.58704 | -3.34030 |
| C | -2.68587 | 1.08244 | -1.33588 |
| H | -2.39024 | 2.12921 | -1.25611 |
| H | -3.52907 | 0.99154 | -2.02403 |
| H | -2.97613 | 0.70636 | -0.35150 |
| Au | -0.87177 | 0.28009 | 2.25502 |
| Cl | -2.32181 | 0.29575 | 3.98409 |
| H | 1.88721 | 0.38321 | 0.66781 |
| H | -1.77015 | -1.20903 | -1.97871 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.53398 | 0.31206 | 0.48794 |
| C | 0.18343 | 0.23251 | -1.10235 |
| P | -1.36686 | 0.04177 | -1.89920 |
| Ge | 1.07383 | 0.46540 | -3.01565 |
| Cl | 1.47308 | -1.73602 | -3.26403 |
| O | -0.93039 | 0.36822 | -3.34117 |
| C | -2.65327 | 1.15417 | -1.33805 |
| H | -2.29524 | 2.18146 | -1.41206 |

| | | | |
|----|----------|----------|----------|
| H | -3.53518 | 1.03269 | -1.97095 |
| H | -2.91485 | 0.93337 | -0.30069 |
| C | -1.98484 | -1.63003 | -1.74602 |
| H | -2.25089 | -1.83755 | -0.70738 |
| H | -2.86393 | -1.74983 | -2.38310 |
| H | -1.19928 | -2.31227 | -2.07430 |
| C | 2.31121 | 0.49624 | 0.76696 |
| H | 2.67511 | -0.38824 | 1.29583 |
| H | 2.84379 | 0.60615 | -0.17710 |
| H | 2.48628 | 1.36318 | 1.40755 |
| Au | -0.87137 | 0.20406 | 2.19106 |
| Cl | -2.37217 | 0.09133 | 3.88062 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.54604 | 0.35161 | 0.41494 |
| C | 0.26940 | 0.11134 | -1.17959 |
| P | -1.26130 | -0.15364 | -2.01453 |
| Ge | 1.18620 | 0.41614 | -3.08006 |
| Cl | 2.03564 | -1.64799 | -3.34944 |
| O | -0.75329 | -0.01473 | -3.46816 |
| C | -2.45638 | 1.13564 | -1.64046 |
| H | -2.00109 | 2.09423 | -1.89328 |
| H | -3.35912 | 1.00211 | -2.23873 |
| H | -2.71060 | 1.12870 | -0.57915 |
| Au | -0.95046 | 0.41985 | 2.05409 |
| Cl | -2.51757 | 0.51887 | 3.69021 |
| C | 2.32394 | 0.60682 | 0.85668 |
| C | 2.40432 | 1.90714 | 1.65973 |
| C | 2.71620 | -0.57747 | 1.74643 |
| C | 3.21614 | 0.67277 | -0.37196 |
| H | 2.14177 | 2.77589 | 1.05148 |
| H | 1.74648 | 1.88826 | 2.53208 |
| H | 3.43011 | 2.04095 | 2.01560 |
| H | 2.68997 | -1.52068 | 1.19622 |
| H | 3.73769 | -0.42419 | 2.10761 |
| H | 2.06314 | -0.66560 | 2.61832 |
| H | 4.25340 | 0.81018 | -0.05142 |
| H | 3.17049 | -0.24577 | -0.96079 |
| H | 2.95908 | 1.51749 | -1.01581 |
| C | -2.06012 | -1.78584 | -1.76035 |
| C | -1.00059 | -2.88123 | -1.86137 |
| C | -2.75202 | -1.84190 | -0.40100 |
| C | -3.08237 | -1.95125 | -2.89002 |
| H | -0.46948 | -2.85115 | -2.81320 |
| H | -0.26108 | -2.80422 | -1.06257 |
| H | -1.49597 | -3.85225 | -1.77281 |
| H | -3.56321 | -1.11688 | -0.31198 |
| H | -3.18548 | -2.83740 | -0.27084 |
| H | -2.05645 | -1.67968 | 0.42600 |
| H | -3.53619 | -2.94227 | -2.80211 |
| H | -3.88910 | -1.21682 | -2.83230 |
| H | -2.61186 | -1.87701 | -3.87161 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.52279 | 0.47564 | 0.28625 |
| C | 0.33261 | 0.03626 | -1.27751 |
| P | -1.15562 | -0.26496 | -2.15774 |
| Ge | 1.37948 | -0.01814 | -3.10958 |
| Cl | 1.95197 | -2.19501 | -3.01999 |
| O | -0.57769 | -0.29953 | -3.58657 |
| C | -2.38784 | 1.02430 | -1.98332 |
| H | -1.93195 | 1.97825 | -2.25197 |
| H | -3.22207 | 0.81180 | -2.65475 |
| H | -2.75055 | 1.07780 | -0.95491 |
| Au | -1.08396 | 0.91011 | 1.75007 |
| Cl | -2.81004 | 1.32077 | 3.15942 |

| | | | |
|---|----------|----------|----------|
| C | 2.24009 | 0.61272 | 0.74801 |
| C | 3.25120 | -0.03385 | 0.03235 |
| C | 2.56059 | 1.38317 | 1.86751 |
| C | 4.56946 | 0.11550 | 0.42422 |
| H | 3.00302 | -0.68065 | -0.80194 |
| C | 3.88320 | 1.53248 | 2.24800 |
| H | 1.77050 | 1.86639 | 2.43327 |
| C | 4.88623 | 0.90201 | 1.52506 |
| H | 5.35279 | -0.39232 | -0.12596 |
| H | 4.13097 | 2.13736 | 3.11215 |
| H | 5.92113 | 1.01394 | 1.82769 |
| C | -1.92850 | -1.82281 | -1.73335 |
| C | -2.72499 | -1.94451 | -0.59445 |
| C | -1.70460 | -2.92549 | -2.55397 |
| C | -3.29735 | -3.16597 | -0.28407 |
| H | -2.89603 | -1.09673 | 0.06086 |
| C | -2.28534 | -4.14369 | -2.23733 |
| H | -1.07483 | -2.82342 | -3.42920 |
| C | -3.07902 | -4.26364 | -1.10645 |
| H | -3.91402 | -3.26007 | 0.60187 |
| H | -2.11249 | -5.00217 | -2.87557 |
| H | -3.52950 | -5.21863 | -0.86092 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.47052 | 0.52779 | 0.81583 |
| C | 0.18058 | -0.06827 | -0.67895 |
| P | -1.23834 | -0.25771 | -1.70381 |
| Ge | 1.38295 | 0.11908 | -2.39667 |
| Cl | 1.70810 | -2.09291 | -2.71613 |
| O | -0.55263 | 0.16279 | -3.02196 |
| C | -2.58726 | 0.87788 | -1.35806 |
| H | -2.19098 | 1.89314 | -1.31101 |
| H | -3.31098 | 0.80489 | -2.17295 |
| H | -3.08467 | 0.63678 | -0.41821 |
| Au | -0.94925 | 1.11041 | 2.41513 |
| Cl | -2.42510 | 1.72455 | 4.02204 |
| C | 2.24456 | 0.73854 | 1.04325 |
| C | 3.06388 | -0.38568 | 1.23214 |
| C | 2.77983 | 2.03652 | 1.06536 |
| C | 4.42275 | -0.17951 | 1.43212 |
| C | 4.14445 | 2.18514 | 1.26426 |
| C | 4.98218 | 1.09185 | 1.45191 |
| H | 5.06340 | -1.04349 | 1.57978 |
| H | 4.56549 | 3.18592 | 1.27051 |
| C | -1.92997 | -1.92495 | -1.77632 |
| C | -2.28082 | -2.59050 | -0.58594 |
| C | -2.17196 | -2.54230 | -3.02370 |
| C | -2.84317 | -3.85764 | -0.65856 |
| C | -2.73726 | -3.81177 | -3.02935 |
| C | -3.07165 | -4.49327 | -1.86863 |
| H | -3.11318 | -4.35784 | 0.26634 |
| H | -2.92690 | -4.28196 | -3.98918 |
| C | 1.91847 | 3.24423 | 0.85125 |
| H | 1.48043 | 3.24702 | -0.15154 |
| H | 1.09142 | 3.28288 | 1.56738 |
| H | 2.49934 | 4.16002 | 0.96265 |
| C | 2.51896 | -1.78255 | 1.22860 |
| H | 1.63712 | -1.87164 | 1.87058 |
| H | 2.22412 | -2.09533 | 0.22301 |
| H | 3.26790 | -2.48553 | 1.59433 |
| C | 6.44635 | 1.28255 | 1.69966 |
| H | 6.63956 | 1.43358 | 2.76638 |
| H | 7.02089 | 0.41091 | 1.38255 |
| H | 6.82843 | 2.15830 | 1.17221 |
| C | -2.05858 | -2.01837 | 0.78114 |
| H | -1.01622 | -2.13561 | 1.08827 |

| | | | |
|---|----------|----------|----------|
| H | -2.29395 | -0.95585 | 0.85793 |
| H | -2.67840 | -2.53580 | 1.51374 |
| C | -1.86661 | -1.93327 | -4.36236 |
| H | -2.26328 | -0.92379 | -4.47080 |
| H | -0.79003 | -1.86539 | -4.52534 |
| H | -2.29604 | -2.55567 | -5.14796 |
| C | -3.64584 | -5.87405 | -1.92281 |
| H | -4.25880 | -6.01598 | -2.81459 |
| H | -2.84542 | -6.61984 | -1.95495 |
| H | -4.25726 | -6.08702 | -1.04452 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.13410 | 0.83689 | 0.03358 |
| C | -0.20865 | -0.44175 | 0.47114 |
| P | 1.46337 | -0.91389 | 0.80891 |
| Cl | -1.31075 | -3.20945 | -1.16339 |
| O | 1.25729 | -2.43828 | 0.60634 |
| C | 3.08576 | -0.48117 | 0.08569 |
| C | 3.62565 | -1.39673 | -0.86177 |
| C | 3.98386 | 0.35161 | 0.80401 |
| C | 4.97434 | -1.70669 | -0.75963 |
| C | 5.32582 | -0.01348 | 0.84232 |
| C | 5.83263 | -1.09989 | 0.14738 |
| H | 5.37288 | -2.45481 | -1.43280 |
| H | 5.99975 | 0.59393 | 1.43046 |
| C | -2.85746 | 0.25013 | 0.09506 |
| C | -3.51498 | -0.16217 | -1.09474 |
| C | -3.43583 | -0.02642 | 1.35838 |
| C | -4.59603 | -1.02615 | -0.96281 |
| C | -4.50299 | -0.91841 | 1.39500 |
| C | -5.06643 | -1.47705 | 0.26129 |
| H | -5.07689 | -1.38470 | -1.85735 |
| H | -4.91434 | -1.18250 | 2.36078 |
| C | -3.17484 | 0.35868 | -2.50553 |
| C | -3.09304 | 0.63159 | 2.71423 |
| C | -6.17869 | -2.51256 | 0.38881 |
| C | 3.65587 | 1.73752 | 1.39157 |
| C | 2.88619 | -1.96741 | -2.08481 |
| C | 7.27685 | -1.56886 | 0.27316 |
| C | -4.39245 | 1.24604 | 3.26916 |
| H | -4.18270 | 1.73965 | 4.22166 |
| H | -4.79331 | 1.99358 | 2.58049 |
| H | -5.16998 | 0.50380 | 3.44765 |
| C | -2.09663 | 1.78709 | 2.66177 |
| H | -1.07173 | 1.46261 | 2.47849 |
| H | -2.36892 | 2.53673 | 1.91455 |
| H | -2.09138 | 2.28997 | 3.63277 |
| C | -2.57158 | -0.41099 | 3.70728 |
| H | -3.28347 | -1.22474 | 3.85625 |
| H | -1.63645 | -0.85324 | 3.35719 |
| H | -2.38757 | 0.05701 | 4.67855 |
| C | -7.36808 | -1.90599 | 1.14208 |
| H | -8.16695 | -2.64622 | 1.23978 |
| H | -7.09168 | -1.58224 | 2.14759 |
| H | -7.76952 | -1.04065 | 0.60890 |
| C | -6.67185 | -3.00463 | -0.96937 |
| H | -7.44865 | -3.75864 | -0.82176 |
| H | -7.10756 | -2.19692 | -1.56315 |
| H | -5.86880 | -3.46599 | -1.54912 |
| C | -5.64073 | -3.71802 | 1.16973 |
| H | -4.78954 | -4.16852 | 0.65390 |
| H | -5.31327 | -3.43657 | 2.17280 |
| H | -6.42093 | -4.47731 | 1.27304 |
| C | -4.06046 | -0.27730 | -3.58194 |
| H | -5.12147 | -0.07229 | -3.42367 |
| H | -3.78957 | 0.15217 | -4.54873 |

| | | | |
|----|----------|----------|----------|
| H | -3.91499 | -1.35827 | -3.64846 |
| C | -3.45570 | 1.86724 | -2.53611 |
| H | -4.50366 | 2.07002 | -2.30165 |
| H | -2.84041 | 2.41873 | -1.82167 |
| H | -3.24331 | 2.26841 | -3.53074 |
| C | -1.73220 | 0.07916 | -2.93435 |
| H | -0.99447 | 0.66055 | -2.37711 |
| H | -1.48429 | -0.97738 | -2.82819 |
| H | -1.60728 | 0.36692 | -3.98202 |
| C | 2.23235 | 2.20044 | 1.11198 |
| H | 2.01078 | 2.13549 | 0.04466 |
| H | 1.46059 | 1.65483 | 1.65211 |
| H | 2.12395 | 3.24934 | 1.39565 |
| C | 4.55213 | 2.74141 | 0.63543 |
| H | 4.31087 | 3.75620 | 0.96187 |
| H | 5.61332 | 2.57200 | 0.81937 |
| H | 4.37942 | 2.68418 | -0.44136 |
| C | 3.98215 | 1.85324 | 2.88342 |
| H | 5.03225 | 1.62948 | 3.08184 |
| H | 3.79475 | 2.87594 | 3.22068 |
| H | 3.38251 | 1.18318 | 3.49965 |
| C | 1.55212 | -1.27763 | -2.34684 |
| H | 1.16975 | -1.59670 | -3.31935 |
| H | 0.78329 | -1.54065 | -1.62584 |
| H | 1.66649 | -0.19050 | -2.37480 |
| C | 2.69755 | -3.48380 | -1.99240 |
| H | 2.05888 | -3.75171 | -1.15336 |
| H | 2.23402 | -3.85287 | -2.91122 |
| H | 3.65841 | -3.99187 | -1.87575 |
| C | 3.75457 | -1.66066 | -3.32173 |
| H | 3.96007 | -0.59076 | -3.40712 |
| H | 4.70736 | -2.19086 | -3.31750 |
| H | 3.21206 | -1.97392 | -4.21720 |
| C | 8.04936 | -0.78622 | 1.33161 |
| H | 8.14101 | 0.27163 | 1.07251 |
| H | 7.57885 | -0.86137 | 2.31526 |
| H | 9.06107 | -1.18959 | 1.41664 |
| C | 7.99349 | -1.39960 | -1.07189 |
| H | 7.51882 | -1.98456 | -1.86195 |
| H | 7.99715 | -0.35271 | -1.38488 |
| H | 9.03128 | -1.73355 | -0.98783 |
| C | 7.28224 | -3.05045 | 0.66851 |
| H | 6.78943 | -3.20050 | 1.63218 |
| H | 6.76721 | -3.66805 | -0.06980 |
| H | 8.31033 | -3.41328 | 0.75139 |
| Au | -0.57822 | 2.91623 | -0.53681 |
| Cl | -0.01672 | 5.05320 | -1.07021 |
| Ge | -0.75737 | -2.46944 | 0.88680 |
| C | 1.66408 | -0.75022 | 2.60225 |
| H | 2.61618 | -1.20583 | 2.87933 |
| H | 1.61017 | 0.26245 | 2.98716 |
| H | 0.85511 | -1.34095 | 3.03908 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.55447 | -0.17113 | 0.65406 |
| C | 0.21775 | 0.55260 | -0.87169 |
| P | -1.25944 | 0.51375 | -1.83581 |
| Ge | 1.26200 | 0.99932 | -2.69697 |
| Cl | 1.41374 | -1.18312 | -3.21662 |
| O | -0.74729 | 1.14365 | -3.13514 |
| C | -2.72725 | 1.32371 | -1.21513 |
| H | -2.51493 | 2.37693 | -1.02603 |
| H | -3.51919 | 1.24019 | -1.96289 |
| H | -3.04860 | 0.84206 | -0.28880 |

| | | | |
|----|----------|----------|----------|
| Au | 0.28482 | 2.19215 | 0.51814 |
| Cl | 0.20773 | 4.26941 | 1.37839 |
| H | 1.98138 | -0.13748 | 0.57559 |
| H | -1.63316 | -0.83295 | -2.01257 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.55636 | -0.08732 | 0.63586 |
| C | 0.15769 | 0.67360 | -0.85298 |
| P | -1.32052 | 0.50588 | -1.81146 |
| Ge | 1.17101 | 1.16266 | -2.67668 |
| Cl | 1.68938 | -1.00423 | -3.08930 |
| O | -0.79574 | 1.01778 | -3.16637 |
| C | -2.74101 | 1.46208 | -1.28042 |
| H | -2.46916 | 2.51645 | -1.21805 |
| H | -3.54200 | 1.34076 | -2.01360 |
| H | -3.08630 | 1.11951 | -0.30310 |
| C | -1.83597 | -1.20698 | -1.90612 |
| H | -2.17053 | -1.55597 | -0.92698 |
| H | -2.64903 | -1.30070 | -2.62914 |
| H | -0.98203 | -1.79819 | -2.24065 |
| C | 2.38950 | -0.12843 | 0.64199 |
| H | 2.68307 | -1.10128 | 0.23351 |
| H | 2.84746 | 0.65615 | 0.04052 |
| H | 2.74802 | -0.06879 | 1.67132 |
| Au | 0.10242 | 2.26098 | 0.59602 |
| Cl | -0.09510 | 4.26590 | 1.60757 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.67708 | -0.12608 | 0.44139 |
| C | 0.09892 | 0.68782 | -0.96299 |
| P | -1.44992 | 0.38463 | -1.79752 |
| Ge | 0.79806 | 1.58215 | -2.79825 |
| Cl | 1.87746 | -0.23716 | -3.59585 |
| O | -1.06826 | 0.91094 | -3.19850 |
| C | -2.81285 | 1.36485 | -1.14876 |
| H | -2.52233 | 2.41615 | -1.17861 |
| H | -3.69039 | 1.22793 | -1.78363 |
| H | -3.05318 | 1.09176 | -0.12119 |
| Au | -0.09969 | 2.12230 | 0.64456 |
| Cl | -0.49272 | 3.97160 | 1.87820 |
| C | -2.00642 | -1.36350 | -1.87968 |
| C | -3.10883 | -1.43509 | -2.94118 |
| C | -0.83780 | -2.25051 | -2.30483 |
| C | -2.54035 | -1.80500 | -0.51734 |
| H | -3.99637 | -0.86398 | -2.66032 |
| H | -2.75536 | -1.07714 | -3.90965 |
| H | -3.41461 | -2.47893 | -3.05484 |
| H | -0.04677 | -2.27230 | -1.55340 |
| H | -1.20629 | -3.27251 | -2.43162 |
| H | -0.39746 | -1.92336 | -3.24733 |
| H | -2.81275 | -2.86274 | -0.57374 |
| H | -1.79035 | -1.70108 | 0.27102 |
| H | -3.43480 | -1.25198 | -0.22351 |
| C | 2.53556 | 0.04235 | 0.54805 |
| C | 3.05969 | -1.30169 | 0.02627 |
| C | 3.16100 | 1.19097 | -0.22346 |
| C | 2.84183 | 0.17231 | 2.04177 |
| H | 2.61336 | -2.14834 | 0.55668 |
| H | 2.87054 | -1.41683 | -1.04327 |
| H | 4.14166 | -1.34892 | 0.18655 |
| H | 2.75922 | 2.15907 | 0.08469 |
| H | 4.24022 | 1.20587 | -0.03685 |
| H | 3.02894 | 1.07543 | -1.30074 |
| H | 3.92345 | 0.11300 | 2.19640 |
| H | 2.49626 | 1.12838 | 2.44290 |
| H | 2.37748 | -0.62831 | 2.62449 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.38564 | 0.35850 | 0.52151 |
| C | 0.20389 | 0.64879 | -1.16499 |
| P | -1.28158 | 0.42048 | -2.10451 |
| Ge | 1.22173 | 0.93348 | -3.04070 |
| Cl | 1.71680 | -1.23327 | -3.45505 |
| O | -0.75251 | 0.77925 | -3.50514 |
| C | -2.68315 | 1.45175 | -1.66659 |
| H | -2.39500 | 2.50198 | -1.73058 |
| H | -3.49668 | 1.24746 | -2.36601 |
| H | -3.01604 | 1.22910 | -0.65112 |
| Au | 0.25778 | 2.61948 | -0.25751 |
| Cl | 0.26224 | 4.84483 | 0.11254 |
| C | -1.85805 | -1.27681 | -2.04039 |
| C | -2.39458 | -1.80199 | -0.86528 |
| C | -1.77830 | -2.06343 | -3.18524 |
| C | -2.85252 | -3.10790 | -0.84037 |
| H | -2.44516 | -1.20061 | 0.03689 |
| C | -2.24283 | -3.36970 | -3.15376 |
| H | -1.34332 | -1.65191 | -4.08749 |
| C | -2.77839 | -3.89023 | -1.98581 |
| H | -3.26559 | -3.51762 | 0.07386 |
| H | -2.17804 | -3.98361 | -4.04432 |
| H | -3.13666 | -4.91311 | -1.96384 |
| C | 2.15907 | 0.19153 | 0.84537 |
| C | 3.09265 | -0.26331 | -0.08656 |
| C | 2.57210 | 0.47623 | 2.14988 |
| C | 4.42143 | -0.40236 | 0.27790 |
| H | 2.77691 | -0.54101 | -1.08547 |
| C | 3.90460 | 0.35183 | 2.50410 |
| H | 1.84566 | 0.80943 | 2.88486 |
| C | 4.82999 | -0.08664 | 1.56703 |
| H | 5.14106 | -0.76191 | -0.44852 |
| H | 4.22108 | 0.59157 | 3.51252 |
| H | 5.87244 | -0.19239 | 1.84510 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.31103 | 0.20241 | 1.01811 |
| C | -0.08898 | 0.70739 | -0.58341 |
| P | -1.47895 | 0.50195 | -1.69024 |
| Ge | 0.98420 | 1.61474 | -2.19122 |
| Cl | 1.95599 | -0.21249 | -3.10023 |
| O | -0.88461 | 1.26001 | -2.89386 |
| C | -3.02501 | 1.31989 | -1.26318 |
| H | -2.83223 | 2.38579 | -1.13019 |
| H | -3.70896 | 1.18006 | -2.10421 |
| H | -3.47715 | 0.91538 | -0.35981 |
| Au | -0.46559 | 2.43901 | 0.66893 |
| Cl | -1.11262 | 4.49783 | 1.34958 |
| C | -1.85201 | -1.23249 | -2.03877 |
| C | -2.31633 | -2.04768 | -0.98789 |
| C | -1.70569 | -1.77564 | -3.33584 |
| C | -2.54754 | -3.39593 | -1.22486 |
| C | -1.96513 | -3.12994 | -3.51088 |
| C | -2.36254 | -3.96350 | -2.47546 |
| H | -2.89373 | -4.01542 | -0.40292 |
| H | -1.85027 | -3.54611 | -4.50680 |
| C | 2.13970 | 0.20792 | 1.06852 |
| C | 2.74642 | -0.95602 | 0.55940 |
| C | 2.91596 | 1.17813 | 1.71962 |
| C | 4.12593 | -1.08144 | 0.63560 |
| C | 4.29504 | 1.00636 | 1.76450 |
| C | 4.92274 | -0.10212 | 1.21412 |
| H | 4.58880 | -1.97961 | 0.23756 |
| H | 4.89541 | 1.76363 | 2.26006 |

| | | | |
|---|----------|----------|----------|
| C | 2.32541 | 2.38731 | 2.37940 |
| H | 2.04948 | 3.15699 | 1.65190 |
| H | 1.42586 | 2.14652 | 2.95236 |
| H | 3.04404 | 2.83563 | 3.06707 |
| C | 1.94026 | -2.07407 | -0.03290 |
| H | 1.09343 | -2.34753 | 0.60681 |
| H | 1.54190 | -1.80390 | -1.01359 |
| H | 2.55808 | -2.96426 | -0.15791 |
| C | 6.41339 | -0.24030 | 1.24331 |
| H | 6.85130 | 0.33001 | 2.06419 |
| H | 6.71513 | -1.28414 | 1.34909 |
| H | 6.85241 | 0.13265 | 0.31265 |
| C | -2.65759 | -1.53800 | 0.38345 |
| H | -2.47903 | -2.31137 | 1.13166 |
| H | -2.08767 | -0.66292 | 0.69239 |
| H | -3.72014 | -1.27902 | 0.43516 |
| C | -1.31669 | -0.99731 | -4.55947 |
| H | -1.91976 | -0.09897 | -4.68884 |
| H | -0.27623 | -0.67404 | -4.51427 |
| H | -1.44318 | -1.62727 | -5.44051 |
| C | -2.57714 | -5.42679 | -2.70329 |
| H | -2.97370 | -5.61999 | -3.70165 |
| H | -1.63074 | -5.96995 | -2.61857 |
| H | -3.26527 | -5.84926 | -1.96948 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.70257 | -0.03970 | 1.14881 |
| C | 0.38736 | 0.12853 | -0.55649 |
| P | -1.09496 | -0.10654 | -1.60631 |
| O | -0.32700 | -0.08970 | -2.95016 |
| Cl | 2.71768 | -1.05434 | -2.97746 |
| Au | 0.21694 | 2.14526 | 0.23079 |
| Cl | -0.25919 | 4.36846 | 0.32805 |
| C | 2.55461 | -0.08254 | 1.24626 |
| C | 3.26581 | -1.21756 | 0.76907 |
| C | 3.29851 | 1.05626 | 1.64131 |
| C | 4.57770 | -1.03849 | 0.35729 |
| C | 4.60403 | 1.17472 | 1.16197 |
| C | 5.24102 | 0.17928 | 0.44319 |
| H | 5.10932 | -1.89215 | -0.04276 |
| H | 5.14568 | 2.08187 | 1.39145 |
| C | 2.90542 | 2.09320 | 2.71621 |
| C | 2.80376 | -2.68224 | 0.90746 |
| C | 6.63239 | 0.34244 | -0.15712 |
| C | -2.13871 | 1.36963 | -1.70222 |
| H | -2.68081 | 1.60805 | -0.79266 |
| H | -1.50078 | 2.21280 | -1.97364 |
| H | -2.84735 | 1.18565 | -2.51318 |
| C | 3.93416 | 1.92004 | 3.85370 |
| H | 3.90367 | 0.90464 | 4.25712 |
| H | 4.95370 | 2.11889 | 3.52290 |
| H | 3.70108 | 2.61692 | 4.66341 |
| C | 2.99380 | 3.53158 | 2.20107 |
| H | 2.28063 | 3.72411 | 1.39861 |
| H | 2.76969 | 4.22883 | 3.01306 |
| H | 3.99249 | 3.76895 | 1.83018 |
| C | 1.54555 | 1.87691 | 3.37468 |
| H | 1.47145 | 2.52640 | 4.25100 |
| H | 0.70350 | 2.13901 | 2.73125 |
| H | 1.41754 | 0.84681 | 3.71741 |
| C | 3.11031 | -3.52119 | -0.33574 |
| H | 2.64024 | -3.10373 | -1.22453 |
| H | 4.18118 | -3.59592 | -0.53017 |
| H | 2.74020 | -4.53950 | -0.18695 |
| C | 3.60827 | -3.25364 | 2.09063 |
| H | 4.68214 | -3.20506 | 1.90326 |

| | | | |
|----|----------|----------|----------|
| H | 3.40211 | -2.69931 | 3.00981 |
| H | 3.33634 | -4.30101 | 2.25302 |
| C | 1.33359 | -2.87601 | 1.25808 |
| H | 1.05679 | -2.35582 | 2.17999 |
| H | 0.66581 | -2.56483 | 0.45454 |
| H | 1.14702 | -3.94002 | 1.43096 |
| C | 7.18968 | 1.74809 | 0.05017 |
| H | 6.53955 | 2.50935 | -0.38802 |
| H | 7.32945 | 1.98137 | 1.10905 |
| H | 8.16602 | 1.82781 | -0.43389 |
| C | 6.55166 | 0.07216 | -1.66427 |
| H | 7.54270 | 0.16840 | -2.11698 |
| H | 6.17763 | -0.93114 | -1.87623 |
| H | 5.88024 | 0.78070 | -2.15441 |
| C | 7.59868 | -0.65831 | 0.48732 |
| H | 7.66993 | -0.49593 | 1.56583 |
| H | 7.28466 | -1.69085 | 0.32211 |
| H | 8.59830 | -0.54359 | 0.05884 |
| C | -2.36933 | -1.43854 | -1.65253 |
| C | -2.33855 | -2.33617 | -2.76084 |
| C | -3.61625 | -1.22405 | -1.00406 |
| C | -3.54463 | -2.64091 | -3.37719 |
| C | -1.11438 | -3.12662 | -3.25922 |
| C | -4.78033 | -1.60173 | -1.66630 |
| C | -3.82313 | -0.77227 | 0.45444 |
| C | -4.77916 | -2.21943 | -2.90527 |
| H | -3.51263 | -3.25976 | -4.26415 |
| C | -0.60397 | -2.63926 | -4.61824 |
| C | -1.53832 | -4.60072 | -3.42644 |
| C | -0.00359 | -3.15698 | -2.21797 |
| H | -5.72572 | -1.40314 | -1.18128 |
| C | -2.53973 | -0.43046 | 1.19073 |
| C | -4.41395 | -1.99372 | 1.18755 |
| C | -4.81177 | 0.39024 | 0.59115 |
| C | -6.04998 | -2.52191 | -3.68914 |
| H | 0.20150 | -3.29395 | -4.96166 |
| H | -1.40397 | -2.67483 | -5.36292 |
| H | -0.22289 | -1.62338 | -4.56684 |
| H | -2.21247 | -4.76008 | -4.26875 |
| H | -0.64370 | -5.19904 | -3.61615 |
| H | -2.01903 | -4.98574 | -2.52381 |
| H | 0.43260 | -2.18304 | -2.01353 |
| H | -0.37064 | -3.59230 | -1.28507 |
| H | 0.81527 | -3.78177 | -2.58015 |
| H | -1.80592 | -1.23382 | 1.10601 |
| H | -2.07994 | 0.50127 | 0.86015 |
| H | -2.75068 | -0.29907 | 2.25449 |
| H | -4.55682 | -1.74990 | 2.24386 |
| H | -5.37830 | -2.29414 | 0.77633 |
| H | -3.73816 | -2.84978 | 1.12347 |
| H | -5.79402 | 0.14642 | 0.18352 |
| H | -4.94727 | 0.62949 | 1.64899 |
| H | -4.46318 | 1.29501 | 0.09100 |
| C | -7.29576 | -1.95846 | -3.01078 |
| C | -6.22025 | -4.03935 | -3.82973 |
| C | -5.93272 | -1.89305 | -5.08273 |
| H | -7.47430 | -2.41879 | -2.03563 |
| H | -7.22903 | -0.87609 | -2.87468 |
| H | -8.17160 | -2.16083 | -3.63160 |
| H | -5.38096 | -4.49532 | -4.35832 |
| H | -6.29990 | -4.51698 | -2.85011 |
| H | -7.13041 | -4.26360 | -4.39266 |
| H | -5.82540 | -0.80774 | -5.01500 |
| H | -5.07177 | -2.28077 | -5.63071 |
| H | -6.82934 | -2.11037 | -5.66947 |
| Ge | 1.44211 | 0.68675 | -2.34723 |

[R-P=C(Ge(II)Cl)-P(S)ClR](AuCl)

Coordination through Ge(II) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.43110 | 0.76476 | 0.31787 |
| C | 0.03493 | 0.37151 | -1.24486 |
| P | -1.52503 | -0.12198 | -1.85741 |
| Ge | 0.87718 | 0.71438 | -3.04612 |
| Cl | 1.40918 | -1.32317 | -3.61901 |
| Au | 2.16742 | 2.57971 | -3.58636 |
| Cl | 3.43869 | 4.40916 | -4.01917 |
| H | 1.76648 | 1.19498 | 0.04769 |
| H | -1.63708 | -1.52299 | -1.88365 |
| Cl | -3.10159 | 0.35164 | -0.71444 |
| S | -1.50127 | 0.70010 | -3.66904 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.45862 | 0.55260 | 0.35067 |
| C | 0.02421 | 0.31097 | -1.23341 |
| P | -1.57339 | -0.07899 | -1.82231 |
| Ge | 0.84573 | 0.68474 | -3.03100 |
| Cl | 1.42279 | -1.33724 | -3.65733 |
| C | -1.90584 | -1.84118 | -1.82265 |
| H | -1.92824 | -2.20744 | -0.79496 |
| H | -2.86278 | -2.02683 | -2.31238 |
| H | -1.09900 | -2.32071 | -2.38123 |
| C | 2.23822 | 0.95899 | 0.26661 |
| H | 2.80757 | 0.02424 | 0.29584 |
| H | 2.50704 | 1.50623 | -0.64005 |
| H | 2.51081 | 1.54446 | 1.14601 |
| Au | 2.19565 | 2.52622 | -3.52896 |
| Cl | 3.53740 | 4.32446 | -3.89631 |
| Cl | -3.07467 | 0.68467 | -0.71250 |
| S | -1.48351 | 0.70872 | -3.66510 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.41020 | 0.51378 | 0.05131 |
| C | 0.27549 | 0.15728 | -1.56836 |
| P | -1.28239 | -0.22317 | -2.30027 |
| Ge | 1.33295 | 0.34248 | -3.27492 |
| Cl | 2.22995 | -1.63556 | -3.54984 |
| Au | 2.50732 | 2.26867 | -3.89951 |
| Cl | 3.64384 | 4.17695 | -4.40505 |
| C | 2.17410 | 0.95607 | 0.44914 |
| C | 3.23362 | 0.26692 | -0.39606 |
| C | 2.25407 | 2.48043 | 0.29646 |
| C | 2.34679 | 0.57618 | 1.92328 |
| H | 3.10757 | -0.81725 | -0.42028 |
| H | 3.24660 | 0.63883 | -1.42282 |
| H | 4.22225 | 0.48152 | 0.02275 |
| H | 1.48063 | 2.99398 | 0.87548 |
| H | 3.22445 | 2.82384 | 0.66939 |
| H | 2.16839 | 2.78869 | -0.74782 |
| H | 3.32446 | 0.92100 | 2.27215 |
| H | 1.58337 | 1.03665 | 2.55614 |
| H | 2.30263 | -0.50619 | 2.07119 |
| C | -2.00109 | -1.87804 | -1.89838 |
| C | -3.23831 | -2.08243 | -2.77042 |
| C | -0.93680 | -2.92305 | -2.23318 |
| C | -2.35997 | -1.93855 | -0.41643 |
| H | -4.02393 | -1.35978 | -2.54442 |
| H | -2.99797 | -2.02094 | -3.83393 |
| H | -3.63400 | -3.08271 | -2.57511 |
| H | -0.03562 | -2.80011 | -1.63068 |

| | | | |
|----|----------|----------|----------|
| H | -1.35522 | -3.91095 | -2.02240 |
| H | -0.64824 | -2.89250 | -3.28452 |
| H | -2.73047 | -2.94349 | -0.19639 |
| H | -1.49359 | -1.75759 | 0.22354 |
| H | -3.14137 | -1.22536 | -0.15221 |
| Cl | -2.71672 | 1.08952 | -1.72539 |
| S | -0.84072 | 0.00753 | -4.24705 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.49886 | 0.57663 | 0.21323 |
| C | 0.07652 | 0.26664 | -1.36877 |
| P | -1.55384 | -0.05971 | -1.91043 |
| Ge | 0.88631 | 0.60358 | -3.17407 |
| Cl | 1.48863 | -1.40917 | -3.82370 |
| Au | 2.20141 | 2.44505 | -3.76313 |
| Cl | 3.51852 | 4.23294 | -4.27026 |
| C | 2.27217 | 0.85014 | 0.19611 |
| C | 2.76192 | 1.70181 | 1.19257 |
| C | 3.16651 | 0.27048 | -0.71009 |
| C | 4.10980 | 2.01152 | 1.24690 |
| H | 2.07652 | 2.13537 | 1.91421 |
| C | 4.51447 | 0.57137 | -0.64140 |
| H | 2.81541 | -0.44383 | -1.44676 |
| C | 4.98400 | 1.44949 | 0.32740 |
| H | 4.47952 | 2.69010 | 2.00641 |
| H | 5.20187 | 0.12400 | -1.34927 |
| H | 6.03986 | 1.69056 | 0.36898 |
| C | -2.05569 | -1.77710 | -1.74491 |
| C | -2.01496 | -2.61118 | -2.85736 |
| C | -2.41067 | -2.28272 | -0.49411 |
| C | -2.33981 | -3.95200 | -2.71758 |
| H | -1.72656 | -2.21330 | -3.82255 |
| C | -2.72977 | -3.62198 | -0.36568 |
| H | -2.44457 | -1.63376 | 0.37343 |
| C | -2.69577 | -4.45584 | -1.47685 |
| H | -2.31159 | -4.60205 | -3.58380 |
| H | -3.00940 | -4.01679 | 0.60382 |
| H | -2.94913 | -5.50444 | -1.37157 |
| Cl | -2.93517 | 0.95122 | -0.83284 |
| S | -1.44857 | 0.57335 | -3.80863 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.53029 | 0.61398 | 0.49233 |
| C | 0.32057 | -0.03896 | -1.02811 |
| P | -1.23339 | -0.32166 | -1.80424 |
| Ge | 1.43850 | 0.15304 | -2.67678 |
| Cl | 1.82412 | -1.95094 | -3.20072 |
| Au | 3.09829 | 1.75308 | -3.08236 |
| Cl | 4.74383 | 3.31512 | -3.36455 |
| C | 2.28695 | 1.06200 | 0.52095 |
| C | 2.59098 | 2.43447 | 0.52787 |
| C | 3.31098 | 0.10526 | 0.58246 |
| C | 3.92043 | 2.82407 | 0.53425 |
| C | 4.62725 | 0.54703 | 0.59782 |
| C | 4.95506 | 1.89640 | 0.54766 |
| H | 4.15630 | 3.88286 | 0.49657 |
| H | 5.42380 | -0.18968 | 0.64209 |
| C | -1.94941 | -1.97503 | -1.90207 |
| C | -3.01212 | -2.17576 | -2.81102 |
| C | -1.48299 | -3.04185 | -1.10719 |
| C | -3.56386 | -3.44464 | -2.91321 |
| C | -2.07532 | -4.28760 | -1.26624 |
| C | -3.10698 | -4.51809 | -2.16360 |
| H | -4.38393 | -3.59335 | -3.60857 |
| H | -1.71383 | -5.10770 | -0.65441 |
| C | -3.58800 | -1.10983 | -3.69582 |

| | | | |
|----|----------|----------|----------|
| H | -3.70107 | -0.14719 | -3.19665 |
| H | -2.95748 | -0.94976 | -4.57403 |
| H | -4.57436 | -1.41699 | -4.04456 |
| C | -0.38950 | -2.92936 | -0.08998 |
| H | 0.55487 | -2.63313 | -0.54832 |
| H | -0.62484 | -2.19787 | 0.68560 |
| H | -0.24074 | -3.89397 | 0.39526 |
| C | -3.69613 | -5.88272 | -2.32946 |
| H | -3.16090 | -6.43615 | -3.10738 |
| H | -3.62503 | -6.46279 | -1.40812 |
| H | -4.74441 | -5.83113 | -2.62783 |
| C | 3.02951 | -1.36766 | 0.63583 |
| H | 2.16500 | -1.59695 | 1.26497 |
| H | 2.82813 | -1.77598 | -0.35930 |
| H | 3.88795 | -1.90574 | 1.04020 |
| C | 1.51201 | 3.47280 | 0.45049 |
| H | 1.15331 | 3.58715 | -0.57725 |
| H | 0.64644 | 3.21598 | 1.07140 |
| H | 1.88260 | 4.44456 | 0.77868 |
| C | 6.37845 | 2.34646 | 0.46786 |
| H | 6.61137 | 2.64004 | -0.56058 |
| H | 6.55884 | 3.21561 | 1.10401 |
| H | 7.06843 | 1.55326 | 0.75895 |
| Cl | -2.67055 | 0.76849 | -0.86021 |
| S | -0.75151 | 0.45606 | -3.60854 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.31651 | 1.58440 | 1.45279 |
| C | 0.23100 | 0.47217 | 0.32987 |
| P | 1.82931 | -0.26199 | 0.12041 |
| Cl | -1.16943 | 0.77956 | -2.70954 |
| C | 3.53611 | 0.39308 | 0.17743 |
| C | 4.15716 | 0.66595 | -1.07878 |
| C | 4.36737 | 0.14277 | 1.30252 |
| C | 5.46907 | 0.24878 | -1.24025 |
| C | 5.67971 | -0.24577 | 1.05558 |
| C | 6.22466 | -0.31119 | -0.21707 |
| H | 5.92928 | 0.39419 | -2.20960 |
| H | 6.30001 | -0.49478 | 1.90523 |
| C | -2.11156 | 1.63568 | 1.09595 |
| C | -2.63239 | 2.65227 | 0.26353 |
| C | -2.96706 | 0.61618 | 1.59304 |
| C | -3.90093 | 2.45794 | -0.27750 |
| C | -4.21277 | 0.48409 | 0.99375 |
| C | -4.67637 | 1.34574 | 0.00696 |
| H | -4.29054 | 3.19729 | -0.95843 |
| H | -4.84983 | -0.33080 | 1.30299 |
| C | -1.92956 | 4.00581 | 0.03932 |
| C | -2.68605 | -0.18325 | 2.88401 |
| C | -6.01065 | 1.06997 | -0.67700 |
| C | 4.03627 | 0.47188 | 2.77226 |
| C | 3.60104 | 1.58294 | -2.18736 |
| C | 7.61560 | -0.86251 | -0.49931 |
| C | -3.80055 | -1.18909 | 3.18637 |
| H | -3.56425 | -1.70005 | 4.12246 |
| H | -4.76868 | -0.70231 | 3.32131 |
| H | -3.89244 | -1.95028 | 2.40723 |
| C | -2.65686 | 0.83751 | 4.03317 |
| H | -1.84110 | 1.55653 | 3.91395 |
| H | -3.59331 | 1.39783 | 4.08392 |
| H | -2.51307 | 0.32213 | 4.98719 |
| C | -1.37580 | -0.97026 | 2.90835 |
| H | -1.27119 | -1.62047 | 2.03770 |
| H | -0.49373 | -0.32614 | 2.96418 |
| H | -1.35462 | -1.59541 | 3.80508 |
| C | -7.12905 | 1.00033 | 0.36952 |

| | | | |
|----|----------|----------|----------|
| H | -8.08654 | 0.80518 | -0.12106 |
| H | -6.96095 | 0.20027 | 1.09260 |
| H | -7.21344 | 1.94199 | 0.91846 |
| C | -6.37418 | 2.14965 | -1.69293 |
| H | -7.32398 | 1.89392 | -2.16846 |
| H | -6.49466 | 3.13048 | -1.22454 |
| H | -5.62282 | 2.23251 | -2.48220 |
| C | -5.91543 | -0.27356 | -1.41099 |
| H | -5.13510 | -0.24515 | -2.17540 |
| H | -5.68257 | -1.09864 | -0.73511 |
| H | -6.86621 | -0.49879 | -1.90252 |
| C | -2.76858 | 4.95135 | -0.82352 |
| H | -3.74957 | 5.14844 | -0.38632 |
| H | -2.24722 | 5.90801 | -0.90345 |
| H | -2.90841 | 4.56676 | -1.83652 |
| C | -1.75250 | 4.68029 | 1.40767 |
| H | -2.71624 | 4.81160 | 1.90499 |
| H | -1.10943 | 4.09720 | 2.07191 |
| H | -1.29312 | 5.66527 | 1.28383 |
| C | -0.56652 | 3.88927 | -0.64251 |
| H | 0.18352 | 3.42294 | 0.00328 |
| H | -0.62265 | 3.30631 | -1.56235 |
| H | -0.18886 | 4.88847 | -0.87899 |
| C | 2.64447 | 1.04808 | 2.99216 |
| H | 2.44011 | 1.87380 | 2.30691 |
| H | 1.85265 | 0.30741 | 2.90160 |
| H | 2.57730 | 1.45018 | 4.00595 |
| C | 5.01499 | 1.60418 | 3.15336 |
| H | 4.80704 | 1.92779 | 4.17668 |
| H | 6.05661 | 1.28563 | 3.10601 |
| H | 4.89395 | 2.46601 | 2.49270 |
| C | 4.26891 | -0.70087 | 3.72775 |
| H | 5.28804 | -1.08596 | 3.66154 |
| H | 4.11231 | -0.36592 | 4.75642 |
| H | 3.58320 | -1.52458 | 3.53368 |
| C | 2.24494 | 2.19837 | -1.86879 |
| H | 2.03422 | 2.98749 | -2.59472 |
| H | 1.42016 | 1.49348 | -1.93932 |
| H | 2.24256 | 2.65822 | -0.87762 |
| C | 3.55974 | 0.91613 | -3.56361 |
| H | 2.83444 | 0.10416 | -3.59303 |
| H | 3.27143 | 1.65492 | -4.31579 |
| H | 4.53425 | 0.51628 | -3.85159 |
| C | 4.58615 | 2.77046 | -2.25516 |
| H | 4.66499 | 3.27173 | -1.28731 |
| H | 5.58772 | 2.46703 | -2.56123 |
| H | 4.21771 | 3.49620 | -2.98480 |
| C | 8.27374 | -1.43856 | 0.75148 |
| H | 8.45154 | -0.67258 | 1.51070 |
| H | 7.67101 | -2.23396 | 1.19677 |
| H | 9.24365 | -1.86625 | 0.48782 |
| C | 8.51355 | 0.25186 | -1.05019 |
| H | 8.12603 | 0.66413 | -1.98383 |
| H | 8.60809 | 1.07092 | -0.33305 |
| H | 9.51378 | -0.14088 | -1.25127 |
| C | 7.49508 | -1.98078 | -1.54208 |
| H | 6.86898 | -2.79610 | -1.17219 |
| H | 7.05700 | -1.61901 | -2.47438 |
| H | 8.48385 | -2.38698 | -1.77109 |
| Ge | -0.73746 | -0.60959 | -1.06275 |
| Au | -2.32090 | -2.28140 | -0.62239 |
| Cl | -3.92575 | -3.82336 | -0.07270 |
| Cl | 1.89993 | -1.79592 | 1.47641 |
| S | 1.50370 | -1.21701 | -1.62817 |

Coordination through S atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.55384 | 0.18513 | 0.72298 |
| C | 0.29881 | 0.26732 | -0.91382 |
| P | -1.20860 | 0.54045 | -1.72220 |
| Ge | 1.55521 | 0.48257 | -2.57201 |
| Cl | 0.95409 | -1.43527 | -3.52419 |
| Au | -1.96233 | 1.46360 | -4.92101 |
| Cl | -3.30319 | 1.12471 | -6.69410 |
| H | -1.66359 | -0.64888 | -2.30594 |
| H | 1.97559 | 0.02390 | 0.67438 |
| Cl | -2.79050 | 1.10593 | -0.62234 |
| S | -0.61781 | 1.86614 | -3.13616 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.56302 | 0.20397 | 0.72679 |
| C | 0.28748 | 0.34193 | -0.90389 |
| P | -1.27143 | 0.51871 | -1.63879 |
| Ge | 1.51076 | 0.74462 | -2.54514 |
| Cl | 1.35208 | -1.25653 | -3.51743 |
| C | -1.97008 | -1.03813 | -2.17861 |
| H | -2.16938 | -1.64839 | -1.29537 |
| H | -2.89164 | -0.84466 | -2.72931 |
| H | -1.23669 | -1.52523 | -2.82452 |
| C | 2.37988 | -0.00800 | 0.84942 |
| H | 2.60103 | -1.08010 | 0.84094 |
| H | 2.92458 | 0.46624 | 0.03054 |
| H | 2.72496 | 0.39333 | 1.80398 |
| Au | -2.02049 | 1.15991 | -4.97878 |
| Cl | -3.27488 | 0.60655 | -6.76415 |
| Cl | -2.70975 | 1.31161 | -0.45528 |
| S | -0.77672 | 1.76592 | -3.17606 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.63953 | -0.16224 | 0.52923 |
| C | 0.20369 | 0.48658 | -0.94163 |
| P | -1.46855 | 0.38520 | -1.45538 |
| Ge | 1.01109 | 1.81325 | -2.34853 |
| Cl | 1.67751 | 0.33119 | -3.87845 |
| Au | -2.54741 | 1.46314 | -4.74453 |
| Cl | -3.55937 | 1.08192 | -6.72222 |
| C | -2.02994 | -1.27423 | -2.08031 |
| C | -3.49632 | -1.19091 | -2.49682 |
| C | -1.15133 | -1.67234 | -3.26277 |
| C | -1.86342 | -2.28009 | -0.94144 |
| H | -4.15076 | -0.95512 | -1.65703 |
| H | -3.65893 | -0.46002 | -3.29230 |
| H | -3.78666 | -2.16881 | -2.88971 |
| H | -0.09562 | -1.72609 | -2.99511 |
| H | -1.47254 | -2.66272 | -3.59671 |
| H | -1.25677 | -0.98651 | -4.10480 |
| H | -2.19624 | -3.25287 | -1.31329 |
| H | -0.82296 | -2.38334 | -0.62935 |
| H | -2.46890 | -2.02847 | -0.06986 |
| C | 2.48764 | -0.03817 | 0.75181 |
| C | 2.97405 | -1.49171 | 0.69442 |
| C | 3.23660 | 0.80892 | -0.25928 |
| C | 2.68974 | 0.51139 | 2.16738 |
| H | 2.43300 | -2.13375 | 1.39550 |
| H | 2.86925 | -1.91146 | -0.30879 |
| H | 4.03424 | -1.52680 | 0.96605 |
| H | 2.90856 | 1.85139 | -0.23973 |
| H | 4.30649 | 0.80505 | -0.02378 |
| H | 3.13386 | 0.41624 | -1.27460 |

| | | | |
|----|----------|----------|----------|
| H | 3.75265 | 0.47178 | 2.42510 |
| H | 2.36381 | 1.55146 | 2.24757 |
| H | 2.14377 | -0.07317 | 2.91279 |
| Cl | -2.76198 | 0.78799 | 0.06408 |
| S | -1.52712 | 1.95215 | -2.77159 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.44416 | -0.04844 | 0.87282 |
| C | 0.16022 | 0.23173 | -0.74429 |
| P | -1.41828 | 0.30584 | -1.46152 |
| Ge | 1.34488 | 1.11951 | -2.19816 |
| Cl | 1.60858 | -0.61910 | -3.57802 |
| Au | -2.47052 | 1.73877 | -4.57231 |
| Cl | -3.80830 | 1.72423 | -6.38579 |
| C | -1.93657 | -1.25751 | -2.17744 |
| C | -2.44427 | -2.24046 | -1.32615 |
| C | -1.76871 | -1.51812 | -3.53302 |
| C | -2.79261 | -3.47528 | -1.84116 |
| H | -2.57675 | -2.04115 | -0.26935 |
| C | -2.12750 | -2.75767 | -4.03895 |
| H | -1.36280 | -0.76366 | -4.19400 |
| C | -2.63805 | -3.73256 | -3.19762 |
| H | -3.19355 | -4.23665 | -1.18274 |
| H | -2.00857 | -2.95339 | -5.09757 |
| H | -2.92057 | -4.69902 | -3.59888 |
| C | 2.24458 | -0.06105 | 0.99578 |
| C | 3.09899 | -0.49693 | -0.02291 |
| C | 2.79389 | 0.37530 | 2.20525 |
| C | 4.47219 | -0.45692 | 0.15487 |
| H | 2.68879 | -0.91752 | -0.93572 |
| C | 4.16732 | 0.42432 | 2.37425 |
| H | 2.13768 | 0.68997 | 3.01087 |
| C | 5.00625 | 0.01188 | 1.34771 |
| H | 5.12686 | -0.80129 | -0.63721 |
| H | 4.58516 | 0.77885 | 3.30927 |
| H | 6.08129 | 0.04193 | 1.48326 |
| Cl | -2.88912 | 0.75511 | -0.13761 |
| S | -1.11177 | 1.84091 | -2.75557 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.14435 | 0.66904 | 0.42163 |
| C | 0.07182 | 0.05350 | -1.12015 |
| P | -1.25892 | -0.04799 | -2.23118 |
| Ge | 1.69886 | -0.06902 | -2.40973 |
| Cl | 1.56227 | -2.28072 | -2.85859 |
| Au | 0.12341 | 2.83342 | -3.27353 |
| Cl | 0.65112 | 4.96009 | -2.72526 |
| C | -1.97193 | -1.70507 | -2.37367 |
| C | -2.43503 | -2.29423 | -1.17410 |
| C | -2.09221 | -2.40874 | -3.59377 |
| C | -2.96387 | -3.57708 | -1.21961 |
| C | -2.63108 | -3.68784 | -3.56285 |
| C | -3.05974 | -4.30094 | -2.39572 |
| H | -3.32049 | -4.01678 | -0.29356 |
| H | -2.72265 | -4.22307 | -4.50229 |
| C | 1.93140 | 0.59782 | 0.77741 |
| C | 2.62998 | 1.81301 | 0.86193 |
| C | 2.57680 | -0.61937 | 1.05690 |
| C | 3.98212 | 1.78443 | 1.17805 |
| C | 3.92891 | -0.59311 | 1.37186 |
| C | 4.65221 | 0.59343 | 1.42474 |
| H | 4.52451 | 2.72352 | 1.23553 |
| H | 4.43051 | -1.53007 | 1.59534 |
| C | 1.95144 | 3.12101 | 0.59054 |
| H | 1.83705 | 3.31066 | -0.48118 |
| H | 0.94585 | 3.15586 | 1.02420 |

| | | | |
|----|----------|----------|----------|
| H | 2.52166 | 3.95180 | 1.00790 |
| C | 1.84388 | -1.92962 | 1.06190 |
| H | 0.93050 | -1.87250 | 1.66254 |
| H | 1.55272 | -2.24292 | 0.05583 |
| H | 2.47028 | -2.71511 | 1.48620 |
| C | 6.11807 | 0.58457 | 1.73040 |
| H | 6.70172 | 0.47043 | 0.81150 |
| H | 6.43231 | 1.51668 | 2.20289 |
| H | 6.38334 | -0.24366 | 2.38995 |
| C | -2.40051 | -1.64050 | 0.17520 |
| H | -1.42192 | -1.76931 | 0.64428 |
| H | -2.61409 | -0.57309 | 0.15301 |
| H | -3.14117 | -2.10787 | 0.82486 |
| C | -1.68749 | -1.89739 | -4.94352 |
| H | -2.12425 | -0.92559 | -5.17451 |
| H | -0.60278 | -1.80342 | -5.02428 |
| H | -2.01717 | -2.60104 | -5.70788 |
| C | -3.59925 | -5.69552 | -2.40952 |
| H | -4.25413 | -5.87941 | -1.55669 |
| H | -4.15670 | -5.89767 | -3.32579 |
| H | -2.78062 | -6.42020 | -2.35967 |
| Cl | -2.84001 | 1.17225 | -1.82180 |
| S | -0.32211 | 0.67667 | -3.91562 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -2.04108 | 1.89965 | 0.25708 |
| C | -1.10123 | 0.52480 | 0.20665 |
| P | 0.64165 | 0.39204 | 0.27366 |
| C | -3.73050 | 1.17616 | 0.29444 |
| C | -4.53426 | 1.25964 | -0.87637 |
| C | -4.17734 | 0.40844 | 1.39172 |
| C | -5.59673 | 0.37953 | -0.99423 |
| C | -5.24394 | -0.47060 | 1.18298 |
| C | -5.92904 | -0.55112 | -0.01291 |
| H | -6.18858 | 0.39880 | -1.89733 |
| H | -5.55527 | -1.09632 | 2.00791 |
| C | -3.74962 | 0.57751 | 2.86624 |
| C | -4.31583 | 2.31293 | -1.97865 |
| C | -7.04234 | -1.56078 | -0.26766 |
| C | -3.01623 | 2.08637 | -2.75386 |
| H | -2.12919 | 2.24301 | -2.13472 |
| H | -2.96140 | 1.07194 | -3.15189 |
| H | -2.95244 | 2.79745 | -3.58286 |
| C | -4.31191 | 3.71170 | -1.34623 |
| H | -5.25129 | 3.90188 | -0.82145 |
| H | -3.49456 | 3.84776 | -0.63511 |
| H | -4.19647 | 4.47092 | -2.12478 |
| C | -5.44677 | 2.30177 | -3.01035 |
| H | -5.47206 | 1.37341 | -3.58559 |
| H | -6.42568 | 2.45624 | -2.55052 |
| H | -5.28178 | 3.11749 | -3.71784 |
| C | -3.28953 | -0.74408 | 3.48833 |
| H | -2.38119 | -1.11549 | 3.00906 |
| H | -3.07347 | -0.59645 | 4.55004 |
| H | -4.04842 | -1.52428 | 3.41164 |
| C | -2.66551 | 1.61919 | 3.12394 |
| H | -1.67839 | 1.28138 | 2.81163 |
| H | -2.88845 | 2.57820 | 2.64378 |
| H | -2.60878 | 1.81290 | 4.19893 |
| C | -4.99914 | 1.07224 | 3.62053 |
| H | -5.34867 | 2.02370 | 3.21176 |
| H | -5.82398 | 0.36142 | 3.56482 |
| H | -4.75570 | 1.22259 | 4.67588 |
| C | -7.24988 | -2.50354 | 0.91445 |
| H | -7.56757 | -1.96906 | 1.81364 |
| H | -8.03220 | -3.22606 | 0.67052 |

| | | | |
|----|----------|----------|----------|
| H | -6.34237 | -3.06578 | 1.14829 |
| C | -6.67438 | -2.40295 | -1.49565 |
| H | -6.56311 | -1.78660 | -2.38982 |
| H | -5.73156 | -2.93212 | -1.34045 |
| H | -7.45690 | -3.14118 | -1.69196 |
| C | -8.35933 | -0.82213 | -0.53293 |
| H | -8.28827 | -0.16361 | -1.40092 |
| H | -9.16036 | -1.54107 | -0.72588 |
| H | -8.64815 | -0.21401 | 0.32805 |
| C | 2.04762 | 1.44876 | -0.18563 |
| C | 2.67348 | 1.14140 | -1.42656 |
| C | 2.81462 | 2.10394 | 0.82244 |
| C | 4.06296 | 1.09130 | -1.44272 |
| C | 4.19200 | 2.02123 | 0.72227 |
| C | 4.84469 | 1.40787 | -0.34358 |
| H | 4.54675 | 0.78921 | -2.36104 |
| H | 4.78793 | 2.46613 | 1.50944 |
| C | 1.97871 | 1.07085 | -2.80076 |
| C | 2.31013 | -0.19735 | -3.59004 |
| C | 2.53882 | 2.28334 | -3.57716 |
| H | 1.89577 | -1.08552 | -3.11482 |
| H | 1.88223 | -0.11966 | -4.59293 |
| H | 3.38586 | -0.34297 | -3.70162 |
| H | 2.33094 | 3.21780 | -3.04992 |
| H | 3.61605 | 2.21390 | -3.73081 |
| H | 2.05919 | 2.33136 | -4.55839 |
| C | 2.26572 | 3.07948 | 1.88301 |
| C | 2.85162 | 4.45514 | 1.49950 |
| C | 2.72148 | 2.74728 | 3.30574 |
| H | 2.56219 | 4.73476 | 0.48369 |
| H | 2.46601 | 5.21451 | 2.18527 |
| H | 3.94034 | 4.47082 | 1.55633 |
| H | 2.31363 | 1.79859 | 3.65229 |
| H | 3.80877 | 2.69377 | 3.38291 |
| H | 2.38273 | 3.53146 | 3.98805 |
| C | 6.35097 | 1.19849 | -0.30674 |
| C | 7.05802 | 2.55690 | -0.22605 |
| C | 6.85800 | 0.45552 | -1.53977 |
| H | 6.77335 | 3.11213 | 0.67033 |
| H | 8.14081 | 2.40968 | -0.19446 |
| H | 6.82459 | 3.17610 | -1.09607 |
| H | 6.37491 | -0.51845 | -1.64742 |
| H | 6.70439 | 1.02873 | -2.45817 |
| H | 7.93197 | 0.28250 | -1.44103 |
| Cl | -2.43315 | -1.56869 | -1.92584 |
| Cl | 0.98834 | -0.04854 | 2.24403 |
| Au | 2.74227 | -2.39295 | 0.08661 |
| Cl | 4.71939 | -3.30536 | 0.70201 |
| C | 0.75294 | 3.25834 | 1.85437 |
| H | 0.39468 | 3.48744 | 0.84828 |
| H | 0.21065 | 2.39507 | 2.23393 |
| H | 0.48141 | 4.10194 | 2.49394 |
| C | 0.46788 | 1.26985 | -2.76541 |
| H | -0.08123 | 0.41039 | -2.38330 |
| H | 0.19921 | 2.15463 | -2.18249 |
| H | 0.11152 | 1.43215 | -3.78570 |
| C | 6.69637 | 0.36358 | 0.93355 |
| H | 6.39292 | 0.86492 | 1.85527 |
| H | 6.20766 | -0.61318 | 0.90203 |
| H | 7.77707 | 0.20465 | 0.98110 |
| Ge | -1.64876 | -1.49925 | 0.17454 |
| S | 0.81337 | -1.43050 | -0.64329 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.40495 | 0.26580 | 0.51080 |
| C | 0.14573 | 0.12163 | -1.09943 |
| P | -1.33747 | 0.05230 | -1.99457 |
| Ge | 1.39965 | 0.36795 | -2.77792 |
| Cl | 1.28785 | -1.78964 | -3.36996 |
| Au | -0.91505 | 0.36172 | 2.26140 |
| Cl | -2.25557 | 0.46033 | 4.06902 |
| H | 1.80965 | 0.34850 | 0.63747 |
| H | -1.64780 | -1.29531 | -2.23667 |
| Cl | -3.00036 | 0.66029 | -1.04067 |
| S | -0.88658 | 1.06576 | -3.63239 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.47566 | 0.36556 | 0.49074 |
| C | 0.13926 | 0.20867 | -1.10405 |
| P | -1.40238 | 0.02837 | -1.88537 |
| Ge | 1.30337 | 0.39334 | -2.84065 |
| Cl | 1.50442 | -1.82535 | -3.17314 |
| C | -1.94753 | -1.67900 | -1.85727 |
| H | -2.14355 | -1.98082 | -0.82694 |
| H | -2.85447 | -1.76859 | -2.45702 |
| H | -1.14554 | -2.28098 | -2.29027 |
| C | 2.26229 | 0.47245 | 0.74373 |
| H | 2.59512 | -0.44301 | 1.24008 |
| H | 2.79529 | 0.59118 | -0.19981 |
| H | 2.47709 | 1.31046 | 1.40964 |
| Au | -0.88211 | 0.38945 | 2.22430 |
| Cl | -2.25799 | 0.37649 | 4.01486 |
| Cl | -2.91766 | 1.02427 | -0.98552 |
| S | -1.01524 | 0.72006 | -3.71134 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.66299 | -0.23996 | 0.47562 |
| C | 0.13912 | 0.32592 | -0.97850 |
| P | -1.50694 | 0.20511 | -1.57105 |
| Ge | 0.86609 | 1.72201 | -2.39008 |
| Cl | 1.73386 | 0.26717 | -3.87195 |
| C | -2.01622 | -1.46684 | -2.19053 |
| C | -3.42250 | -1.32701 | -2.77258 |
| C | -1.03173 | -1.87343 | -3.28516 |
| C | -2.00014 | -2.48635 | -1.05742 |
| H | -4.16094 | -1.08113 | -2.00826 |
| H | -3.46224 | -0.57097 | -3.55941 |
| H | -3.70192 | -2.28654 | -3.21581 |
| H | -0.01129 | -1.96319 | -2.91048 |
| H | -1.34110 | -2.84886 | -3.67080 |
| H | -1.02358 | -1.16432 | -4.11343 |
| H | -2.32538 | -3.44868 | -1.46267 |
| H | -0.99871 | -2.62712 | -0.64694 |
| H | -2.67579 | -2.22107 | -0.24337 |
| C | 2.47647 | -0.04779 | 0.78641 |
| C | 3.02599 | -1.47438 | 0.90611 |
| C | 3.20209 | 0.70955 | -0.31287 |
| C | 2.61938 | 0.67514 | 2.12863 |
| H | 2.50240 | -2.05146 | 1.67221 |
| H | 2.96063 | -2.01341 | -0.04171 |
| H | 4.08086 | -1.41842 | 1.19152 |
| H | 2.85569 | 1.74278 | -0.39296 |
| H | 4.26922 | 0.74481 | -0.07266 |
| H | 3.10129 | 0.22316 | -1.28550 |
| H | 3.67994 | 0.71723 | 2.39353 |
| H | 2.24214 | 1.69921 | 2.08013 |

| | | | |
|----|----------|----------|----------|
| H | 2.09315 | 0.15291 | 2.93113 |
| Cl | -2.86134 | 0.62065 | -0.11175 |
| Au | -0.51553 | -1.21128 | 2.07949 |
| Cl | -1.69333 | -2.21127 | 3.73470 |
| S | -1.55277 | 1.60530 | -2.99109 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.47361 | 0.56891 | 0.11707 |
| C | 0.34035 | 0.02702 | -1.42883 |
| P | -1.12657 | -0.28581 | -2.31223 |
| Ge | 1.69179 | -0.11914 | -3.01870 |
| Cl | 2.06893 | -2.34105 | -2.87864 |
| Au | -1.12110 | 1.19068 | 1.51404 |
| Cl | -2.76256 | 1.77794 | 2.95523 |
| Cl | -2.57534 | 1.07991 | -1.92968 |
| C | 2.17699 | 0.62716 | 0.63787 |
| C | 3.15623 | -0.20677 | 0.09002 |
| C | 2.51840 | 1.53943 | 1.63988 |
| C | 4.46606 | -0.10124 | 0.52422 |
| H | 2.88933 | -0.96574 | -0.63733 |
| C | 3.83230 | 1.64265 | 2.06126 |
| H | 1.75171 | 2.16787 | 2.08115 |
| C | 4.80531 | 0.82596 | 1.50102 |
| H | 5.22284 | -0.75350 | 0.10483 |
| H | 4.09670 | 2.35704 | 2.83174 |
| H | 5.83293 | 0.90303 | 1.83733 |
| C | -1.87515 | -1.85414 | -1.85431 |
| C | -1.61460 | -2.97954 | -2.63001 |
| C | -2.65041 | -1.95333 | -0.69896 |
| C | -2.13871 | -4.20536 | -2.25016 |
| H | -1.00226 | -2.89426 | -3.51920 |
| C | -3.16651 | -3.18231 | -0.32894 |
| H | -2.85865 | -1.07801 | -0.09431 |
| C | -2.91186 | -4.30666 | -1.10411 |
| H | -1.93868 | -5.08255 | -2.85380 |
| H | -3.77266 | -3.26042 | 0.56570 |
| H | -3.32094 | -5.26684 | -0.81120 |
| S | -0.51141 | -0.19511 | -4.20201 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.51993 | 0.55454 | 0.63997 |
| C | 0.42469 | -0.26154 | -0.78234 |
| P | -0.92456 | -0.48313 | -1.87126 |
| Ge | 2.01237 | -0.48879 | -2.11711 |
| Cl | 1.98381 | -2.74981 | -2.09680 |
| Au | -1.07702 | 1.25867 | 1.99161 |
| Cl | -2.68466 | 1.94991 | 3.42595 |
| C | 2.25371 | 0.80101 | 1.06269 |
| C | 2.99513 | -0.23066 | 1.65436 |
| C | 2.82204 | 2.06584 | 0.83664 |
| C | 4.31503 | 0.02585 | 2.00374 |
| C | 4.14420 | 2.26774 | 1.20070 |
| C | 4.90702 | 1.26294 | 1.78683 |
| H | 4.89587 | -0.76801 | 2.46313 |
| H | 4.59229 | 3.24041 | 1.02155 |
| C | -1.81704 | -2.05371 | -1.88786 |
| C | -1.71822 | -2.99198 | -0.84048 |
| C | -2.65392 | -2.31262 | -2.99615 |
| C | -2.42710 | -4.18051 | -0.95112 |
| C | -3.34051 | -3.51814 | -3.03873 |
| C | -3.23403 | -4.47305 | -2.03980 |
| H | -2.34734 | -4.90037 | -0.14299 |
| H | -3.98668 | -3.70989 | -3.88956 |
| C | 2.03867 | 3.17211 | 0.19768 |
| H | 1.77826 | 2.92956 | -0.83719 |
| H | 1.10200 | 3.36432 | 0.73090 |

| | | | |
|----|----------|----------|----------|
| H | 2.61211 | 4.09921 | 0.18814 |
| C | 2.40781 | -1.58624 | 1.90383 |
| H | 1.39274 | -1.52189 | 2.30733 |
| H | 2.35789 | -2.17025 | 0.97956 |
| H | 3.01442 | -2.14473 | 2.61740 |
| C | 6.32280 | 1.52249 | 2.19860 |
| H | 6.35437 | 2.06422 | 3.14892 |
| H | 6.87713 | 0.59233 | 2.32955 |
| H | 6.84489 | 2.13365 | 1.45972 |
| C | -0.90575 | -2.79607 | 0.40130 |
| H | 0.15471 | -2.69583 | 0.16726 |
| H | -1.21698 | -1.90904 | 0.95741 |
| H | -1.02768 | -3.65728 | 1.05825 |
| C | -2.86242 | -1.37615 | -4.15023 |
| H | -2.95636 | -0.33297 | -3.84802 |
| H | -2.03212 | -1.43518 | -4.85766 |
| H | -3.77598 | -1.64983 | -4.67918 |
| C | -3.95598 | -5.77944 | -2.13704 |
| H | -4.86024 | -5.69168 | -2.74121 |
| H | -3.31764 | -6.53354 | -2.60800 |
| H | -4.23259 | -6.15606 | -1.15088 |
| Cl | -2.38558 | 0.88783 | -1.47080 |
| S | 0.03726 | -0.05967 | -3.57882 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.10410 | 0.77572 | 0.12485 |
| C | -0.37231 | -0.68442 | 0.33634 |
| P | 1.29132 | -1.22826 | 0.46696 |
| Cl | -2.04971 | -2.69047 | -1.78087 |
| C | 2.91634 | -0.49582 | 0.06998 |
| C | 3.47690 | -0.90038 | -1.18065 |
| C | 3.79053 | -0.03560 | 1.09326 |
| C | 4.82740 | -1.20982 | -1.20069 |
| C | 5.13341 | -0.38659 | 0.98647 |
| C | 5.66150 | -1.06339 | -0.09973 |
| H | 5.25056 | -1.56582 | -2.13134 |
| H | 5.79353 | -0.09465 | 1.79075 |
| C | -2.89247 | 0.45982 | 0.16895 |
| C | -3.65887 | 0.41563 | -1.02636 |
| C | -3.44901 | -0.01066 | 1.38555 |
| C | -4.83849 | -0.31902 | -1.00086 |
| C | -4.61470 | -0.76406 | 1.30924 |
| C | -5.29649 | -0.98738 | 0.12461 |
| H | -5.40868 | -0.40135 | -1.91096 |
| H | -5.01190 | -1.18419 | 2.22431 |
| C | -3.31909 | 1.19830 | -2.30864 |
| C | -2.97106 | 0.33415 | 2.81312 |
| C | -6.51610 | -1.90173 | 0.10323 |
| C | 3.47795 | 0.99173 | 2.20370 |
| C | 2.79549 | -0.82793 | -2.56409 |
| C | 7.10544 | -1.54388 | -0.15861 |
| C | -4.17979 | 0.90566 | 3.57912 |
| H | -3.86157 | 1.20751 | 4.58021 |
| H | -4.58457 | 1.78455 | 3.07167 |
| H | -4.98743 | 0.18372 | 3.69746 |
| C | -1.90053 | 1.42023 | 2.88759 |
| H | -0.91523 | 1.07581 | 2.57142 |
| H | -2.17084 | 2.30666 | 2.30771 |
| H | -1.78742 | 1.73625 | 3.92820 |
| C | -2.46668 | -0.91138 | 3.54608 |
| H | -3.21976 | -1.70171 | 3.56248 |
| H | -1.56888 | -1.31465 | 3.07434 |
| H | -2.22021 | -0.66007 | 4.58165 |
| C | -7.58833 | -1.36153 | 1.05642 |
| H | -8.46238 | -2.01848 | 1.04756 |
| H | -7.22795 | -1.30384 | 2.08550 |

| | | | |
|----|----------|----------|----------|
| H | -7.91174 | -0.36159 | 0.75671 |
| C | -7.12755 | -2.02058 | -1.29022 |
| H | -7.97819 | -2.70531 | -1.25569 |
| H | -7.49531 | -1.05950 | -1.65890 |
| H | -6.41148 | -2.41811 | -2.01341 |
| C | -6.08394 | -3.30102 | 0.55937 |
| H | -5.31600 | -3.70672 | -0.10341 |
| H | -5.67841 | -3.28856 | 1.57326 |
| H | -6.94090 | -3.98022 | 0.54975 |
| C | -4.37037 | 0.99379 | -3.40386 |
| H | -5.36703 | 1.31023 | -3.08828 |
| H | -4.09312 | 1.60519 | -4.26526 |
| H | -4.41885 | -0.04468 | -3.74004 |
| C | -3.32436 | 2.69490 | -1.96840 |
| H | -4.30258 | 3.00016 | -1.58847 |
| H | -2.57763 | 2.95370 | -1.21452 |
| H | -3.10462 | 3.28425 | -2.86243 |
| C | -1.98144 | 0.79592 | -2.93184 |
| H | -1.12297 | 1.04276 | -2.30458 |
| H | -1.94791 | -0.27343 | -3.14199 |
| H | -1.83870 | 1.34604 | -3.86624 |
| C | 2.04532 | 1.50717 | 2.23390 |
| H | 1.71809 | 1.81022 | 1.23650 |
| H | 1.33428 | 0.79548 | 2.64370 |
| H | 2.00230 | 2.40070 | 2.86074 |
| C | 4.33823 | 2.22648 | 1.85174 |
| H | 4.15294 | 3.01140 | 2.58944 |
| H | 5.40583 | 2.00555 | 1.85475 |
| H | 4.07200 | 2.62135 | 0.86873 |
| C | 3.87985 | 0.50721 | 3.59952 |
| H | 4.93881 | 0.24880 | 3.65658 |
| H | 3.70013 | 1.30653 | 4.32319 |
| H | 3.30250 | -0.36397 | 3.90790 |
| C | 1.35274 | -0.33932 | -2.55337 |
| H | 1.05596 | -0.10875 | -3.57945 |
| H | 0.64624 | -1.08100 | -2.18488 |
| H | 1.25045 | 0.58317 | -1.97501 |
| C | 2.87287 | -2.14739 | -3.33553 |
| H | 2.29436 | -2.92844 | -2.84247 |
| H | 2.46321 | -2.00388 | -4.33878 |
| H | 3.90003 | -2.49979 | -3.44800 |
| C | 3.58747 | 0.24554 | -3.34198 |
| H | 3.55203 | 1.20847 | -2.82689 |
| H | 4.63425 | -0.02635 | -3.48131 |
| H | 3.13829 | 0.37348 | -4.33029 |
| C | 7.84840 | -1.30557 | 1.15318 |
| H | 7.94094 | -0.24122 | 1.38379 |
| H | 7.35493 | -1.79983 | 1.99373 |
| H | 8.85981 | -1.71134 | 1.07710 |
| C | 7.85043 | -0.80674 | -1.27807 |
| H | 7.40061 | -0.98927 | -2.25593 |
| H | 7.85226 | 0.27201 | -1.10428 |
| H | 8.88881 | -1.14626 | -1.32177 |
| C | 7.11000 | -3.04951 | -0.45025 |
| H | 6.59479 | -3.60287 | 0.33847 |
| H | 6.61689 | -3.27955 | -1.39672 |
| H | 8.13820 | -3.41655 | -0.50917 |
| Cl | 1.43221 | -1.65980 | 2.47905 |
| Au | -0.13343 | 2.74595 | -0.25101 |
| Cl | 0.88841 | 4.73695 | -0.63753 |
| Ge | -1.24633 | -2.63098 | 0.32575 |
| S | 1.12356 | -3.04083 | -0.35681 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.35501 | -0.10812 | 0.70139 |
| C | 0.12830 | 0.51893 | -0.89323 |
| P | -1.31906 | 0.48494 | -1.87039 |
| Ge | 1.39656 | 0.94751 | -2.54549 |
| Cl | 1.32299 | -1.15776 | -3.33347 |
| Au | 0.19914 | 2.23972 | 0.39055 |
| Cl | 0.24377 | 4.31826 | 1.23622 |
| H | 1.78351 | -0.14506 | 0.67229 |
| H | -1.51637 | -0.84028 | -2.28876 |
| Cl | -3.07584 | 0.84634 | -0.94252 |
| S | -0.88229 | 1.71475 | -3.35561 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.40701 | 0.06140 | 0.70115 |
| C | 0.07869 | 0.67299 | -0.87985 |
| P | -1.41701 | 0.51518 | -1.77788 |
| Ge | 1.28100 | 1.14367 | -2.56053 |
| Cl | 1.60410 | -1.00565 | -3.18852 |
| C | -1.79956 | -1.21367 | -2.06624 |
| H | -2.01772 | -1.70199 | -1.11502 |
| H | -2.66542 | -1.27219 | -2.72708 |
| H | -0.92855 | -1.66723 | -2.54433 |
| C | 2.23020 | -0.12584 | 0.72153 |
| H | 2.44585 | -1.16209 | 0.44041 |
| H | 2.75232 | 0.53995 | 0.03399 |
| H | 2.59321 | 0.03231 | 1.73871 |
| Au | 0.13505 | 2.40838 | 0.39145 |
| Cl | 0.16524 | 4.46779 | 1.29367 |
| Cl | -3.07759 | 1.19150 | -0.82092 |
| S | -1.02456 | 1.53165 | -3.44177 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.54041 | 0.09381 | 0.52283 |
| C | 0.04197 | 0.74293 | -1.00389 |
| P | -1.54613 | 0.41190 | -1.71783 |
| Ge | 0.90843 | 1.69259 | -2.69872 |
| Cl | 1.87311 | -0.10878 | -3.66427 |
| Au | -0.03902 | 2.39742 | 0.40189 |
| Cl | -0.14982 | 4.36105 | 1.49858 |
| C | -1.98399 | -1.38200 | -1.91222 |
| C | -3.26204 | -1.44820 | -2.74843 |
| C | -0.84130 | -2.07141 | -2.65362 |
| C | -2.20504 | -2.03226 | -0.54948 |
| H | -4.10680 | -0.97357 | -2.24660 |
| H | -3.12862 | -0.98556 | -3.72786 |
| H | -3.51081 | -2.50151 | -2.90394 |
| H | 0.08886 | -2.05983 | -2.08401 |
| H | -1.12545 | -3.11478 | -2.81701 |
| H | -0.64506 | -1.61433 | -3.62374 |
| H | -2.41956 | -3.09233 | -0.71187 |
| H | -1.32247 | -1.96666 | 0.08985 |
| H | -3.04970 | -1.59505 | -0.01667 |
| C | 2.40515 | 0.07132 | 0.62389 |
| C | 2.78098 | -1.33807 | 0.14896 |
| C | 3.15897 | 1.11812 | -0.17783 |
| C | 2.71716 | 0.21990 | 2.11499 |
| H | 2.23507 | -2.11552 | 0.69229 |
| H | 2.59837 | -1.46042 | -0.92112 |
| H | 3.84802 | -1.50184 | 0.33066 |
| H | 2.85843 | 2.13427 | 0.08685 |
| H | 4.23062 | 1.02584 | 0.02949 |
| H | 3.03687 | 0.97487 | -1.25344 |
| H | 3.78748 | 0.06251 | 2.27798 |

| | | | |
|----|----------|----------|----------|
| H | 2.46408 | 1.21788 | 2.48134 |
| H | 2.17563 | -0.51203 | 2.72059 |
| Cl | -3.07892 | 1.13091 | -0.57625 |
| S | -1.45263 | 1.39045 | -3.45147 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.27494 | 0.58089 | 0.51121 |
| C | 0.13287 | 0.69275 | -1.20807 |
| P | -1.35332 | 0.47072 | -2.11201 |
| Ge | 1.39966 | 0.84224 | -2.91313 |
| Cl | 1.62370 | -1.35577 | -3.39486 |
| Au | 0.30239 | 2.73943 | -0.50611 |
| Cl | 0.51238 | 4.96699 | -0.25411 |
| C | -1.86086 | -1.25367 | -2.12669 |
| C | -2.25519 | -1.86073 | -0.93463 |
| C | -1.84909 | -1.97430 | -3.31458 |
| C | -2.63569 | -3.19018 | -0.93858 |
| H | -2.27214 | -1.29669 | -0.00830 |
| C | -2.23762 | -3.30541 | -3.30957 |
| H | -1.52794 | -1.49626 | -4.23158 |
| C | -2.62800 | -3.91158 | -2.12633 |
| H | -2.94188 | -3.66487 | -0.01392 |
| H | -2.22795 | -3.86922 | -4.23467 |
| H | -2.92812 | -4.95320 | -2.12583 |
| C | 2.03058 | 0.29715 | 0.84597 |
| C | 2.87154 | -0.44548 | 0.01567 |
| C | 2.52054 | 0.79054 | 2.05859 |
| C | 4.19015 | -0.66141 | 0.38260 |
| H | 2.49224 | -0.88279 | -0.90117 |
| C | 3.84279 | 0.58512 | 2.41153 |
| H | 1.86571 | 1.35111 | 2.71852 |
| C | 4.67858 | -0.13995 | 1.57246 |
| H | 4.83735 | -1.24159 | -0.26487 |
| H | 4.22160 | 0.98686 | 3.34402 |
| H | 5.71242 | -0.30703 | 1.85230 |
| Cl | -2.95695 | 1.41341 | -1.28369 |
| S | -0.88372 | 1.20321 | -3.89858 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.24666 | 0.48768 | 1.07895 |
| C | -0.09571 | 0.68983 | -0.60987 |
| P | -1.52610 | 0.50805 | -1.62663 |
| Ge | 1.24927 | 1.30286 | -2.14127 |
| Cl | 1.63717 | -0.66675 | -3.19212 |
| Au | -0.23823 | 2.67441 | 0.27251 |
| Cl | -0.47039 | 4.87692 | 0.72310 |
| C | -1.86147 | -1.21994 | -2.05906 |
| C | -2.14087 | -2.11585 | -1.00100 |
| C | -1.83047 | -1.69853 | -3.39097 |
| C | -2.26811 | -3.46954 | -1.28188 |
| C | -1.98257 | -3.06382 | -3.59863 |
| C | -2.17139 | -3.97183 | -2.56867 |
| H | -2.46913 | -4.14806 | -0.45870 |
| H | -1.95249 | -3.42705 | -4.62067 |
| C | 2.06413 | 0.31454 | 1.12372 |
| C | 2.58661 | -0.91704 | 0.68171 |
| C | 2.90423 | 1.25841 | 1.73653 |
| C | 3.95476 | -1.13042 | 0.76894 |
| C | 4.26769 | 0.99547 | 1.79451 |
| C | 4.81728 | -0.17812 | 1.29758 |
| H | 4.35512 | -2.07996 | 0.42651 |
| H | 4.91826 | 1.73174 | 2.25703 |
| C | 2.39173 | 2.53090 | 2.33873 |
| H | 2.22147 | 3.30324 | 1.58289 |
| H | 1.44378 | 2.38615 | 2.86384 |
| H | 3.11162 | 2.92828 | 3.05571 |

| | | | |
|----|----------|----------|----------|
| C | 1.70695 | -2.02285 | 0.17617 |
| H | 0.84378 | -2.18290 | 0.83110 |
| H | 1.32825 | -1.81936 | -0.82786 |
| H | 2.26481 | -2.95913 | 0.13476 |
| C | 6.29472 | -0.41602 | 1.33676 |
| H | 6.76924 | 0.15030 | 2.13979 |
| H | 6.52501 | -1.47379 | 1.47693 |
| H | 6.75858 | -0.10359 | 0.39588 |
| C | -2.41314 | -1.71299 | 0.41777 |
| H | -2.20968 | -2.54884 | 1.08833 |
| H | -1.83530 | -0.86176 | 0.77134 |
| H | -3.46729 | -1.44481 | 0.53110 |
| C | -1.68319 | -0.86067 | -4.62654 |
| H | -2.39316 | -0.03435 | -4.65396 |
| H | -0.68247 | -0.43626 | -4.70959 |
| H | -1.85945 | -1.48664 | -5.50180 |
| C | -2.27049 | -5.43908 | -2.84062 |
| H | -2.75185 | -5.63440 | -3.80043 |
| H | -1.27256 | -5.88691 | -2.87976 |
| H | -2.83169 | -5.95389 | -2.05937 |
| Cl | -3.28361 | 1.16263 | -0.79778 |
| S | -1.01861 | 1.80198 | -3.06373 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.67710 | 0.17138 | 1.07823 |
| C | 0.40520 | 0.14580 | -0.64979 |
| P | -1.12049 | -0.08069 | -1.59917 |
| Cl | 2.82145 | -1.08469 | -3.04991 |
| Au | 0.37785 | 2.26707 | -0.09613 |
| Cl | 0.19374 | 4.52900 | -0.03306 |
| C | 2.51722 | 0.04287 | 1.20675 |
| C | 3.19299 | -1.12698 | 0.76007 |
| C | 3.29640 | 1.15863 | 1.60442 |
| C | 4.51795 | -1.00611 | 0.37209 |
| C | 4.61876 | 1.21248 | 1.16039 |
| C | 5.22986 | 0.18419 | 0.46612 |
| H | 5.02278 | -1.88483 | -0.00749 |
| H | 5.19295 | 2.09773 | 1.39442 |
| C | 2.91961 | 2.23319 | 2.64697 |
| C | 2.67371 | -2.56842 | 0.93151 |
| C | 6.64004 | 0.28445 | -0.10282 |
| C | 3.86710 | 1.98902 | 3.84046 |
| H | 3.72943 | 0.98544 | 4.25137 |
| H | 4.91572 | 2.09657 | 3.56140 |
| H | 3.65125 | 2.71421 | 4.62981 |
| C | 3.14733 | 3.65574 | 2.12932 |
| H | 2.50481 | 3.88753 | 1.27967 |
| H | 2.91775 | 4.37320 | 2.92189 |
| H | 4.18345 | 3.82194 | 1.82991 |
| C | 1.50994 | 2.13948 | 3.22347 |
| H | 1.43733 | 2.81628 | 4.07908 |
| H | 0.73482 | 2.45028 | 2.52137 |
| H | 1.27958 | 1.13372 | 3.58454 |
| C | 2.98382 | -3.45863 | -0.27433 |
| H | 2.56450 | -3.04861 | -1.19152 |
| H | 4.05623 | -3.58711 | -0.42763 |
| H | 2.56324 | -4.45448 | -0.10895 |
| C | 3.42640 | -3.12544 | 2.15530 |
| H | 4.50587 | -3.11708 | 1.99645 |
| H | 3.21361 | -2.53464 | 3.04994 |
| H | 3.11574 | -4.15758 | 2.34352 |
| C | 1.18914 | -2.69915 | 1.24766 |
| H | 0.90058 | -2.11916 | 2.13067 |
| H | 0.55684 | -2.41256 | 0.40841 |
| H | 0.96513 | -3.74495 | 1.47696 |
| C | 7.25911 | 1.66058 | 0.12593 |

| | | | |
|----|----------|----------|----------|
| H | 6.65774 | 2.45456 | -0.32353 |
| H | 7.38420 | 1.88178 | 1.18925 |
| H | 8.24954 | 1.69498 | -0.33415 |
| C | 6.57678 | 0.02717 | -1.61320 |
| H | 7.58075 | 0.07506 | -2.04449 |
| H | 6.15552 | -0.95390 | -1.84006 |
| H | 5.95381 | 0.77302 | -2.11202 |
| C | 7.54425 | -0.76500 | 0.55419 |
| H | 7.59861 | -0.61473 | 1.63543 |
| H | 7.18851 | -1.78104 | 0.37223 |
| H | 8.55734 | -0.69208 | 0.14911 |
| C | -2.35368 | -1.46487 | -1.67172 |
| C | -2.32877 | -2.30514 | -2.82637 |
| C | -3.58230 | -1.34479 | -0.96571 |
| C | -3.53899 | -2.57090 | -3.44792 |
| C | -1.13193 | -3.14531 | -3.31012 |
| C | -4.75253 | -1.67995 | -1.63881 |
| C | -3.74757 | -1.07490 | 0.54149 |
| C | -4.76739 | -2.18280 | -2.92958 |
| H | -3.51559 | -3.14376 | -4.36665 |
| C | -0.70394 | -2.85502 | -4.74997 |
| C | -1.59831 | -4.61649 | -3.24870 |
| C | 0.05393 | -3.06351 | -2.36449 |
| H | -5.68981 | -1.53778 | -1.11964 |
| C | -2.45267 | -0.75577 | 1.26864 |
| C | -4.24794 | -2.41253 | 1.12670 |
| C | -4.78110 | 0.00785 | 0.86235 |
| C | -6.04762 | -2.41052 | -3.72143 |
| H | 0.01982 | -3.60880 | -5.07069 |
| H | -1.55418 | -2.89752 | -5.43483 |
| H | -0.23639 | -1.87756 | -4.84423 |
| H | -2.36626 | -4.84658 | -3.98793 |
| H | -0.74105 | -5.26466 | -3.44917 |
| H | -1.99091 | -4.86717 | -2.26031 |
| H | 0.49887 | -2.07281 | -2.30802 |
| H | -0.23350 | -3.39106 | -1.36298 |
| H | 0.84616 | -3.72626 | -2.71867 |
| H | -1.67561 | -1.48900 | 1.04202 |
| H | -2.07899 | 0.24282 | 1.05017 |
| H | -2.62210 | -0.79021 | 2.34757 |
| H | -4.35959 | -2.31284 | 2.20986 |
| H | -5.21249 | -2.70728 | 0.71164 |
| H | -3.53505 | -3.21700 | 0.92984 |
| H | -5.76519 | -0.22219 | 0.45099 |
| H | -4.89287 | 0.08764 | 1.94681 |
| H | -4.47370 | 0.98227 | 0.48387 |
| C | -7.28240 | -1.90274 | -2.98183 |
| C | -6.22883 | -3.90835 | -3.99572 |
| C | -5.93789 | -1.65942 | -5.05400 |
| H | -7.45571 | -2.44923 | -2.05120 |
| H | -7.20497 | -0.83805 | -2.74815 |
| H | -8.16544 | -2.04131 | -3.60985 |
| H | -5.40166 | -4.31894 | -4.57797 |
| H | -6.29712 | -4.47284 | -3.06255 |
| H | -7.14888 | -4.07537 | -4.56230 |
| H | -5.81949 | -0.58580 | -4.88997 |
| H | -5.08527 | -2.00359 | -5.64270 |
| H | -6.84210 | -1.81645 | -5.64823 |
| Ge | 1.72078 | 0.72972 | -2.25028 |
| Cl | -2.43847 | 1.46280 | -1.22391 |
| S | -0.41809 | 0.33249 | -3.42710 |

[R-P=C(Ge(II)Cl)-P(S)MeR](AuCl)

Coordination through Ge(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.40301 | 0.90251 | 0.24315 |
| C | 0.03379 | 0.50646 | -1.32529 |
| P | -1.55421 | 0.08076 | -1.96107 |
| Ge | 0.96087 | 0.74887 | -3.09381 |
| Cl | 1.43375 | -1.33601 | -3.55485 |
| C | -2.97853 | 0.67566 | -1.04442 |
| H | -2.93766 | 1.76399 | -0.99189 |
| H | -3.89208 | 0.36644 | -1.55564 |
| H | -2.96277 | 0.25251 | -0.03721 |
| Au | 2.38080 | 2.51766 | -3.63886 |
| Cl | 3.76394 | 4.26812 | -4.07860 |
| H | 1.76108 | 1.28521 | 0.02005 |
| H | -1.69073 | -1.32220 | -1.95541 |
| S | -1.36547 | 0.81169 | -3.82225 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.43164 | 0.57740 | 0.28206 |
| C | 0.03861 | 0.35603 | -1.31429 |
| P | -1.57794 | 0.00019 | -1.92069 |
| Ge | 0.92512 | 0.67508 | -3.08507 |
| Cl | 1.53113 | -1.36991 | -3.61434 |
| C | -2.91467 | 0.81354 | -1.03229 |
| H | -2.74653 | 1.89024 | -1.04828 |
| H | -3.86608 | 0.58550 | -1.51675 |
| H | -2.93634 | 0.45929 | 0.00081 |
| C | -1.91656 | -1.76668 | -1.87452 |
| H | -1.98075 | -2.10244 | -0.83709 |
| H | -2.85486 | -1.97312 | -2.39296 |
| H | -1.09848 | -2.28118 | -2.38055 |
| C | 2.21645 | 0.97372 | 0.26801 |
| H | 2.77684 | 0.03989 | 0.37896 |
| H | 2.53375 | 1.47036 | -0.65148 |
| H | 2.44858 | 1.60462 | 1.12775 |
| Au | 2.30656 | 2.49380 | -3.58540 |
| Cl | 3.66306 | 4.28652 | -3.95176 |
| S | -1.36285 | 0.68353 | -3.81347 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.42465 | 0.44757 | 0.09617 |
| C | 0.23946 | 0.15700 | -1.52973 |
| P | -1.36582 | -0.18372 | -2.21209 |
| Ge | 1.23646 | 0.40300 | -3.26111 |
| Cl | 2.18235 | -1.54261 | -3.61484 |
| C | -2.59269 | 1.02108 | -1.66349 |
| H | -2.22634 | 2.01104 | -1.93616 |
| H | -3.54777 | 0.84320 | -2.15933 |
| H | -2.71613 | 0.96525 | -0.58084 |
| Au | 2.34671 | 2.38296 | -3.84069 |
| Cl | 3.40080 | 4.35415 | -4.29834 |
| C | 2.19270 | 0.90401 | 0.46978 |
| C | 3.23388 | 0.27254 | -0.44071 |
| C | 2.25137 | 2.43400 | 0.38995 |
| C | 2.41583 | 0.45423 | 1.91681 |
| H | 3.12311 | -0.81120 | -0.51176 |
| H | 3.20522 | 0.69136 | -1.44887 |
| H | 4.23273 | 0.48409 | -0.04496 |
| H | 1.48987 | 2.90827 | 1.01653 |
| H | 3.22847 | 2.77291 | 0.74935 |
| H | 2.12987 | 2.79045 | -0.63531 |
| H | 3.39946 | 0.79449 | 2.25358 |
| H | 1.66636 | 0.87195 | 2.59457 |

| | | | |
|---|----------|----------|----------|
| H | 2.38911 | -0.63468 | 2.01141 |
| C | -2.02141 | -1.87485 | -1.84584 |
| C | -3.24636 | -2.10866 | -2.73003 |
| C | -0.93738 | -2.89715 | -2.17591 |
| C | -2.40063 | -1.96028 | -0.36838 |
| H | -4.06459 | -1.42243 | -2.50070 |
| H | -3.00090 | -2.02064 | -3.79045 |
| H | -3.61271 | -3.12405 | -2.55548 |
| H | -0.05131 | -2.76731 | -1.55272 |
| H | -1.33748 | -3.89886 | -1.99622 |
| H | -0.62568 | -2.83618 | -3.21964 |
| H | -2.71131 | -2.98539 | -0.14811 |
| H | -1.55943 | -1.72262 | 0.28725 |
| H | -3.23483 | -1.30311 | -0.11494 |
| S | -0.94156 | 0.06228 | -4.18150 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.47888 | 0.57550 | 0.14639 |
| C | 0.09452 | 0.26922 | -1.44347 |
| P | -1.55477 | -0.04073 | -1.98829 |
| Ge | 0.93634 | 0.55176 | -3.23993 |
| Cl | 1.55427 | -1.48375 | -3.80180 |
| C | -2.80184 | 0.92108 | -1.11334 |
| H | -2.55151 | 1.97819 | -1.20441 |
| H | -3.77855 | 0.72908 | -1.56060 |
| H | -2.82258 | 0.63818 | -0.05924 |
| Au | 2.26679 | 2.37473 | -3.85518 |
| Cl | 3.58357 | 4.16027 | -4.38580 |
| C | 2.25154 | 0.86528 | 0.19107 |
| C | 2.70693 | 1.71527 | 1.20405 |
| C | 3.17446 | 0.29378 | -0.69011 |
| C | 4.05145 | 2.03023 | 1.30083 |
| H | 1.99834 | 2.14307 | 1.90656 |
| C | 4.51855 | 0.60157 | -0.58082 |
| H | 2.84837 | -0.41758 | -1.44092 |
| C | 4.95553 | 1.47667 | 0.40548 |
| H | 4.39508 | 2.70676 | 2.07442 |
| H | 5.22819 | 0.16135 | -1.27104 |
| H | 6.00858 | 1.72226 | 0.47957 |
| C | -2.02620 | -1.77215 | -1.80560 |
| C | -2.16557 | -2.59171 | -2.91937 |
| C | -2.22852 | -2.28980 | -0.52582 |
| C | -2.52151 | -3.92208 | -2.75402 |
| H | -1.98611 | -2.18799 | -3.90886 |
| C | -2.58157 | -3.61834 | -0.36851 |
| H | -2.09663 | -1.66562 | 0.35207 |
| C | -2.73089 | -4.43375 | -1.48328 |
| H | -2.62852 | -4.55999 | -3.62328 |
| H | -2.73644 | -4.02030 | 0.62582 |
| H | -3.00561 | -5.47465 | -1.35714 |
| S | -1.37354 | 0.52275 | -3.92059 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.53451 | 0.56808 | 0.50897 |
| C | 0.31042 | -0.02134 | -1.03365 |
| P | -1.28154 | -0.28507 | -1.77927 |
| Ge | 1.41450 | 0.20152 | -2.68185 |
| Cl | 1.82325 | -1.90029 | -3.21317 |
| C | -2.53233 | 0.68780 | -0.90893 |
| H | -2.25615 | 1.74139 | -0.95392 |
| H | -3.52188 | 0.53660 | -1.33707 |
| H | -2.54449 | 0.35811 | 0.13314 |
| Au | 3.06568 | 1.81379 | -3.07717 |
| Cl | 4.69505 | 3.40088 | -3.34177 |
| C | 2.28511 | 1.04711 | 0.54024 |
| C | 2.58115 | 2.42049 | 0.54295 |

| | | | |
|---|----------|----------|----------|
| C | 3.31414 | 0.09696 | 0.60027 |
| C | 3.90821 | 2.81796 | 0.54732 |
| C | 4.62867 | 0.54569 | 0.61168 |
| C | 4.94852 | 1.89636 | 0.56035 |
| H | 4.13801 | 3.87796 | 0.50598 |
| H | 5.42927 | -0.18696 | 0.65134 |
| C | -1.96166 | -1.96517 | -1.90067 |
| C | -3.02543 | -2.16723 | -2.80623 |
| C | -1.50236 | -3.03727 | -1.10919 |
| C | -3.60217 | -3.42821 | -2.89049 |
| C | -2.11661 | -4.27527 | -1.24674 |
| C | -3.16291 | -4.49906 | -2.12888 |
| H | -4.42288 | -3.57291 | -3.58624 |
| H | -1.75829 | -5.09565 | -0.63308 |
| C | -3.56664 | -1.12174 | -3.73935 |
| H | -3.61875 | -0.11986 | -3.31385 |
| H | -2.94234 | -1.04633 | -4.63327 |
| H | -4.57389 | -1.39601 | -4.05509 |
| C | -0.38175 | -2.93795 | -0.11978 |
| H | 0.54844 | -2.63424 | -0.60154 |
| H | -0.59111 | -2.21646 | 0.67280 |
| H | -0.21866 | -3.90854 | 0.34893 |
| C | -3.77719 | -5.85588 | -2.27062 |
| H | -3.21376 | -6.45678 | -2.99117 |
| H | -3.77276 | -6.39622 | -1.32241 |
| H | -4.80574 | -5.79318 | -2.62903 |
| C | 3.03895 | -1.37729 | 0.64600 |
| H | 2.17882 | -1.61370 | 1.27904 |
| H | 2.83112 | -1.77778 | -0.35100 |
| H | 3.90176 | -1.91558 | 1.04079 |
| C | 1.49631 | 3.45265 | 0.46531 |
| H | 1.12183 | 3.54697 | -0.55904 |
| H | 0.64355 | 3.20227 | 1.10605 |
| H | 1.86786 | 4.43174 | 0.76970 |
| C | 6.36901 | 2.35578 | 0.47725 |
| H | 6.59251 | 2.66995 | -0.54710 |
| H | 6.55003 | 3.21379 | 1.12840 |
| H | 7.06537 | 1.56111 | 0.74855 |
| S | -0.77095 | 0.49359 | -3.59592 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.22934 | 1.82487 | 1.18770 |
| C | 0.22279 | 0.47305 | 0.31926 |
| P | 1.82346 | -0.30819 | 0.17758 |
| Cl | -1.26759 | 0.57189 | -2.69150 |
| C | 3.52768 | 0.37237 | 0.20894 |
| C | 4.17345 | 0.61620 | -1.03835 |
| C | 4.34236 | 0.13377 | 1.34929 |
| C | 5.49041 | 0.19942 | -1.16921 |
| C | 5.65926 | -0.26137 | 1.13545 |
| C | 6.22961 | -0.34159 | -0.12533 |
| H | 5.96556 | 0.32386 | -2.13428 |
| H | 6.26425 | -0.49880 | 1.99957 |
| C | -2.05010 | 1.83947 | 0.97126 |
| C | -2.64147 | 2.72825 | 0.04448 |
| C | -2.85454 | 0.88411 | 1.64518 |
| C | -3.92803 | 2.43693 | -0.40013 |
| C | -4.12338 | 0.64507 | 1.13453 |
| C | -4.65641 | 1.35244 | 0.06440 |
| H | -4.37340 | 3.07431 | -1.14706 |
| H | -4.72834 | -0.12327 | 1.59477 |
| C | -1.98354 | 4.05291 | -0.38956 |
| C | -2.47353 | 0.21364 | 2.98598 |
| C | -6.01313 | 0.95886 | -0.50884 |
| C | 3.98274 | 0.47640 | 2.81113 |
| C | 3.63181 | 1.49033 | -2.18730 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 7.62895 | -0.88942 | -0.37356 | H | 8.15799 | 0.62036 | -1.86808 |
| C | -3.73962 | -0.09037 | 3.80120 | H | 8.60669 | 1.05184 | -0.21447 |
| H | -3.44521 | -0.40452 | 4.80554 | H | 9.53717 | -0.16603 | -1.09957 |
| H | -4.38394 | 0.78695 | 3.89390 | C | 7.53665 | -2.02264 | -1.40274 |
| H | -4.32278 | -0.90721 | 3.37351 | H | 6.91075 | -2.83838 | -1.03311 |
| C | -1.64065 | 1.16697 | 3.84687 | H | 7.11226 | -1.67740 | -2.34749 |
| H | -0.64520 | 1.36596 | 3.43064 | H | 8.53244 | -2.42401 | -1.60874 |
| H | -2.14112 | 2.12897 | 3.98017 | Ge | -0.73984 | -0.72115 | -0.99629 |
| H | -1.47485 | 0.72322 | 4.83229 | Au | -2.23623 | -2.45952 | -0.50204 |
| C | -1.72182 | -1.10894 | 2.82356 | Cl | -3.73144 | -4.09929 | 0.07373 |
| H | -2.29996 | -1.82494 | 2.23585 | S | 1.49085 | -1.28144 | -1.59073 |
| H | -0.76059 | -0.96754 | 2.33191 | C | 1.83236 | -1.69945 | 1.34572 |
| H | -1.53977 | -1.54974 | 3.80861 | H | 1.84333 | -1.40815 | 2.39070 |
| C | -7.08210 | 1.02017 | 0.58855 | H | 0.92493 | -2.27010 | 1.13917 |
| H | -8.05504 | 0.73738 | 0.17742 | H | 2.69795 | -2.32264 | 1.11704 |
| H | -6.86146 | 0.33752 | 1.41122 | | | | |
| H | -7.16651 | 2.02972 | 0.99950 | | | | |
| C | -6.44675 | 1.87585 | -1.64952 | | | | |
| H | -7.40806 | 1.53576 | -2.04180 | | | | |
| H | -6.57407 | 2.91042 | -1.31895 | | | | |
| H | -5.73033 | 1.86131 | -2.47459 | | | | |
| C | -5.91853 | -0.47341 | -1.04939 | | | | |
| H | -5.17159 | -0.54228 | -1.84371 | | | | |
| H | -5.63896 | -1.19042 | -0.27526 | | | | |
| H | -6.88349 | -0.78298 | -1.46067 | | | | |
| C | -2.91505 | 4.89270 | -1.26662 | | | | |
| H | -3.85927 | 5.11931 | -0.76665 | | | | |
| H | -2.42393 | 5.84277 | -1.48970 | | | | |
| H | -3.13279 | 4.40483 | -2.21953 | | | | |
| C | -1.69098 | 4.87756 | 0.87277 | | | | |
| H | -2.60588 | 5.05216 | 1.44395 | | | | |
| H | -0.97330 | 4.38194 | 1.53081 | | | | |
| H | -1.26965 | 5.84830 | 0.59600 | | | | |
| C | -0.68989 | 3.86676 | -1.18160 | | | | |
| H | 0.10483 | 3.41580 | -0.58123 | | | | |
| H | -0.84102 | 3.23477 | -2.05677 | | | | |
| H | -0.31745 | 4.84213 | -1.50895 | | | | |
| C | 2.61009 | 1.11454 | 2.99144 | | | | |
| H | 2.48303 | 1.97334 | 2.32969 | | | | |
| H | 1.76994 | 0.44116 | 2.83360 | | | | |
| H | 2.51783 | 1.47907 | 4.01744 | | | | |
| C | 4.98500 | 1.57380 | 3.23107 | | | | |
| H | 4.74980 | 1.90714 | 4.24540 | | | | |
| H | 6.01577 | 1.21938 | 3.22518 | | | | |
| H | 4.91968 | 2.43729 | 2.56526 | | | | |
| C | 4.15713 | -0.70398 | 3.77156 | | | | |
| H | 5.17431 | -1.09876 | 3.74225 | | | | |
| H | 3.96390 | -0.37410 | 4.79557 | | | | |
| H | 3.47986 | -1.53001 | 3.55489 | | | | |
| C | 2.26173 | 2.09897 | -1.92048 | | | | |
| H | 2.06073 | 2.86348 | -2.67478 | | | | |
| H | 1.44904 | 1.37932 | -1.98606 | | | | |
| H | 2.23197 | 2.58747 | -0.94350 | | | | |
| C | 3.62693 | 0.77468 | -3.53983 | | | | |
| H | 2.91983 | -0.05363 | -3.54979 | | | | |
| H | 3.33391 | 1.48018 | -4.32166 | | | | |
| H | 4.61439 | 0.38750 | -3.79997 | | | | |
| C | 4.60511 | 2.68582 | -2.27524 | | | | |
| H | 4.65282 | 3.22438 | -1.32546 | | | | |
| H | 5.61795 | 2.38365 | -2.54368 | | | | |
| H | 4.24795 | 3.37915 | -3.04110 | | | | |
| C | 8.26663 | -1.44386 | 0.89746 | | | | |
| H | 8.42452 | -0.66643 | 1.64945 | | | | |
| H | 7.66091 | -2.23750 | 1.34211 | | | | |
| H | 9.24432 | -1.86852 | 0.65876 | | | | |
| C | 8.53088 | 0.22275 | -0.92224 | | | | |

| Coordination through S atom | | | | | | | |
|------------------------------------|----------|----------|----------|--|--|--|--|
| R= H | | | | | | | |
| P | 0.53048 | 0.29204 | 0.66447 | | | | |
| C | 0.32219 | 0.31560 | -0.98108 | | | | |
| P | -1.17988 | 0.63163 | -1.82089 | | | | |
| Ge | 1.64395 | 0.35904 | -2.58722 | | | | |
| Cl | 0.94469 | -1.58491 | -3.42000 | | | | |
| C | -2.57101 | 1.32231 | -0.92136 | | | | |
| H | -2.28125 | 2.27535 | -0.47830 | | | | |
| H | -3.39665 | 1.47588 | -1.61957 | | | | |
| H | -2.87642 | 0.62431 | -0.13816 | | | | |
| Au | -1.90789 | 1.42868 | -5.01356 | | | | |
| Cl | -3.40531 | 1.09029 | -6.66138 | | | | |
| H | -1.63290 | -0.58277 | -2.35987 | | | | |
| H | 1.94817 | 0.08967 | 0.67930 | | | | |
| S | -0.44939 | 1.82150 | -3.30783 | | | | |

| R = Me | | | | | | | |
|---------------|----------|----------|----------|--|--|--|--|
| P | 0.51695 | 0.21422 | 0.63591 | | | | |
| C | 0.30736 | 0.35554 | -1.00325 | | | | |
| P | -1.26055 | 0.56368 | -1.75489 | | | | |
| Ge | 1.59378 | 0.66325 | -2.60671 | | | | |
| Cl | 1.41868 | -1.39640 | -3.45746 | | | | |
| C | -2.51007 | 1.42371 | -0.78619 | | | | |
| H | -2.12591 | 2.39798 | -0.48476 | | | | |
| H | -3.40419 | 1.55630 | -1.39913 | | | | |
| H | -2.75665 | 0.83511 | 0.10050 | | | | |
| C | -1.96328 | -1.01686 | -2.23499 | | | | |
| H | -2.19499 | -1.58241 | -1.32891 | | | | |
| H | -2.86775 | -0.84950 | -2.82272 | | | | |
| H | -1.22827 | -1.55691 | -2.83258 | | | | |
| C | 2.32609 | 0.00073 | 0.85278 | | | | |
| H | 2.53901 | -1.07053 | 0.92308 | | | | |
| H | 2.90886 | 0.42044 | 0.03076 | | | | |
| H | 2.63319 | 0.45969 | 1.79458 | | | | |
| Au | -1.99513 | 1.06592 | -5.11027 | | | | |
| Cl | -3.37293 | 0.49923 | -6.80224 | | | | |
| S | -0.66502 | 1.68633 | -3.36847 | | | | |

| R = t-Bu | | | | | | | |
|-----------------|----------|----------|----------|--|--|--|--|
| P | 0.65973 | -0.24848 | 0.47361 | | | | |
| C | 0.19729 | 0.47478 | -0.95169 | | | | |
| P | -1.50630 | 0.38108 | -1.42214 | | | | |
| Ge | 0.98242 | 1.84618 | -2.32243 | | | | |
| Cl | 1.66483 | 0.37100 | -3.85817 | | | | |
| Au | -2.46963 | 1.40005 | -4.79533 | | | | |
| Cl | -3.41336 | 0.96734 | -6.79875 | | | | |
| C | -2.05101 | -1.27626 | -2.06302 | | | | |

| | | | |
|---|----------|----------|----------|
| C | -3.51029 | -1.18634 | -2.50845 |
| C | -1.15916 | -1.70050 | -3.22440 |
| C | -1.92475 | -2.28411 | -0.91887 |
| H | -4.18660 | -0.96962 | -1.67909 |
| H | -3.65850 | -0.44228 | -3.29473 |
| H | -3.79840 | -2.15624 | -2.92247 |
| H | -0.10973 | -1.76309 | -2.93409 |
| H | -1.48417 | -2.68870 | -3.56123 |
| H | -1.23633 | -1.01703 | -4.07158 |
| H | -2.22388 | -3.26269 | -1.30428 |
| H | -0.90068 | -2.37171 | -0.55224 |
| H | -2.57863 | -2.05091 | -0.07630 |
| C | 2.50038 | -0.06405 | 0.72940 |
| C | 3.05098 | -1.49113 | 0.62504 |
| C | 3.22097 | 0.85013 | -0.24316 |
| C | 2.66521 | 0.44239 | 2.16519 |
| H | 2.53321 | -2.18010 | 1.29849 |
| H | 2.96950 | -1.87905 | -0.39306 |
| H | 4.11029 | -1.49098 | 0.90239 |
| H | 2.84923 | 1.87649 | -0.18954 |
| H | 4.28868 | 0.88124 | 0.00065 |
| H | 3.14031 | 0.49122 | -1.27284 |
| H | 3.72600 | 0.43704 | 2.43487 |
| H | 2.29620 | 1.46506 | 2.27755 |
| H | 2.13589 | -0.19013 | 2.88309 |
| S | -1.55091 | 1.93718 | -2.78057 |
| C | -2.61332 | 0.83130 | -0.06645 |
| H | -2.52870 | 0.10869 | 0.74659 |
| H | -2.31125 | 1.81462 | 0.29419 |
| H | -3.64251 | 0.88146 | -0.42326 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.42790 | 0.78655 | 0.36118 |
| C | 0.40889 | 0.28157 | -1.22508 |
| P | -1.03938 | 0.34346 | -2.20474 |
| Ge | 1.91607 | 0.08074 | -2.63930 |
| Cl | 1.79049 | -2.13455 | -2.93489 |
| C | -2.25901 | 1.58608 | -1.73922 |
| H | -1.78083 | 2.56563 | -1.72736 |
| H | -3.06959 | 1.58608 | -2.47016 |
| H | -2.66042 | 1.35001 | -0.75156 |
| Au | -1.30446 | -0.09414 | -5.70267 |
| Cl | -2.49942 | -0.96692 | -7.40909 |
| C | -1.89854 | -1.23433 | -2.22290 |
| C | -1.42728 | -2.29717 | -1.45847 |
| C | -3.05060 | -1.38322 | -2.99587 |
| C | -2.11233 | -3.50229 | -1.46318 |
| H | -0.52249 | -2.18648 | -0.87533 |
| C | -3.72459 | -2.59089 | -2.99887 |
| H | -3.41187 | -0.57315 | -3.61960 |
| C | -3.25654 | -3.64927 | -2.23125 |
| H | -1.74046 | -4.33146 | -0.87318 |
| H | -4.60834 | -2.70846 | -3.61406 |
| H | -3.78376 | -4.59628 | -2.24082 |
| C | 2.13300 | 0.53259 | 0.89797 |
| C | 2.61493 | 1.38896 | 1.89211 |
| C | 2.97012 | -0.47043 | 0.39858 |
| C | 3.91992 | 1.27788 | 2.34200 |
| H | 1.96340 | 2.15342 | 2.30428 |
| C | 4.27142 | -0.58513 | 0.85879 |
| H | 2.58997 | -1.19296 | -0.31697 |
| C | 4.74908 | 0.29307 | 1.82254 |
| H | 4.29002 | 1.95554 | 3.10255 |
| H | 4.91224 | -1.36755 | 0.46924 |
| H | 5.76813 | 0.20023 | 2.18025 |
| S | -0.15715 | 0.87091 | -3.99063 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.21167 | 0.53470 | 0.49646 |
| C | 0.11491 | 0.06811 | -1.09549 |
| P | -1.28700 | 0.02368 | -2.15867 |
| Ge | 1.72697 | 0.07540 | -2.38366 |
| Cl | 1.69030 | -2.14007 | -2.85079 |
| C | -2.64857 | 1.14446 | -1.76367 |
| H | -2.23510 | 2.13469 | -1.56737 |
| H | -3.30204 | 1.19315 | -2.63726 |
| H | -3.21553 | 0.79509 | -0.90332 |
| Au | -0.00183 | 2.92807 | -3.20475 |
| Cl | 0.40097 | 5.06879 | -2.59947 |
| C | -1.99457 | -1.64968 | -2.32970 |
| C | -2.58113 | -2.19764 | -1.16754 |
| C | -1.99072 | -2.40786 | -3.52454 |
| C | -3.11286 | -3.48116 | -1.21358 |
| C | -2.55092 | -3.67828 | -3.50297 |
| C | -3.10629 | -4.24504 | -2.36572 |
| H | -3.54967 | -3.88781 | -0.30653 |
| H | -2.54286 | -4.25154 | -4.42435 |
| C | 2.01248 | 0.52242 | 0.79659 |
| C | 2.69172 | 1.74950 | 0.86277 |
| C | 2.68504 | -0.68300 | 1.05524 |
| C | 4.05071 | 1.74394 | 1.14644 |
| C | 4.04469 | -0.63497 | 1.33655 |
| C | 4.74715 | 0.56356 | 1.37596 |
| H | 4.57881 | 2.69188 | 1.19141 |
| H | 4.56846 | -1.56421 | 1.54073 |
| C | 1.98142 | 3.04429 | 0.60978 |
| H | 1.78639 | 3.20382 | -0.45529 |
| H | 1.01087 | 3.08003 | 1.11658 |
| H | 2.57151 | 3.89120 | 0.96163 |
| C | 1.97326 | -2.00403 | 1.05210 |
| H | 1.04218 | -1.95988 | 1.62599 |
| H | 1.71222 | -2.31996 | 0.03820 |
| H | 2.60145 | -2.77900 | 1.49316 |
| C | 6.22013 | 0.58205 | 1.64602 |
| H | 6.78377 | 0.54085 | 0.70866 |
| H | 6.51862 | 1.49450 | 2.16532 |
| H | 6.52618 | -0.27430 | 2.24938 |
| C | -2.72909 | -1.48975 | 0.14961 |
| H | -1.98503 | -0.71946 | 0.34013 |
| H | -3.71839 | -1.02759 | 0.22731 |
| H | -2.65245 | -2.21061 | 0.96495 |
| C | -1.42928 | -1.96519 | -4.84316 |
| H | -1.87608 | -1.03621 | -5.19821 |
| H | -0.34965 | -1.81794 | -4.78895 |
| H | -1.62187 | -2.73413 | -5.59143 |
| C | -3.65681 | -5.63573 | -2.38689 |
| H | -4.30762 | -5.82151 | -1.53155 |
| H | -4.22456 | -5.82323 | -3.30054 |
| H | -2.84553 | -6.36920 | -2.35357 |
| S | -0.36422 | 0.75778 | -3.86615 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -1.99909 | 1.86324 | 0.37895 |
| C | -1.05993 | 0.49325 | 0.26419 |
| P | 0.70144 | 0.36263 | 0.36902 |
| C | -3.70665 | 1.16953 | 0.36470 |
| C | -4.49038 | 1.28214 | -0.81390 |
| C | -4.19690 | 0.41759 | 1.45652 |
| C | -5.56789 | 0.42182 | -0.95781 |
| C | -5.27575 | -0.43699 | 1.22536 |
| C | -5.93341 | -0.50654 | 0.01064 |
| H | -6.14537 | 0.46122 | -1.86964 |

| | | | |
|---|----------|----------|----------|
| H | -5.62050 | -1.05932 | 2.03730 |
| C | -3.71745 | 0.56214 | 2.91951 |
| C | -4.25660 | 2.36445 | -1.88551 |
| C | -7.05715 | -1.49833 | -0.26945 |
| C | -2.94996 | 2.16733 | -2.65443 |
| H | -2.07121 | 2.28949 | -2.01794 |
| H | -2.89494 | 1.17307 | -3.09962 |
| H | -2.87419 | 2.91665 | -3.44815 |
| C | -4.25783 | 3.74222 | -1.20779 |
| H | -5.20006 | 3.91503 | -0.68196 |
| H | -3.44428 | 3.85330 | -0.48788 |
| H | -4.13834 | 4.52650 | -1.96058 |
| C | -5.37771 | 2.38693 | -2.92767 |
| H | -5.40177 | 1.47425 | -3.52761 |
| H | -6.36053 | 2.53432 | -2.47384 |
| H | -5.20137 | 3.22026 | -3.61161 |
| C | -2.66342 | -0.47945 | 3.30162 |
| H | -1.73501 | -0.32494 | 2.75335 |
| H | -2.44162 | -0.41121 | 4.37102 |
| H | -3.01495 | -1.49220 | 3.09286 |
| C | -3.17717 | 1.96460 | 3.20343 |
| H | -2.24619 | 2.18667 | 2.67107 |
| H | -3.90477 | 2.73426 | 2.93568 |
| H | -2.95087 | 2.06213 | 4.26872 |
| C | -4.90717 | 0.38022 | 3.87732 |
| H | -5.75010 | 1.01632 | 3.59817 |
| H | -5.25660 | -0.65211 | 3.92440 |
| H | -4.59361 | 0.65385 | 4.88769 |
| C | -7.30135 | -2.44338 | 0.90391 |
| H | -7.62881 | -1.90833 | 1.79923 |
| H | -8.08875 | -3.15382 | 0.64120 |
| H | -6.40645 | -3.01923 | 1.15287 |
| C | -6.67934 | -2.34050 | -1.49433 |
| H | -6.53739 | -1.72137 | -2.38216 |
| H | -5.74996 | -2.88810 | -1.32244 |
| H | -7.47060 | -3.06351 | -1.71154 |
| C | -8.35827 | -0.73968 | -0.55587 |
| H | -8.26118 | -0.07889 | -1.41960 |
| H | -9.16640 | -1.44574 | -0.76647 |
| H | -8.65361 | -0.13061 | 0.30224 |
| C | 2.08557 | 1.48157 | -0.05491 |
| C | 2.71244 | 1.30580 | -1.32275 |
| C | 2.85305 | 2.04127 | 1.00227 |
| C | 4.09840 | 1.28881 | -1.35282 |
| C | 4.23793 | 1.98998 | 0.89359 |
| C | 4.88965 | 1.50837 | -0.23218 |
| H | 4.58255 | 1.09538 | -2.30176 |
| H | 4.82758 | 2.35293 | 1.72440 |
| C | 2.00755 | 1.34281 | -2.69250 |
| C | 2.36171 | 0.15541 | -3.59063 |
| C | 2.52700 | 2.63107 | -3.36664 |
| H | 1.99273 | -0.78287 | -3.17856 |
| H | 1.90429 | 0.29723 | -4.57332 |
| H | 3.43877 | 0.06132 | -3.74079 |
| H | 2.29803 | 3.51121 | -2.76048 |
| H | 3.60458 | 2.60625 | -3.53262 |
| H | 2.03808 | 2.74936 | -4.33733 |
| C | 2.29851 | 2.88664 | 2.16738 |
| C | 2.90897 | 4.29218 | 1.98025 |
| C | 2.72465 | 2.37500 | 3.54658 |
| H | 2.65786 | 4.69930 | 0.99822 |
| H | 2.50576 | 4.96495 | 2.74209 |
| H | 3.99469 | 4.28786 | 2.07690 |
| H | 2.31410 | 1.39259 | 3.77818 |
| H | 3.81055 | 2.30316 | 3.62913 |
| H | 2.38212 | 3.07056 | 4.31729 |

| | | | |
|----|----------|----------|----------|
| C | 6.39683 | 1.30920 | -0.30166 |
| C | 6.99871 | 2.28170 | -1.32321 |
| C | 6.67974 | -0.13379 | -0.73954 |
| H | 6.80936 | 3.32011 | -1.03912 |
| H | 8.08075 | 2.13689 | -1.38190 |
| H | 6.58900 | 2.12513 | -2.32316 |
| H | 6.25222 | -0.85722 | -0.04145 |
| H | 6.26527 | -0.34479 | -1.72737 |
| H | 7.75911 | -0.30082 | -0.78879 |
| Cl | -2.34693 | -1.45288 | -2.06868 |
| Au | 2.67634 | -2.49329 | 0.05883 |
| Cl | 4.52856 | -3.54639 | 0.82201 |
| C | 0.78981 | 3.10436 | 2.12002 |
| H | 0.47599 | 3.50023 | 1.15212 |
| H | 0.19774 | 2.21421 | 2.32343 |
| H | 0.51031 | 3.83763 | 2.88062 |
| C | 0.49417 | 1.49728 | -2.62180 |
| H | -0.02490 | 0.59432 | -2.30348 |
| H | 0.21298 | 2.32195 | -1.96207 |
| H | 0.11688 | 1.73347 | -3.61974 |
| C | 7.07090 | 1.54417 | 1.04742 |
| H | 6.96695 | 2.57889 | 1.38539 |
| H | 6.66913 | 0.88272 | 1.81882 |
| H | 8.13976 | 1.33727 | 0.95934 |
| Ge | -1.56134 | -1.53346 | 0.02806 |
| S | 0.87753 | -1.36586 | -0.76895 |
| C | 1.03500 | -0.25109 | 2.04657 |
| H | 2.09633 | -0.48452 | 2.13560 |
| H | 0.72638 | 0.44828 | 2.81824 |
| H | 0.46548 | -1.17595 | 2.15381 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.46370 | 0.28087 | 0.46656 |
| C | 0.20187 | 0.15525 | -1.14340 |
| P | -1.31374 | 0.20301 | -2.02218 |
| Ge | 1.48288 | 0.27385 | -2.80796 |
| Cl | 1.19473 | -1.89368 | -3.32034 |
| C | -2.73110 | 0.94877 | -1.21023 |
| H | -2.49982 | 1.98338 | -0.95562 |
| H | -3.57778 | 0.92385 | -1.89979 |
| H | -2.97892 | 0.39037 | -0.30441 |
| Au | -0.90253 | 0.44803 | 2.18593 |
| Cl | -2.34596 | 0.62392 | 3.91094 |
| H | 1.86818 | 0.28826 | 0.62150 |
| H | -1.68961 | -1.13642 | -2.23961 |
| S | -0.73083 | 1.10583 | -3.70506 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.50492 | 0.35272 | 0.43452 |
| C | 0.17466 | 0.23970 | -1.16264 |
| P | -1.40000 | 0.08397 | -1.92511 |
| Ge | 1.35047 | 0.38183 | -2.88996 |
| Cl | 1.57884 | -1.85502 | -3.09784 |
| C | -2.70015 | 1.10350 | -1.21096 |
| H | -2.38354 | 2.14634 | -1.22217 |
| H | -3.60181 | 0.99410 | -1.81769 |
| H | -2.90716 | 0.79055 | -0.18490 |
| C | -1.95466 | -1.62332 | -1.81330 |
| H | -2.15825 | -1.87734 | -0.77051 |
| H | -2.85961 | -1.74498 | -2.41194 |
| H | -1.16301 | -2.26148 | -2.20841 |
| C | 2.28681 | 0.46292 | 0.72161 |
| H | 2.61650 | -0.45426 | 1.21622 |

| | | | |
|----|----------|---------|----------|
| H | 2.82979 | 0.58857 | -0.21548 |
| H | 2.49073 | 1.29903 | 1.39329 |
| Au | -0.90904 | 0.33785 | 2.13290 |
| Cl | -2.40817 | 0.30852 | 3.82605 |
| S | -0.95057 | 0.62597 | -3.80732 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.51129 | 0.42466 | 0.30127 |
| C | 0.29935 | 0.12630 | -1.30088 |
| P | -1.27538 | -0.11810 | -2.07489 |
| Ge | 1.47345 | 0.39252 | -3.03603 |
| Cl | 2.23824 | -1.72106 | -3.22833 |
| C | -2.49893 | 1.10509 | -1.55773 |
| H | -2.05969 | 2.09302 | -1.69768 |
| H | -3.38250 | 1.01841 | -2.19161 |
| H | -2.77396 | 0.97577 | -0.50952 |
| Au | -1.06124 | 0.65698 | 1.85474 |
| Cl | -2.69865 | 0.92254 | 3.40064 |
| C | 2.26472 | 0.60537 | 0.86561 |
| C | 2.36185 | 1.95322 | 1.58484 |
| C | 2.49826 | -0.53270 | 1.86566 |
| C | 3.26975 | 0.52724 | -0.27122 |
| H | 2.20938 | 2.79002 | 0.89930 |
| H | 1.63441 | 2.03649 | 2.39595 |
| H | 3.36132 | 2.04943 | 2.01918 |
| H | 2.45762 | -1.51050 | 1.38047 |
| H | 3.49343 | -0.41396 | 2.30486 |
| H | 1.76943 | -0.51763 | 2.67984 |
| H | 4.27971 | 0.59999 | 0.14425 |
| H | 3.20489 | -0.41720 | -0.81552 |
| H | 3.15044 | 1.35184 | -0.97800 |
| C | -1.99993 | -1.80325 | -1.79129 |
| C | -0.98904 | -2.85632 | -2.23336 |
| C | -2.35001 | -1.99803 | -0.31934 |
| C | -3.26077 | -1.89837 | -2.65303 |
| H | -0.71897 | -2.74497 | -3.28405 |
| H | -0.06956 | -2.81303 | -1.64801 |
| H | -1.43699 | -3.84447 | -2.09496 |
| H | -3.07746 | -1.27164 | 0.04763 |
| H | -2.79229 | -2.99140 | -0.20007 |
| H | -1.46749 | -1.95618 | 0.32128 |
| H | -3.64768 | -2.91867 | -2.58395 |
| H | -4.04996 | -1.22556 | -2.31125 |
| H | -3.04981 | -1.69286 | -3.70482 |
| S | -0.79302 | 0.15657 | -4.01298 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.48849 | 0.48543 | 0.20189 |
| C | 0.31778 | 0.06438 | -1.37497 |
| P | -1.21220 | -0.19317 | -2.20910 |
| Ge | 1.60868 | 0.02358 | -3.01580 |
| Cl | 2.06901 | -2.19142 | -2.94139 |
| C | -2.46222 | 1.05651 | -1.86039 |
| H | -2.04686 | 2.03193 | -2.11474 |
| H | -3.33366 | 0.85511 | -2.48645 |
| H | -2.75288 | 1.04913 | -0.80839 |
| Au | -1.11781 | 0.94560 | 1.65849 |
| Cl | -2.82869 | 1.37886 | 3.07869 |
| C | 2.19899 | 0.57851 | 0.69828 |
| C | 3.19944 | -0.16478 | 0.06617 |
| C | 2.52337 | 1.42091 | 1.76441 |
| C | 4.51291 | -0.03756 | 0.48387 |
| H | 2.94857 | -0.87138 | -0.71747 |
| C | 3.84057 | 1.54639 | 2.16969 |
| H | 1.74097 | 1.97828 | 2.26922 |
| C | 4.83458 | 0.82074 | 1.52717 |

| | | | |
|---|----------|----------|----------|
| H | 5.28697 | -0.61975 | -0.00194 |
| H | 4.09135 | 2.20674 | 2.99131 |
| H | 5.86513 | 0.91470 | 1.85004 |
| C | -1.92427 | -1.79109 | -1.77179 |
| C | -2.70557 | -1.91889 | -0.62270 |
| C | -1.65607 | -2.90519 | -2.56105 |
| C | -3.22069 | -3.15633 | -0.27562 |
| H | -2.91194 | -1.06486 | 0.01276 |
| C | -2.17501 | -4.14024 | -2.20566 |
| H | -1.03893 | -2.80029 | -3.44537 |
| C | -2.95680 | -4.26587 | -1.06728 |
| H | -3.82870 | -3.25182 | 0.61620 |
| H | -1.96422 | -5.00670 | -2.82124 |
| H | -3.36192 | -5.23312 | -0.79259 |
| S | -0.61390 | -0.10493 | -4.12559 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.52009 | 0.53305 | 0.64793 |
| C | 0.40454 | -0.24155 | -0.79442 |
| P | -0.99509 | -0.43515 | -1.85670 |
| Ge | 1.97635 | -0.43169 | -2.14756 |
| Cl | 1.94746 | -2.69934 | -2.12797 |
| C | -2.27483 | 0.78024 | -1.46826 |
| H | -1.84290 | 1.78020 | -1.51426 |
| H | -3.10340 | 0.70100 | -2.17116 |
| H | -2.64868 | 0.58774 | -0.45937 |
| Au | -1.07989 | 1.19059 | 2.03155 |
| Cl | -2.73150 | 1.84097 | 3.43902 |
| C | 2.25380 | 0.80117 | 1.06139 |
| C | 3.01254 | -0.23464 | 1.62323 |
| C | 2.80627 | 2.07693 | 0.86014 |
| C | 4.33238 | 0.02952 | 1.96811 |
| C | 4.12829 | 2.28707 | 1.21957 |
| C | 4.90781 | 1.27816 | 1.77609 |
| H | 4.92657 | -0.76820 | 2.40304 |
| H | 4.56349 | 3.26890 | 1.05937 |
| C | -1.84865 | -2.04215 | -1.87802 |
| C | -1.76275 | -2.97194 | -0.82215 |
| C | -2.67524 | -2.32002 | -2.98813 |
| C | -2.48747 | -4.15291 | -0.91245 |
| C | -3.38034 | -3.51740 | -3.01380 |
| C | -3.29733 | -4.45351 | -1.99669 |
| H | -2.41517 | -4.86158 | -0.09356 |
| H | -4.01690 | -3.71939 | -3.86970 |
| C | 2.00731 | 3.18784 | 0.24927 |
| H | 1.75484 | 2.96701 | -0.79245 |
| H | 1.06676 | 3.35153 | 0.78515 |
| H | 2.56668 | 4.12347 | 0.26547 |
| C | 2.44474 | -1.60348 | 1.84383 |
| H | 1.43808 | -1.56183 | 2.27080 |
| H | 2.37970 | -2.15923 | 0.90318 |
| H | 3.07264 | -2.17654 | 2.52678 |
| C | 6.32444 | 1.54514 | 2.18042 |
| H | 6.35888 | 2.09734 | 3.12454 |
| H | 6.88140 | 0.61762 | 2.31833 |
| H | 6.84239 | 2.14948 | 1.43282 |
| C | -0.93417 | -2.77663 | 0.40969 |
| H | 0.12288 | -2.67986 | 0.15915 |
| H | -1.23112 | -1.88800 | 0.97154 |
| H | -1.04942 | -3.63612 | 1.07030 |
| C | -2.84046 | -1.43003 | -4.18750 |
| H | -2.88655 | -0.36666 | -3.95502 |
| H | -2.00625 | -1.55798 | -4.88116 |
| H | -3.76062 | -1.69188 | -4.71142 |
| C | -4.03897 | -5.75088 | -2.07117 |
| H | -4.90430 | -5.67881 | -2.73167 |

| | | | |
|---|----------|----------|----------|
| H | -3.39016 | -6.54074 | -2.46218 |
| H | -4.38180 | -6.07017 | -1.08526 |
| S | -0.01253 | -0.01548 | -3.57672 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.08895 | 0.76522 | 0.08690 |
| C | -0.32615 | -0.64996 | 0.43387 |
| P | 1.35210 | -1.14820 | 0.71706 |
| Cl | -1.90963 | -2.91871 | -1.50395 |
| C | 2.97605 | -0.48954 | 0.16082 |
| C | 3.52686 | -1.04757 | -1.03045 |
| C | 3.86928 | 0.07586 | 1.11251 |
| C | 4.87651 | -1.36759 | -1.02579 |
| C | 5.20758 | -0.30224 | 1.04837 |
| C | 5.72212 | -1.10423 | 0.04333 |
| H | 5.28698 | -1.83773 | -1.91047 |
| H | 5.87505 | 0.07245 | 1.81176 |
| C | -2.87546 | 0.42237 | 0.13426 |
| C | -3.61489 | 0.23249 | -1.06373 |
| C | -3.45600 | 0.08792 | 1.38376 |
| C | -4.78593 | -0.51184 | -0.98117 |
| C | -4.61335 | -0.68267 | 1.36860 |
| C | -5.26382 | -1.05143 | 0.20340 |
| H | -5.33281 | -0.70712 | -1.88835 |
| H | -5.02764 | -1.00170 | 2.31633 |
| C | -3.26050 | 0.87679 | -2.41769 |
| C | -3.01456 | 0.58652 | 2.77826 |
| C | -6.47188 | -1.97963 | 0.26142 |
| C | 3.56116 | 1.22507 | 2.09703 |
| C | 2.82955 | -1.15241 | -2.40170 |
| C | 7.16216 | -1.60041 | 0.02778 |
| C | -4.24263 | 1.23181 | 3.44925 |
| H | -3.95341 | 1.63007 | 4.42521 |
| H | -4.62710 | 2.05750 | 2.84583 |
| H | -5.05757 | 0.52720 | 3.61220 |
| C | -1.94614 | 1.67782 | 2.77426 |
| H | -0.95170 | 1.30566 | 2.52704 |
| H | -2.19337 | 2.49617 | 2.09333 |
| H | -1.87247 | 2.10343 | 3.77878 |
| C | -2.52924 | -0.57473 | 3.64927 |
| H | -3.28778 | -1.35389 | 3.74502 |
| H | -1.63526 | -1.03602 | 3.22546 |
| H | -2.28701 | -0.21446 | 4.65329 |
| C | -7.57232 | -1.34863 | 1.12213 |
| H | -8.43860 | -2.01418 | 1.17001 |
| H | -7.23663 | -1.16795 | 2.14535 |
| H | -7.89959 | -0.39424 | 0.70222 |
| C | -7.04932 | -2.26702 | -1.12196 |
| H | -7.89239 | -2.95550 | -1.02723 |
| H | -7.41961 | -1.36014 | -1.60704 |
| H | -6.31180 | -2.73456 | -1.77865 |
| C | -6.03441 | -3.31079 | 0.88531 |
| H | -5.24719 | -3.77947 | 0.29020 |
| H | -5.65131 | -3.17539 | 1.89896 |
| H | -6.88311 | -3.99854 | 0.93661 |
| C | -4.27179 | 0.51482 | -3.50981 |
| H | -5.28607 | 0.83501 | -3.26121 |
| H | -3.98519 | 1.03074 | -4.42868 |
| H | -4.28130 | -0.55676 | -3.72328 |
| C | -3.32191 | 2.40097 | -2.24675 |
| H | -4.31888 | 2.71374 | -1.92625 |
| H | -2.60344 | 2.76533 | -1.50909 |
| H | -3.09630 | 2.89456 | -3.19575 |
| C | -1.89226 | 0.45773 | -2.95740 |
| H | -1.06142 | 0.82514 | -2.35262 |
| H | -1.80721 | -0.62706 | -3.02512 |

| | | | |
|----|----------|----------|----------|
| H | -1.75087 | 0.88764 | -3.95309 |
| C | 2.17806 | 1.83939 | 1.91730 |
| H | 2.06436 | 2.22770 | 0.90357 |
| H | 1.34368 | 1.16960 | 2.11010 |
| H | 2.06458 | 2.68582 | 2.59868 |
| C | 4.53247 | 2.37018 | 1.73276 |
| H | 4.28303 | 3.25165 | 2.32909 |
| H | 5.57357 | 2.11660 | 1.93319 |
| H | 4.44089 | 2.64078 | 0.67907 |
| C | 3.82287 | 0.85688 | 3.56124 |
| H | 4.84207 | 0.49078 | 3.70150 |
| H | 3.70454 | 1.74576 | 4.18644 |
| H | 3.14499 | 0.09284 | 3.93909 |
| C | 1.38492 | -0.67392 | -2.42581 |
| H | 1.06327 | -0.58589 | -3.46638 |
| H | 0.69636 | -1.36627 | -1.94438 |
| H | 1.28636 | 0.31570 | -1.97189 |
| C | 2.90092 | -2.55946 | -3.00023 |
| H | 2.33872 | -3.27233 | -2.39760 |
| H | 2.46820 | -2.54666 | -4.00404 |
| H | 3.92823 | -2.91813 | -3.09089 |
| C | 3.60556 | -0.18539 | -3.32123 |
| H | 3.57413 | 0.83539 | -2.93258 |
| H | 4.65153 | -0.47069 | -3.44042 |
| H | 3.14178 | -0.18527 | -4.31114 |
| C | 7.91743 | -1.22409 | 1.29958 |
| H | 8.01858 | -0.14146 | 1.41046 |
| H | 7.42782 | -1.61891 | 2.19344 |
| H | 8.92566 | -1.64301 | 1.26174 |
| C | 7.90297 | -0.99661 | -1.17140 |
| H | 7.44119 | -1.27961 | -2.11927 |
| H | 7.91541 | 0.09457 | -1.11577 |
| H | 8.93803 | -1.34865 | -1.18759 |
| C | 7.15580 | -3.12887 | -0.09610 |
| H | 6.64406 | -3.58876 | 0.75274 |
| H | 6.65304 | -3.45858 | -1.00732 |
| H | 8.18117 | -3.50755 | -0.12222 |
| Au | -0.18965 | 2.74069 | -0.41920 |
| Cl | 0.75032 | 4.74833 | -0.92422 |
| Ge | -1.17409 | -2.59744 | 0.60361 |
| S | 1.20050 | -3.07789 | 0.10774 |
| C | 1.44691 | -1.34512 | 2.52415 |
| H | 0.64420 | -2.03959 | 2.77874 |
| H | 2.39958 | -1.81974 | 2.76162 |
| H | 1.32241 | -0.42978 | 3.09361 |

Coordination through $\pi(C=P)$ bond

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.37679 | -0.07447 | 0.68499 |
| C | 0.21246 | 0.55587 | -0.91295 |
| P | -1.25666 | 0.62144 | -1.89331 |
| Ge | 1.54949 | 0.84041 | -2.52697 |
| Cl | 1.33378 | -1.30380 | -3.19227 |
| C | -2.77743 | 1.19493 | -1.12210 |
| H | -2.65762 | 2.23081 | -0.80316 |
| H | -3.58698 | 1.12949 | -1.85231 |
| H | -3.01010 | 0.56423 | -0.26070 |
| Au | 0.34147 | 2.28250 | 0.37300 |
| Cl | 0.41231 | 4.39704 | 1.13555 |
| H | 1.80271 | -0.18061 | 0.69889 |
| H | -1.53126 | -0.71336 | -2.24777 |
| S | -0.64309 | 1.70001 | -3.45441 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.45301 | 0.02967 | 0.63598 |
| C | 0.16700 | 0.68727 | -0.93119 |
| P | -1.34971 | 0.56725 | -1.84106 |
| Ge | 1.42769 | 1.09208 | -2.57482 |
| Cl | 1.74727 | -1.10482 | -3.05059 |
| C | -2.79466 | 1.34774 | -1.09742 |
| H | -2.61037 | 2.41445 | -0.96983 |
| H | -3.64992 | 1.20637 | -1.76227 |
| H | -3.00604 | 0.89162 | -0.12761 |
| C | -1.76896 | -1.17300 | -2.03310 |
| H | -2.03168 | -1.60156 | -1.06323 |
| H | -2.61161 | -1.26138 | -2.72144 |
| H | -0.90106 | -1.68713 | -2.44877 |
| C | 2.27471 | -0.15836 | 0.71443 |
| H | 2.50076 | -1.18400 | 0.40453 |
| H | 2.81703 | 0.52954 | 0.06521 |
| H | 2.60441 | -0.03274 | 1.74735 |
| Au | 0.19369 | 2.39223 | 0.39085 |
| Cl | 0.13641 | 4.46872 | 1.26329 |
| S | -0.82666 | 1.41691 | -3.58217 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.58789 | 0.05346 | 0.41309 |
| C | 0.10983 | 0.74679 | -1.09681 |
| P | -1.50456 | 0.44289 | -1.81725 |
| Ge | 1.02403 | 1.63711 | -2.79284 |
| Cl | 2.02046 | -0.22159 | -3.62655 |
| C | -2.85577 | 1.25314 | -0.92831 |
| H | -2.68680 | 2.32979 | -0.95048 |
| H | -3.79906 | 1.03596 | -1.43300 |
| H | -2.90151 | 0.91259 | 0.10688 |
| Au | 0.00613 | 2.36509 | 0.35554 |
| Cl | -0.22095 | 4.34693 | 1.40888 |
| C | -1.95463 | -1.35703 | -1.92151 |
| C | -3.13162 | -1.48069 | -2.89094 |
| C | -0.76712 | -2.14592 | -2.46312 |
| C | -2.35720 | -1.87596 | -0.54148 |
| H | -4.02015 | -0.94893 | -2.54320 |
| H | -2.87366 | -1.11558 | -3.88628 |
| H | -3.39647 | -2.53835 | -2.97562 |
| H | 0.08314 | -2.13024 | -1.77974 |
| H | -1.07335 | -3.18760 | -2.59534 |
| H | -0.42751 | -1.76267 | -3.42612 |
| H | -2.55165 | -2.94953 | -0.61979 |
| H | -1.56808 | -1.73747 | 0.20101 |
| H | -3.26987 | -1.40457 | -0.17193 |
| C | 2.44928 | 0.04719 | 0.57620 |
| C | 2.85935 | -1.35331 | 0.10412 |
| C | 3.21587 | 1.11075 | -0.19091 |
| C | 2.71000 | 0.18621 | 2.07805 |
| H | 2.30661 | -2.14077 | 0.62583 |
| H | 2.71158 | -1.47064 | -0.97170 |
| H | 3.92226 | -1.50415 | 0.31886 |
| H | 2.89641 | 2.12083 | 0.07547 |
| H | 4.28170 | 1.02751 | 0.04837 |
| H | 3.12651 | 0.97932 | -1.27083 |
| H | 3.77602 | 0.03803 | 2.27491 |
| H | 2.43511 | 1.17839 | 2.44479 |
| H | 2.15658 | -0.55658 | 2.65933 |
| S | -1.27396 | 1.26416 | -3.64113 |

R = Ph

| | | | |
|---|---------|---------|---------|
| P | 0.33359 | 0.49628 | 0.48547 |
|---|---------|---------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.20083 | 0.66566 | -1.22685 |
| P | -1.33025 | 0.48613 | -2.10726 |
| Ge | 1.46094 | 0.84036 | -2.92385 |
| Cl | 1.69367 | -1.37032 | -3.37153 |
| C | -2.73813 | 1.38542 | -1.42363 |
| H | -2.52033 | 2.45376 | -1.42699 |
| H | -3.61030 | 1.18325 | -2.04868 |
| H | -2.93906 | 1.05344 | -0.40306 |
| Au | 0.33978 | 2.69552 | -0.44911 |
| Cl | 0.46323 | 4.93242 | -0.19107 |
| C | -1.83217 | -1.24895 | -2.10636 |
| C | -2.22949 | -1.84512 | -0.90946 |
| C | -1.83962 | -1.98383 | -3.28547 |
| C | -2.63739 | -3.16773 | -0.89943 |
| H | -2.21103 | -1.28630 | 0.02073 |
| C | -2.25265 | -3.30761 | -3.26926 |
| H | -1.50987 | -1.51904 | -4.20676 |
| C | -2.65113 | -3.89828 | -2.08057 |
| H | -2.94246 | -3.63023 | 0.03193 |
| H | -2.25377 | -3.87960 | -4.18955 |
| H | -2.96935 | -4.93448 | -2.07039 |
| C | 2.08943 | 0.24268 | 0.84776 |
| C | 2.96378 | -0.44885 | 0.00836 |
| C | 2.54449 | 0.70591 | 2.08537 |
| C | 4.28066 | -0.64416 | 0.39305 |
| H | 2.61205 | -0.86258 | -0.93018 |
| C | 3.86488 | 0.52132 | 2.45674 |
| H | 1.86325 | 1.22624 | 2.75160 |
| C | 4.73407 | -0.15289 | 1.60932 |
| H | 4.95424 | -1.18467 | -0.26185 |
| H | 4.21616 | 0.89942 | 3.40972 |
| H | 5.76664 | -0.30383 | 1.90283 |
| S | -0.81289 | 1.15658 | -3.92397 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.25447 | 0.42776 | 1.04715 |
| C | -0.08205 | 0.71087 | -0.62967 |
| P | -1.53630 | 0.55171 | -1.65841 |
| Ge | 1.29215 | 1.38155 | -2.09184 |
| Cl | 1.76288 | -0.59031 | -3.11766 |
| C | -3.11097 | 1.19443 | -1.03245 |
| H | -2.98535 | 2.25084 | -0.79220 |
| H | -3.83556 | 1.09552 | -1.84473 |
| H | -3.47202 | 0.65326 | -0.16074 |
| Au | -0.30713 | 2.64139 | 0.36278 |
| Cl | -0.73387 | 4.81305 | 0.83765 |
| C | -1.83994 | -1.19815 | -2.08936 |
| C | -2.17974 | -2.07393 | -1.03522 |
| C | -1.76135 | -1.70575 | -3.40858 |
| C | -2.35089 | -3.42764 | -1.29926 |
| C | -1.95721 | -3.06740 | -3.60470 |
| C | -2.22857 | -3.95288 | -2.57304 |
| H | -2.59880 | -4.08608 | -0.47209 |
| H | -1.89108 | -3.44774 | -4.61898 |
| C | 2.07781 | 0.29747 | 1.10106 |
| C | 2.60968 | -0.93761 | 0.68090 |
| C | 2.91408 | 1.26055 | 1.68775 |
| C | 3.97916 | -1.14148 | 0.77068 |
| C | 4.27916 | 1.00687 | 1.75055 |
| C | 4.83583 | -0.17427 | 1.28020 |
| H | 4.38518 | -2.09354 | 0.44214 |
| H | 4.92600 | 1.75819 | 2.19381 |
| C | 2.39833 | 2.54732 | 2.25603 |
| H | 2.19795 | 3.28701 | 1.47483 |
| H | 1.46810 | 2.40904 | 2.81340 |
| H | 3.13104 | 2.98389 | 2.93633 |

| | | | |
|---|----------|----------|----------|
| C | 1.73688 | -2.05190 | 0.18288 |
| H | 0.88119 | -2.22129 | 0.84578 |
| H | 1.34818 | -1.84656 | -0.81726 |
| H | 2.30298 | -2.98287 | 0.13354 |
| C | 6.31495 | -0.40169 | 1.32301 |
| H | 6.78621 | 0.18328 | 2.11459 |
| H | 6.55221 | -1.45500 | 1.48393 |
| H | 6.77635 | -0.10485 | 0.37591 |
| C | -2.45176 | -1.65778 | 0.38297 |
| H | -2.15195 | -2.45096 | 1.06950 |
| H | -1.93812 | -0.75425 | 0.70272 |
| H | -3.52536 | -1.49981 | 0.52865 |
| C | -1.50891 | -0.89749 | -4.64753 |
| H | -2.19841 | -0.05915 | -4.74555 |
| H | -0.49840 | -0.48933 | -4.66177 |
| H | -1.63009 | -1.53860 | -5.52136 |
| C | -2.37673 | -5.41890 | -2.83169 |
| H | -2.89253 | -5.60556 | -3.77557 |
| H | -1.39440 | -5.89653 | -2.89903 |
| H | -2.93000 | -5.91260 | -2.03148 |
| S | -0.93745 | 1.81378 | -3.11335 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.70686 | -0.02716 | 1.03587 |
| C | 0.42586 | 0.14718 | -0.68284 |
| P | -1.12795 | -0.04551 | -1.64941 |
| Cl | 2.93137 | -0.96013 | -2.97015 |
| Au | 0.27974 | 2.17230 | 0.11541 |
| Cl | -0.16518 | 4.40129 | 0.23899 |
| C | 2.55565 | -0.06817 | 1.18253 |
| C | 3.28734 | -1.19988 | 0.73071 |
| C | 3.28518 | 1.07299 | 1.60328 |
| C | 4.60930 | -1.01527 | 0.35465 |
| C | 4.60283 | 1.19659 | 1.16150 |
| C | 5.26440 | 0.20499 | 0.45884 |
| H | 5.15421 | -1.86729 | -0.03142 |
| H | 5.13577 | 2.10327 | 1.41197 |
| C | 2.86562 | 2.09412 | 2.68386 |
| C | 2.82825 | -2.66599 | 0.85503 |
| C | 6.67175 | 0.37555 | -0.10045 |
| C | 3.85610 | 1.88555 | 3.84945 |
| H | 3.80138 | 0.86276 | 4.23113 |
| H | 4.88748 | 2.07846 | 3.55356 |
| H | 3.60580 | 2.56904 | 4.66545 |
| C | 2.98647 | 3.54185 | 2.20297 |
| H | 2.30498 | 3.75898 | 1.37987 |
| H | 2.73987 | 4.22335 | 3.02178 |
| H | 4.00017 | 3.77750 | 1.87434 |
| C | 1.48348 | 1.88034 | 3.29493 |
| H | 1.38836 | 2.51505 | 4.18002 |
| H | 0.66487 | 2.16245 | 2.63018 |
| H | 1.33492 | 0.84591 | 3.61563 |
| C | 3.09696 | -3.47955 | -0.41234 |
| H | 2.58735 | -3.05448 | -1.27469 |
| H | 4.16045 | -3.52783 | -0.65086 |
| H | 2.75055 | -4.50688 | -0.26710 |
| C | 3.66118 | -3.26442 | 2.00484 |
| H | 4.72965 | -3.22876 | 1.78756 |
| H | 3.48975 | -2.72148 | 2.93782 |
| H | 3.37982 | -4.31038 | 2.15973 |
| C | 1.36921 | -2.85499 | 1.25030 |
| H | 1.12901 | -2.34893 | 2.18968 |
| H | 0.67820 | -2.51885 | 0.47636 |
| H | 1.17525 | -3.92058 | 1.40369 |
| C | 7.21683 | 1.78292 | 0.12701 |
| H | 6.57592 | 2.54271 | -0.32696 |

| | | | |
|----|----------|----------|----------|
| H | 7.32606 | 2.01341 | 1.19013 |
| H | 8.20594 | 1.86819 | -0.32933 |
| C | 6.63571 | 0.10950 | -1.61000 |
| H | 7.63925 | 0.21149 | -2.03301 |
| H | 6.27190 | -0.89446 | -1.83587 |
| H | 5.97516 | 0.81596 | -2.11739 |
| C | 7.62308 | -0.62313 | 0.56898 |
| H | 7.66255 | -0.46384 | 1.64959 |
| H | 7.31855 | -1.65649 | 0.39154 |
| H | 8.63410 | -0.50281 | 0.16982 |
| C | -2.37431 | -1.42674 | -1.67657 |
| C | -2.35153 | -2.33036 | -2.77890 |
| C | -3.61757 | -1.22831 | -1.01371 |
| C | -3.55765 | -2.61484 | -3.40497 |
| C | -1.16143 | -3.20697 | -3.21164 |
| C | -4.78423 | -1.57421 | -1.68869 |
| C | -3.80842 | -0.85741 | 0.47042 |
| C | -4.78663 | -2.16898 | -2.94032 |
| H | -3.52912 | -3.24253 | -4.28705 |
| C | -0.77324 | -3.03871 | -4.68206 |
| C | -1.62990 | -4.66464 | -3.00809 |
| C | 0.05740 | -3.04876 | -2.31877 |
| H | -5.72843 | -1.37494 | -1.20109 |
| C | -2.51533 | -0.56634 | 1.21367 |
| C | -4.38684 | -2.12785 | 1.12893 |
| C | -4.80458 | 0.28402 | 0.69720 |
| C | -6.05738 | -2.43020 | -3.73834 |
| H | -0.02119 | -3.78728 | -4.94491 |
| H | -1.62970 | -3.18440 | -5.34443 |
| H | -0.35256 | -2.05394 | -4.87528 |
| H | -2.44220 | -4.94367 | -3.68016 |
| H | -0.78971 | -5.33612 | -3.20394 |
| H | -1.96623 | -4.83145 | -1.98172 |
| H | 0.53757 | -2.07705 | -2.40590 |
| H | -0.20639 | -3.23732 | -1.27607 |
| H | 0.80875 | -3.78722 | -2.60668 |
| H | -1.78547 | -1.36422 | 1.06588 |
| H | -2.05074 | 0.38138 | 0.94366 |
| H | -2.71486 | -0.50681 | 2.28618 |
| H | -4.51580 | -1.95433 | 2.20084 |
| H | -5.35583 | -2.40216 | 0.71055 |
| H | -3.71035 | -2.97588 | 0.99946 |
| H | -5.79025 | 0.05590 | 0.28854 |
| H | -4.92779 | 0.44892 | 1.77062 |
| H | -4.47523 | 1.22491 | 0.25494 |
| C | -7.29503 | -1.84767 | -3.06120 |
| C | -6.26283 | -3.94067 | -3.90468 |
| C | -5.91221 | -1.78249 | -5.12064 |
| H | -7.49456 | -2.32069 | -2.09621 |
| H | -7.20214 | -0.76999 | -2.90493 |
| H | -8.16970 | -2.01667 | -3.69349 |
| H | -5.43261 | -4.40776 | -4.43790 |
| H | -6.35880 | -4.43266 | -2.93367 |
| H | -7.17520 | -4.13361 | -4.47553 |
| H | -5.77997 | -0.70126 | -5.03484 |
| H | -5.05480 | -2.18157 | -5.66602 |
| H | -6.80793 | -1.96963 | -5.71902 |
| Ge | 1.69932 | 0.80814 | -2.26908 |
| S | -0.33868 | 0.21244 | -3.49826 |
| C | -2.23786 | 1.39370 | -1.52088 |
| H | -2.68252 | 1.53441 | -0.54097 |
| H | -1.66787 | 2.28035 | -1.79746 |
| H | -3.02141 | 1.23466 | -2.26456 |

E = Sn(II)**[R-P=C(Sn(II)Cl)-P(O)ClR](AuCl)****Coordination through Sn(II) atom****R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.62299 | -0.11936 | 1.17170 |
| C | 0.46874 | -0.20995 | -0.47570 |
| P | -1.00898 | -0.20105 | -1.41453 |
| Cl | 1.76906 | -2.39992 | -2.79309 |
| Sn | 1.66528 | -0.10131 | -2.35345 |
| O | -0.50492 | 0.08468 | -2.81819 |
| Au | 3.24817 | 1.65597 | -3.16505 |
| Cl | 4.67816 | 3.27994 | -3.83372 |
| Cl | -2.37544 | 1.11793 | -0.80137 |
| H | 2.05016 | -0.12229 | 1.23741 |
| H | -1.73264 | -1.40193 | -1.34112 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.65946 | -0.14886 | 1.15963 |
| C | 0.48873 | -0.22294 | -0.48386 |
| P | -1.00156 | -0.25811 | -1.40336 |
| Cl | 1.81396 | -2.37672 | -2.83387 |
| Sn | 1.64410 | -0.07304 | -2.37048 |
| O | -0.50118 | 0.05217 | -2.81306 |
| C | 2.46780 | -0.12916 | 1.43822 |
| H | 2.76991 | -1.12754 | 1.77171 |
| H | 3.04254 | 0.14274 | 0.55247 |
| H | 2.69412 | 0.56299 | 2.25265 |
| C | -1.89561 | -1.80031 | -1.33073 |
| H | -2.25224 | -1.98145 | -0.31621 |
| H | -2.73826 | -1.75694 | -2.02276 |
| H | -1.20560 | -2.59022 | -1.63613 |
| Au | 3.23474 | 1.67259 | -3.19774 |
| Cl | 4.68802 | 3.28445 | -3.85656 |
| Cl | -2.33130 | 1.12381 | -0.80231 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.72093 | -0.59641 | 0.91863 |
| C | 0.69392 | -0.19926 | -0.68803 |
| P | -0.72888 | -0.20434 | -1.72694 |
| Cl | 2.77861 | -1.50383 | -3.18190 |
| Sn | 1.93129 | 0.54328 | -2.37694 |
| O | -0.13138 | 0.25781 | -3.05750 |
| Au | 3.03394 | 2.75363 | -2.79506 |
| Cl | 4.02733 | 4.77494 | -3.08968 |
| C | 2.47070 | -0.43984 | 1.54790 |
| C | 2.83160 | -1.83722 | 2.06427 |
| C | 3.49848 | 0.03614 | 0.54065 |
| C | 2.38115 | 0.53565 | 2.72692 |
| H | 2.09030 | -2.21376 | 2.77466 |
| H | 2.92146 | -2.55819 | 1.24806 |
| H | 3.79490 | -1.79369 | 2.58217 |
| H | 3.27574 | 1.04177 | 0.17238 |
| H | 4.48450 | 0.08770 | 1.01363 |
| H | 3.58986 | -0.65361 | -0.30399 |
| H | 3.34740 | 0.57393 | 3.23946 |
| H | 2.13673 | 1.54816 | 2.39669 |
| H | 1.62943 | 0.22401 | 3.45735 |
| C | -1.67731 | -1.75612 | -1.91724 |
| C | -2.72788 | -1.52955 | -3.00610 |
| C | -0.67739 | -2.82631 | -2.36531 |
| C | -2.33231 | -2.15127 | -0.59746 |
| H | -3.46805 | -0.78453 | -2.70986 |
| H | -2.27126 | -1.21469 | -3.94588 |
| H | -3.25086 | -2.47376 | -3.18072 |

| | | | |
|----|----------|----------|----------|
| H | 0.09118 | -3.01079 | -1.61289 |
| H | -1.22568 | -3.75859 | -2.52503 |
| H | -0.18216 | -2.55770 | -3.29928 |
| H | -2.84896 | -3.10434 | -0.73968 |
| H | -1.59904 | -2.28734 | 0.20097 |
| H | -3.06781 | -1.41513 | -0.26990 |
| Cl | -2.06127 | 1.16827 | -1.07359 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.85065 | -0.00992 | 1.38093 |
| C | 0.44323 | -0.32759 | -0.19516 |
| P | -1.15545 | -0.41561 | -0.90099 |
| Cl | 1.62148 | -2.59892 | -2.60840 |
| Sn | 1.35688 | -0.28760 | -2.20239 |
| O | -0.83910 | -0.29604 | -2.38998 |
| Au | 2.71232 | 1.45764 | -3.38060 |
| Cl | 3.96225 | 3.05807 | -4.39710 |
| C | 2.65268 | -0.05090 | 1.40164 |
| C | 3.28123 | 0.76472 | 2.34662 |
| C | 3.43454 | -0.84877 | 0.56039 |
| C | 4.66370 | 0.82717 | 2.40845 |
| H | 2.68112 | 1.36597 | 3.02257 |
| C | 4.81489 | -0.79563 | 0.63614 |
| H | 2.96230 | -1.54816 | -0.12274 |
| C | 5.42960 | 0.05078 | 1.55104 |
| H | 5.14420 | 1.47965 | 3.12793 |
| H | 5.41461 | -1.41914 | -0.01648 |
| H | 6.51132 | 0.09494 | 1.60233 |
| C | -2.09203 | -1.89037 | -0.54174 |
| C | -2.10108 | -2.90500 | -1.49624 |
| C | -2.74615 | -2.05910 | 0.67783 |
| C | -2.77417 | -4.08671 | -1.22710 |
| H | -1.58575 | -2.76600 | -2.43856 |
| C | -3.41078 | -3.24384 | 0.93719 |
| H | -2.74344 | -1.26623 | 1.41722 |
| C | -3.42523 | -4.25587 | -0.01500 |
| H | -2.78742 | -4.87630 | -1.96884 |
| H | -3.92338 | -3.37793 | 1.88230 |
| H | -3.95009 | -5.18158 | 0.19131 |
| Cl | -2.32001 | 1.10798 | -0.28460 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.95963 | -0.30883 | 1.98639 |
| C | 0.37042 | -0.45452 | 0.44326 |
| P | -1.21479 | -0.40858 | -0.31431 |
| Cl | 1.55676 | -2.09253 | -2.43560 |
| Sn | 1.35661 | 0.04571 | -1.45181 |
| O | -0.83467 | 0.16722 | -1.67833 |
| Au | 2.82493 | 1.98260 | -2.06638 |
| Cl | 4.20355 | 3.74392 | -2.48678 |
| C | 2.74496 | -0.13747 | 1.65314 |
| C | 3.31807 | 1.14158 | 1.73884 |
| C | 3.53272 | -1.25583 | 1.34196 |
| C | 4.66871 | 1.28724 | 1.45930 |
| C | 4.88320 | -1.05871 | 1.07728 |
| C | 5.46640 | 0.20186 | 1.11446 |
| H | 5.10674 | 2.27997 | 1.49720 |
| H | 5.49849 | -1.92047 | 0.83651 |
| C | -2.12965 | -1.94550 | -0.40249 |
| C | -2.60431 | -2.43473 | -1.64139 |
| C | -2.36873 | -2.66591 | 0.78648 |
| C | -3.27721 | -3.64982 | -1.64327 |
| C | -3.05014 | -3.87174 | 0.71275 |
| C | -3.50343 | -4.38940 | -0.49117 |
| H | -3.64770 | -4.02612 | -2.59138 |
| H | -3.23646 | -4.41824 | 1.63192 |

| | | | |
|----|----------|----------|----------|
| Cl | -2.44169 | 0.92717 | 0.59388 |
| C | -1.91475 | -2.21092 | 2.14000 |
| H | -0.86311 | -2.46207 | 2.30501 |
| H | -2.02072 | -1.13640 | 2.29300 |
| H | -2.49496 | -2.71143 | 2.91577 |
| C | -4.20562 | -5.70882 | -0.55024 |
| H | -3.49161 | -6.51109 | -0.76121 |
| H | -4.69385 | -5.94451 | 0.39651 |
| H | -4.95632 | -5.72530 | -1.34209 |
| C | -2.44976 | -1.73983 | -2.96264 |
| H | -2.79439 | -0.70648 | -2.93357 |
| H | -1.40610 | -1.71610 | -3.28034 |
| H | -3.02456 | -2.27400 | -3.71925 |
| C | 2.48827 | 2.34554 | 2.07119 |
| H | 1.93753 | 2.69909 | 1.19354 |
| H | 1.75241 | 2.13355 | 2.85440 |
| H | 3.11535 | 3.16920 | 2.41375 |
| C | 2.95974 | -2.64268 | 1.29893 |
| H | 2.30064 | -2.83381 | 2.15164 |
| H | 2.37215 | -2.81129 | 0.39199 |
| H | 3.75626 | -3.38735 | 1.32061 |
| C | 6.91207 | 0.39850 | 0.78005 |
| H | 7.01455 | 0.92963 | -0.17066 |
| H | 7.41613 | 0.99943 | 1.54055 |
| H | 7.43572 | -0.55417 | 0.69227 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.18588 | 2.27013 | 1.12057 |
| C | 0.26410 | 0.79941 | 0.48854 |
| P | 1.78830 | -0.06250 | 0.26080 |
| Cl | -1.16024 | 0.33551 | -2.78457 |
| O | 1.38974 | -0.97023 | -0.90658 |
| C | 3.51729 | 0.45998 | 0.06468 |
| C | 4.06992 | 0.33166 | -1.24520 |
| C | 4.39881 | 0.50012 | 1.17691 |
| C | 5.37064 | -0.13739 | -1.34088 |
| C | 5.69914 | 0.04482 | 0.98692 |
| C | 6.18145 | -0.38024 | -0.23963 |
| H | 5.77446 | -0.30754 | -2.33012 |
| H | 6.35882 | 0.02893 | 1.84285 |
| C | -1.99897 | 2.20449 | 0.83817 |
| C | -2.55833 | 2.94094 | -0.23212 |
| C | -2.80133 | 1.29115 | 1.56476 |
| C | -3.80513 | 2.54388 | -0.70703 |
| C | -4.02261 | 0.92627 | 1.00912 |
| C | -4.52170 | 1.48966 | -0.15787 |
| H | -4.22538 | 3.06592 | -1.55158 |
| H | -4.61827 | 0.18061 | 1.51895 |
| C | -1.89353 | 4.19648 | -0.82879 |
| C | -2.48515 | 0.77468 | 2.98517 |
| C | -5.83361 | 0.98452 | -0.74937 |
| C | 4.13217 | 1.16744 | 2.54082 |
| C | 3.41870 | 0.80808 | -2.55855 |
| C | 7.56124 | -0.99859 | -0.42238 |
| C | -3.77244 | 0.82375 | 3.82687 |
| H | -3.52941 | 0.58890 | 4.86605 |
| H | -4.23112 | 1.81494 | 3.79840 |
| H | -4.51424 | 0.09396 | 3.50215 |
| C | -1.48053 | 1.66034 | 3.72067 |
| H | -0.46353 | 1.58500 | 3.31856 |
| H | -1.77836 | 2.71171 | 3.70968 |
| H | -1.40737 | 1.33916 | 4.76318 |
| C | -1.97732 | -0.66854 | 2.98322 |
| H | -2.67054 | -1.33714 | 2.46827 |
| H | -1.00227 | -0.75236 | 2.50081 |
| H | -1.86966 | -1.02692 | 4.01116 |

| | | | |
|----|----------|----------|----------|
| C | -6.96108 | 1.14659 | 0.27716 |
| H | -7.90367 | 0.78663 | -0.14392 |
| H | -6.76821 | 0.57675 | 1.18809 |
| H | -7.09111 | 2.19557 | 0.55575 |
| C | -6.22677 | 1.74159 | -2.01515 |
| H | -7.15589 | 1.32557 | -2.41152 |
| H | -6.39928 | 2.80372 | -1.82124 |
| H | -5.46602 | 1.65025 | -2.79433 |
| C | -5.67730 | -0.49915 | -1.10447 |
| H | -4.89157 | -0.64290 | -1.85000 |
| H | -5.42361 | -1.10722 | -0.23404 |
| H | -6.61227 | -0.88610 | -1.51873 |
| C | -2.80942 | 4.90101 | -1.83253 |
| H | -3.77000 | 5.17574 | -1.39095 |
| H | -2.32314 | 5.82127 | -2.16404 |
| H | -2.99422 | 4.29167 | -2.72016 |
| C | -1.62068 | 5.19609 | 0.30404 |
| H | -2.54613 | 5.45755 | 0.82270 |
| H | -0.91915 | 4.80440 | 1.04396 |
| H | -1.18747 | 6.11319 | -0.10490 |
| C | -0.58909 | 3.89011 | -1.56893 |
| H | 0.20531 | 3.55099 | -0.89779 |
| H | -0.73204 | 3.12010 | -2.32821 |
| H | -0.22128 | 4.79923 | -2.05375 |
| C | 2.75131 | 1.79105 | 2.68283 |
| H | 2.52099 | 2.44862 | 1.84158 |
| H | 1.95809 | 1.05319 | 2.78995 |
| H | 2.72695 | 2.40725 | 3.58497 |
| C | 5.12764 | 2.34343 | 2.62575 |
| H | 4.96393 | 2.88667 | 3.56029 |
| H | 6.16595 | 2.01155 | 2.60808 |
| H | 4.98137 | 3.04025 | 1.79690 |
| C | 4.39041 | 0.22934 | 3.72323 |
| H | 5.40604 | -0.17003 | 3.71478 |
| H | 4.26281 | 0.78045 | 4.65878 |
| H | 3.69705 | -0.61116 | 3.72874 |
| C | 2.23040 | 1.73597 | -2.32356 |
| H | 1.91411 | 2.16350 | -3.27774 |
| H | 1.35404 | 1.23542 | -1.92225 |
| H | 2.50432 | 2.56252 | -1.66235 |
| C | 3.03326 | -0.35574 | -3.47571 |
| H | 2.26832 | -0.98428 | -3.02605 |
| H | 2.65010 | 0.03437 | -4.42237 |
| H | 3.90339 | -0.97835 | -3.69907 |
| C | 4.45811 | 1.67304 | -3.30098 |
| H | 4.82994 | 2.48222 | -2.66773 |
| H | 5.31334 | 1.10041 | -3.66025 |
| H | 3.97942 | 2.11931 | -4.17602 |
| C | 8.28650 | -1.19807 | 0.90568 |
| H | 8.49216 | -0.24865 | 1.40678 |
| H | 7.71576 | -1.83301 | 1.58790 |
| H | 9.24726 | -1.68565 | 0.72550 |
| C | 8.42018 | -0.09148 | -1.31174 |
| H | 7.97977 | 0.04417 | -2.30138 |
| H | 8.54511 | 0.89594 | -0.86056 |
| H | 9.41181 | -0.53169 | -1.44652 |
| C | 7.40079 | -2.36712 | -1.09575 |
| H | 6.80003 | -3.03953 | -0.47887 |
| H | 6.91594 | -2.28493 | -2.07043 |
| H | 8.38103 | -2.82707 | -1.24668 |
| Au | -2.20344 | -2.73916 | -0.17893 |
| Cl | -3.53515 | -4.51082 | 0.35366 |
| Sn | -0.79756 | -0.72731 | -0.70657 |
| Cl | 1.88480 | -1.34726 | 1.85155 |

Coordination through O atom**R= H**

| | | | |
|----|----------|----------|----------|
| P | 0.72527 | -0.02047 | 1.06870 |
| C | 0.51102 | -0.15236 | -0.56938 |
| P | -0.99308 | 0.00727 | -1.40894 |
| Cl | 1.18388 | -2.45767 | -2.93096 |
| Sn | 1.76630 | -0.18509 | -2.49632 |
| O | -0.54690 | 0.49003 | -2.79687 |
| Au | -1.84188 | 0.77350 | -4.44094 |
| Cl | -3.19320 | 1.07450 | -6.17671 |
| Cl | -2.34218 | 1.23247 | -0.59621 |
| H | -1.70584 | -1.19668 | -1.49971 |
| H | 2.14521 | -0.20309 | 1.10154 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.72897 | -0.07462 | 1.05993 |
| C | 0.51549 | -0.14741 | -0.57906 |
| P | -1.01160 | -0.01425 | -1.38472 |
| Cl | 1.37878 | -2.39803 | -2.98859 |
| Sn | 1.72565 | -0.06897 | -2.52882 |
| O | -0.57159 | 0.42656 | -2.80087 |
| C | 2.53077 | -0.31855 | 1.30282 |
| H | 2.69305 | -1.35698 | 1.61002 |
| H | 3.12135 | -0.11912 | 0.40796 |
| H | 2.87293 | 0.31720 | 2.12256 |
| C | -1.96569 | -1.51845 | -1.43867 |
| H | -2.27800 | -1.79064 | -0.42961 |
| H | -2.83794 | -1.36644 | -2.07739 |
| H | -1.32218 | -2.29428 | -1.86063 |
| Au | -1.86365 | 0.68521 | -4.44506 |
| Cl | -3.22153 | 0.95680 | -6.18261 |
| Cl | -2.25539 | 1.36207 | -0.61157 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.79051 | -0.60970 | 0.94337 |
| C | 0.44557 | -0.10446 | -0.59654 |
| P | -1.17225 | -0.08674 | -1.24758 |
| Cl | 2.00710 | -1.10748 | -3.50919 |
| Sn | 1.39851 | 0.94306 | -2.41355 |
| O | -0.94211 | 0.61487 | -2.60662 |
| Au | -2.27481 | 1.46369 | -3.99676 |
| Cl | -3.64207 | 2.38151 | -5.48972 |
| C | 2.63807 | -0.49809 | 1.20389 |
| C | 3.09463 | -1.94592 | 1.41582 |
| C | 3.42369 | 0.14251 | 0.07662 |
| C | 2.82048 | 0.29222 | 2.50306 |
| H | 2.52228 | -2.44136 | 2.20509 |
| H | 2.99892 | -2.53586 | 0.50113 |
| H | 4.14768 | -1.95563 | 1.71543 |
| H | 3.11353 | 1.17879 | -0.09203 |
| H | 4.48906 | 0.16956 | 0.32902 |
| H | 3.33292 | -0.42902 | -0.85234 |
| H | 3.87528 | 0.27998 | 2.79518 |
| H | 2.51570 | 1.33565 | 2.38849 |
| H | 2.24263 | -0.14000 | 3.32442 |
| C | -2.04540 | -1.68626 | -1.44439 |
| C | -3.39951 | -1.45197 | -2.11505 |
| C | -1.15917 | -2.56290 | -2.33378 |
| C | -2.23755 | -2.33194 | -0.07413 |
| H | -4.05989 | -0.83545 | -1.50371 |
| H | -3.29975 | -0.98338 | -3.09630 |
| H | -3.87919 | -2.42468 | -2.25483 |
| H | -0.17792 | -2.74308 | -1.89198 |
| H | -1.65812 | -3.52721 | -2.46218 |

| | | | |
|----|----------|----------|----------|
| H | -1.00984 | -2.12392 | -3.32098 |
| H | -2.72895 | -3.29772 | -0.21929 |
| H | -1.28878 | -2.51460 | 0.43469 |
| H | -2.87045 | -1.72793 | 0.57822 |
| Cl | -2.40128 | 1.07058 | -0.13670 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.71433 | 0.22445 | 0.86664 |
| C | 0.53476 | -0.25601 | -0.71074 |
| P | -0.91456 | -0.20128 | -1.65136 |
| Cl | 1.82109 | -2.82567 | -2.70486 |
| Sn | 1.96053 | -0.43600 | -2.47731 |
| O | -0.34752 | -0.12352 | -3.08367 |
| Au | -1.41959 | 0.07833 | -4.88460 |
| Cl | -2.51560 | 0.28842 | -6.80757 |
| C | 2.46307 | -0.09898 | 1.20297 |
| C | 3.19380 | -1.13067 | 0.60344 |
| C | 3.09453 | 0.72818 | 2.13500 |
| C | 4.53581 | -1.30035 | 0.90202 |
| H | 2.69598 | -1.83660 | -0.05531 |
| C | 4.44043 | 0.56418 | 2.42079 |
| H | 2.52846 | 1.51330 | 2.62682 |
| C | 5.16186 | -0.44702 | 1.80187 |
| H | 5.09168 | -2.10855 | 0.44077 |
| H | 4.92650 | 1.22216 | 3.13176 |
| H | 6.21226 | -0.58168 | 2.03307 |
| C | -2.01363 | -1.59133 | -1.45537 |
| C | -2.93121 | -1.63600 | -0.40643 |
| C | -1.89294 | -2.66407 | -2.33653 |
| C | -3.73008 | -2.75330 | -0.24597 |
| H | -3.02908 | -0.79821 | 0.27421 |
| C | -2.70241 | -3.77619 | -2.16848 |
| H | -1.17401 | -2.63098 | -3.14545 |
| C | -3.61672 | -3.82108 | -1.12757 |
| H | -4.44883 | -2.78890 | 0.56398 |
| H | -2.61743 | -4.60712 | -2.85824 |
| H | -4.24955 | -4.69219 | -1.00241 |
| Cl | -2.04064 | 1.42719 | -1.27582 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.59263 | -0.06959 | 1.29882 |
| C | 0.33723 | -0.34726 | -0.31271 |
| P | -1.04718 | -0.25722 | -1.35769 |
| Cl | 2.00528 | -2.52554 | -2.42781 |
| Sn | 1.93496 | -0.17463 | -1.90746 |
| O | -0.36121 | 0.11880 | -2.68677 |
| Au | -0.96916 | 1.37434 | -4.26944 |
| Cl | -1.54267 | 2.70501 | -5.95668 |
| C | 2.41764 | -0.19300 | 1.39436 |
| C | 3.04895 | -1.44623 | 1.46237 |
| C | 3.17060 | 0.98919 | 1.48077 |
| C | 4.43332 | -1.48576 | 1.57531 |
| C | 4.55211 | 0.89730 | 1.59012 |
| C | 5.20332 | -0.32972 | 1.63080 |
| H | 4.92379 | -2.45298 | 1.63260 |
| H | 5.13482 | 1.81167 | 1.65299 |
| C | -2.06259 | -1.73280 | -1.44813 |
| C | -2.75496 | -2.13459 | -0.28343 |
| C | -2.14484 | -2.51125 | -2.62726 |
| C | -3.48799 | -3.31130 | -0.31203 |
| C | -2.90589 | -3.67322 | -2.58581 |
| C | -3.58012 | -4.09676 | -1.45082 |
| H | -4.00724 | -3.61821 | 0.59038 |
| H | -2.96519 | -4.27355 | -3.48772 |
| Cl | -2.28292 | 1.28182 | -0.89829 |
| C | 2.50961 | 2.33539 | 1.43833 |

| | | | |
|---|----------|----------|----------|
| H | 2.16076 | 2.58188 | 0.43038 |
| H | 1.63500 | 2.37851 | 2.09562 |
| H | 3.20079 | 3.11981 | 1.74846 |
| C | 6.69622 | -0.40582 | 1.72056 |
| H | 7.13992 | -0.46820 | 0.72199 |
| H | 7.11200 | 0.47714 | 2.20864 |
| H | 7.01733 | -1.28957 | 2.27463 |
| C | 2.26611 | -2.72512 | 1.43067 |
| H | 1.39802 | -2.68231 | 2.09573 |
| H | 1.89333 | -2.94018 | 0.42528 |
| H | 2.88767 | -3.56467 | 1.74398 |
| C | -2.78899 | -1.34517 | 0.99061 |
| H | -3.50560 | -0.52329 | 0.91942 |
| H | -3.09878 | -1.98630 | 1.81633 |
| H | -1.82733 | -0.90718 | 1.26162 |
| C | -1.48144 | -2.19071 | -3.93296 |
| H | -1.80782 | -1.22898 | -4.33486 |
| H | -0.39588 | -2.15528 | -3.84019 |
| H | -1.73263 | -2.95938 | -4.66335 |
| C | -4.40332 | -5.34552 | -1.46536 |
| H | -4.49237 | -5.77666 | -0.46712 |
| H | -5.41534 | -5.13121 | -1.82294 |
| H | -3.97505 | -6.09624 | -2.13151 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.88951 | 2.17246 | -0.11508 |
| C | 0.96328 | 0.80172 | -0.22639 |
| P | -0.75000 | 0.52089 | -0.33576 |
| C | 3.56695 | 1.40509 | -0.15668 |
| C | 4.31865 | 1.31745 | 1.04474 |
| C | 4.01811 | 0.73315 | -1.31281 |
| C | 5.32798 | 0.36921 | 1.10731 |
| C | 5.01788 | -0.23360 | -1.15905 |
| C | 5.64946 | -0.47437 | 0.04696 |
| H | 5.87967 | 0.25946 | 2.02933 |
| H | 5.32550 | -0.79267 | -2.03227 |
| C | 3.64804 | 1.08455 | -2.77142 |
| C | 4.09953 | 2.25872 | 2.24348 |
| C | 6.70167 | -1.56252 | 0.23206 |
| C | 2.75934 | 2.01368 | 2.94222 |
| H | 1.90532 | 2.29153 | 2.31880 |
| H | 2.63918 | 0.96400 | 3.21475 |
| H | 2.70088 | 2.62417 | 3.84812 |
| C | 4.17906 | 3.71371 | 1.76143 |
| H | 5.14596 | 3.91589 | 1.29411 |
| H | 3.39721 | 3.95735 | 1.03905 |
| H | 4.06211 | 4.39285 | 2.61044 |
| C | 5.18662 | 2.08529 | 3.30706 |
| H | 5.14489 | 1.10315 | 3.78358 |
| H | 6.18926 | 2.23556 | 2.89969 |
| H | 5.03265 | 2.83203 | 4.08920 |
| C | 3.00556 | -0.09631 | -3.50335 |
| H | 2.01462 | -0.32207 | -3.10249 |
| H | 2.88187 | 0.14452 | -4.56289 |
| H | 3.61382 | -1.00045 | -3.43704 |
| C | 2.74054 | 2.30177 | -2.93348 |
| H | 1.70758 | 2.10114 | -2.64689 |
| H | 3.10812 | 3.16573 | -2.37191 |
| H | 2.71924 | 2.59032 | -3.98819 |
| C | 4.96419 | 1.45016 | -3.48492 |
| H | 5.46023 | 2.28442 | -2.98285 |
| H | 5.66568 | 0.61664 | -3.52228 |
| H | 4.75021 | 1.74997 | -4.51416 |
| C | 6.89520 | -2.40063 | -1.02877 |
| H | 7.26734 | -1.80315 | -1.86519 |
| H | 7.63110 | -3.18441 | -0.83504 |

| | | | |
|----|----------|----------|----------|
| H | 5.96748 | -2.88903 | -1.33784 |
| C | 6.26305 | -2.49566 | 1.36723 |
| H | 6.15115 | -1.96057 | 2.31199 |
| H | 5.30425 | -2.96800 | 1.14205 |
| H | 7.00794 | -3.28270 | 1.51348 |
| C | 8.04542 | -0.91890 | 0.59428 |
| H | 7.98191 | -0.34050 | 1.51813 |
| H | 8.80540 | -1.69201 | 0.73715 |
| H | 8.38608 | -0.24916 | -0.19936 |
| C | -2.22260 | 1.35676 | 0.31007 |
| C | -2.82677 | 0.75087 | 1.45228 |
| C | -3.01931 | 2.18119 | -0.52670 |
| C | -4.20843 | 0.65693 | 1.46366 |
| C | -4.39931 | 2.04048 | -0.43855 |
| C | -5.01802 | 1.19737 | 0.47196 |
| H | -4.67427 | 0.13472 | 2.28956 |
| H | -5.01219 | 2.62292 | -1.11244 |
| C | -2.09946 | 0.34889 | 2.74996 |
| C | -2.20158 | -1.14626 | 3.05707 |
| C | -2.79271 | 1.12568 | 3.88849 |
| H | -1.63779 | -1.74294 | 2.34090 |
| H | -1.79465 | -1.34257 | 4.05269 |
| H | -3.23760 | -1.49083 | 3.04310 |
| H | -2.77830 | 2.20187 | 3.69892 |
| H | -3.82901 | 0.82174 | 4.03704 |
| H | -2.25671 | 0.93701 | 4.82213 |
| C | -2.51744 | 3.36226 | -1.38030 |
| C | -3.14406 | 4.61898 | -0.73988 |
| C | -2.97649 | 3.28833 | -2.83873 |
| H | -2.84862 | 4.71290 | 0.30787 |
| H | -2.79517 | 5.50725 | -1.27357 |
| H | -4.23333 | 4.60618 | -0.78337 |
| H | -2.54454 | 2.43227 | -3.35586 |
| H | -4.06250 | 3.21779 | -2.92031 |
| H | -2.66591 | 4.19522 | -3.36459 |
| C | -6.51628 | 0.93013 | 0.47430 |
| C | -7.13898 | 1.51099 | 1.74977 |
| C | -6.74458 | -0.58629 | 0.43841 |
| H | -6.98942 | 2.59240 | 1.80502 |
| H | -8.21452 | 1.31491 | 1.76131 |
| H | -6.71062 | 1.06464 | 2.64943 |
| H | -6.29451 | -1.03963 | -0.44718 |
| H | -6.31475 | -1.08372 | 1.30964 |
| H | -7.81704 | -0.79882 | 0.42809 |
| Cl | 2.09631 | -1.64996 | 2.04255 |
| O | -0.81877 | -0.96411 | 0.10189 |
| Cl | -1.08189 | 0.40369 | -2.35430 |
| Au | -2.43141 | -2.24458 | -0.38147 |
| Cl | -4.11346 | -3.61938 | -0.88931 |
| C | -1.01109 | 3.58617 | -1.32715 |
| H | -0.64581 | 3.61626 | -0.29791 |
| H | -0.44614 | 2.83950 | -1.88168 |
| H | -0.77692 | 4.55285 | -1.77987 |
| C | -0.64048 | 0.78628 | 2.78700 |
| H | 0.00714 | 0.19730 | 2.14097 |
| H | -0.53632 | 1.84520 | 2.53573 |
| H | -0.25117 | 0.64594 | 3.79822 |
| C | -7.21381 | 1.55247 | -0.73227 |
| H | -7.15214 | 2.64412 | -0.72639 |
| H | -6.79567 | 1.18544 | -1.67275 |
| H | -8.27320 | 1.28693 | -0.71503 |
| Sn | 1.56005 | -1.41106 | -0.29431 |

Coordination through P(sp²) atom**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.61606 | 0.00599 | 0.92159 |
| C | 0.37971 | -0.26051 | -0.67361 |
| P | -1.10853 | -0.26698 | -1.56923 |
| Cl | 1.25717 | -2.76501 | -2.78383 |
| Sn | 1.55367 | -0.38915 | -2.69486 |
| O | -0.67389 | -0.00820 | -2.99563 |
| Au | -0.71856 | 0.42027 | 2.61556 |
| Cl | -2.07960 | 0.83991 | 4.36269 |
| Cl | -2.48762 | 1.04382 | -0.95144 |
| H | -1.79144 | -1.48340 | -1.41736 |
| H | 2.01221 | -0.07699 | 1.11822 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.71735 | 0.05040 | 0.87419 |
| C | 0.41972 | -0.18975 | -0.71286 |
| P | -1.12671 | -0.28768 | -1.51000 |
| Cl | 1.37422 | -2.81369 | -2.64303 |
| Sn | 1.46961 | -0.40826 | -2.77777 |
| O | -0.75629 | -0.20560 | -2.98281 |
| C | 2.49248 | 0.01494 | 1.21667 |
| H | 2.69803 | -0.81769 | 1.89436 |
| H | 3.07259 | -0.10093 | 0.30213 |
| H | 2.77316 | 0.93640 | 1.73189 |
| C | -2.04595 | -1.76246 | -1.10989 |
| H | -2.31650 | -1.76124 | -0.05308 |
| H | -2.94509 | -1.79736 | -1.72738 |
| H | -1.40259 | -2.61516 | -1.33926 |
| Au | -0.68770 | 0.33804 | 2.54877 |
| Cl | -2.12832 | 0.59681 | 4.27079 |
| Cl | -2.35947 | 1.22834 | -1.01941 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.74285 | 0.11358 | 0.77398 |
| C | 0.51468 | -0.37019 | -0.77289 |
| P | -0.99398 | -0.56500 | -1.63897 |
| Cl | 2.11293 | -2.91488 | -2.59003 |
| Sn | 1.68497 | -0.55052 | -2.78451 |
| O | -0.53204 | -0.70280 | -3.08482 |
| Au | -0.74787 | 0.71450 | 2.29772 |
| Cl | -2.26087 | 1.33794 | 3.86408 |
| C | 2.51987 | 0.14121 | 1.29128 |
| C | 2.80218 | 1.53687 | 1.85284 |
| C | 2.64807 | -0.90220 | 2.40698 |
| C | 3.46851 | -0.18278 | 0.14971 |
| H | 2.72602 | 2.30785 | 1.08239 |
| H | 2.11554 | 1.79439 | 2.66272 |
| H | 3.81937 | 1.55878 | 2.25487 |
| H | 2.47508 | -1.91465 | 2.03505 |
| H | 3.66248 | -0.85948 | 2.81491 |
| H | 1.95017 | -0.70922 | 3.22538 |
| H | 4.49589 | -0.18053 | 0.52613 |
| H | 3.27655 | -1.17129 | -0.27479 |
| H | 3.41674 | 0.56881 | -0.64313 |
| C | -2.08690 | -1.95366 | -1.15575 |
| C | -1.24607 | -3.23020 | -1.23696 |
| C | -2.63822 | -1.76783 | 0.25263 |
| C | -3.22178 | -2.00825 | -2.18161 |
| H | -0.84101 | -3.39270 | -2.23610 |
| H | -0.41194 | -3.21853 | -0.53338 |
| H | -1.89019 | -4.07713 | -0.98495 |
| H | -3.22971 | -0.85672 | 0.35216 |
| H | -3.28762 | -2.61692 | 0.48312 |

| | | | |
|----|----------|----------|----------|
| H | -1.84672 | -1.74842 | 1.00451 |
| H | -3.83455 | -2.88759 | -1.96531 |
| H | -3.86449 | -1.12826 | -2.12561 |
| H | -2.84045 | -2.10072 | -3.19981 |
| Cl | -2.13316 | 1.10135 | -1.45847 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.73638 | 0.19153 | 0.58064 |
| C | 0.55600 | -0.47601 | -0.90235 |
| P | -0.90957 | -0.74675 | -1.80121 |
| Cl | 1.99249 | -3.34448 | -2.23877 |
| Sn | 1.81379 | -0.99534 | -2.77088 |
| O | -0.39568 | -1.07748 | -3.19367 |
| Au | -0.78631 | 1.09734 | 1.90145 |
| Cl | -2.38097 | 1.98721 | 3.23868 |
| C | 2.44210 | 0.13175 | 1.10508 |
| C | 2.87708 | 1.06935 | 2.04361 |
| C | 3.33050 | -0.83138 | 0.61850 |
| C | 4.19769 | 1.06947 | 2.45965 |
| H | 2.17844 | 1.79905 | 2.43997 |
| C | 4.64572 | -0.83070 | 1.04787 |
| H | 2.98035 | -1.60581 | -0.05608 |
| C | 5.08122 | 0.12318 | 1.95975 |
| H | 4.53603 | 1.80513 | 3.17958 |
| H | 5.33083 | -1.58512 | 0.67939 |
| H | 6.11264 | 0.11875 | 2.29320 |
| C | -1.95991 | -2.03095 | -1.14581 |
| C | -2.84440 | -1.78977 | -0.09529 |
| C | -1.82300 | -3.31200 | -1.67728 |
| C | -3.59272 | -2.83378 | 0.41863 |
| H | -2.95538 | -0.79292 | 0.31631 |
| C | -2.58126 | -4.34885 | -1.15696 |
| H | -1.12662 | -3.49087 | -2.48729 |
| C | -3.46183 | -4.11075 | -0.11249 |
| H | -4.28196 | -2.64858 | 1.23377 |
| H | -2.48046 | -5.34554 | -1.56979 |
| H | -4.05241 | -4.92495 | 0.29187 |
| Cl | -2.06494 | 0.90734 | -1.85400 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.66149 | 0.34741 | 1.16106 |
| C | 0.31775 | -0.43175 | -0.23455 |
| P | -1.06364 | -0.60503 | -1.28400 |
| Cl | 1.72198 | -3.08022 | -2.00214 |
| Sn | 1.75714 | -0.66311 | -2.01735 |
| O | -0.40207 | -0.45719 | -2.64717 |
| Au | -0.61538 | 1.38413 | 2.63821 |
| Cl | -1.89376 | 2.45039 | 4.17309 |
| C | 2.44656 | 0.29454 | 1.40782 |
| C | 3.18496 | 1.48280 | 1.27626 |
| C | 3.07475 | -0.91314 | 1.75457 |
| C | 4.55755 | 1.43250 | 1.47126 |
| C | 4.45083 | -0.90441 | 1.94521 |
| C | 5.20918 | 0.25141 | 1.80746 |
| H | 5.13467 | 2.34512 | 1.35763 |
| H | 4.94379 | -1.83323 | 2.21532 |
| C | -2.01293 | -2.11601 | -1.09680 |
| C | -2.51057 | -2.47058 | 0.17443 |
| C | -2.27142 | -2.94062 | -2.21591 |
| C | -3.22325 | -3.65256 | 0.31054 |
| C | -2.99210 | -4.11029 | -2.00898 |
| C | -3.46626 | -4.49477 | -0.76370 |
| H | -3.60691 | -3.91454 | 1.29155 |
| H | -3.19584 | -4.74194 | -2.86768 |
| Cl | -2.39378 | 0.91583 | -1.07225 |
| C | 2.52773 | 2.78200 | 0.91836 |

| | | | |
|---|----------|----------|----------|
| H | 2.00779 | 2.72306 | -0.04258 |
| H | 1.78500 | 3.07464 | 1.66727 |
| H | 3.26459 | 3.58233 | 0.84840 |
| C | 2.31192 | -2.19191 | 1.93519 |
| H | 1.42115 | -2.04482 | 2.55319 |
| H | 1.97918 | -2.60368 | 0.97833 |
| H | 2.93551 | -2.94093 | 2.42395 |
| C | 6.68668 | 0.23357 | 2.04832 |
| H | 6.90886 | 0.48305 | 3.09059 |
| H | 7.11118 | -0.75165 | 1.84955 |
| H | 7.20111 | 0.96430 | 1.42188 |
| C | -2.30832 | -1.64289 | 1.40589 |
| H | -3.02458 | -1.93162 | 2.17527 |
| H | -1.30725 | -1.79194 | 1.81886 |
| H | -2.43444 | -0.57395 | 1.22954 |
| C | -1.83994 | -2.65445 | -3.62485 |
| H | -2.11953 | -1.65424 | -3.95385 |
| H | -0.75662 | -2.73344 | -3.72832 |
| H | -2.30062 | -3.38046 | -4.29518 |
| C | -4.20752 | -5.78175 | -0.58480 |
| H | -4.76060 | -6.05190 | -1.48582 |
| H | -3.50902 | -6.59739 | -0.37290 |
| H | -4.90842 | -5.72602 | 0.24962 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.05258 | 0.96593 | 0.06589 |
| C | -0.26220 | -0.42349 | 0.41998 |
| P | 1.36296 | -1.05293 | 0.55902 |
| Cl | -1.63010 | -2.92839 | -1.83415 |
| O | 1.16105 | -2.47781 | 0.05881 |
| C | 3.00951 | -0.48049 | 0.05086 |
| C | 3.55242 | -1.14377 | -1.08942 |
| C | 3.89320 | 0.16130 | 0.95820 |
| C | 4.90260 | -1.45535 | -1.06119 |
| C | 5.23803 | -0.19183 | 0.90169 |
| C | 5.75440 | -1.07240 | -0.03360 |
| H | 5.30899 | -2.01849 | -1.89117 |
| H | 5.90682 | 0.25648 | 1.62246 |
| C | -2.82099 | 0.52957 | 0.11808 |
| C | -3.54566 | 0.30016 | -1.08116 |
| C | -3.37458 | 0.15008 | 1.36638 |
| C | -4.67312 | -0.51103 | -1.00137 |
| C | -4.48918 | -0.68219 | 1.34900 |
| C | -5.12419 | -1.07580 | 0.18211 |
| H | -5.20657 | -0.73463 | -1.91005 |
| H | -4.88430 | -1.02721 | 2.29587 |
| C | -3.22239 | 0.96323 | -2.43391 |
| C | -2.94108 | 0.65320 | 2.76099 |
| C | -6.29258 | -2.05432 | 0.23840 |
| C | 3.57281 | 1.35199 | 1.88454 |
| C | 2.82231 | -1.42524 | -2.41740 |
| C | 7.20254 | -1.54518 | -0.01943 |
| C | -4.19329 | 1.20844 | 3.46612 |
| H | -3.90740 | 1.61811 | 4.43810 |
| H | -4.64817 | 2.01058 | 2.88015 |
| H | -4.95409 | 0.44881 | 3.64420 |
| C | -1.94156 | 1.80782 | 2.74994 |
| H | -0.93065 | 1.50047 | 2.47849 |
| H | -2.25576 | 2.62017 | 2.08964 |
| H | -1.86789 | 2.22145 | 3.75935 |
| C | -2.36469 | -0.48872 | 3.60252 |
| H | -3.06213 | -1.32556 | 3.67959 |
| H | -1.43069 | -0.86076 | 3.17648 |
| H | -2.15159 | -0.13593 | 4.61559 |
| C | -7.41788 | -1.46700 | 1.09819 |
| H | -8.25810 | -2.16522 | 1.14364 |

| | | | |
|----|----------|----------|----------|
| H | -7.09109 | -1.27453 | 2.12213 |
| H | -7.78062 | -0.52546 | 0.67863 |
| C | -6.85680 | -2.36418 | -1.14559 |
| H | -7.67100 | -3.08663 | -1.05189 |
| H | -7.26392 | -1.47284 | -1.62970 |
| H | -6.10088 | -2.80043 | -1.80295 |
| C | -5.80596 | -3.36772 | 0.86313 |
| H | -5.00955 | -3.81357 | 0.26217 |
| H | -5.42167 | -3.21768 | 1.87435 |
| H | -6.62992 | -4.08413 | 0.92179 |
| C | -4.21080 | 0.54786 | -3.52795 |
| H | -5.24122 | 0.81277 | -3.28057 |
| H | -3.95132 | 1.07947 | -4.44584 |
| H | -4.16163 | -0.52240 | -3.74261 |
| C | -3.36450 | 2.48188 | -2.26298 |
| H | -4.37782 | 2.74175 | -1.94654 |
| H | -2.66923 | 2.88399 | -1.52285 |
| H | -3.16157 | 2.98648 | -3.21120 |
| C | -1.83277 | 0.61423 | -2.97168 |
| H | -1.01990 | 1.02533 | -2.36964 |
| H | -1.69394 | -0.46514 | -3.03955 |
| H | -1.71415 | 1.04842 | -3.96834 |
| C | 2.13080 | 1.83587 | 1.83172 |
| H | 1.80538 | 1.97794 | 0.79845 |
| H | 1.43106 | 1.17739 | 2.34111 |
| H | 2.06175 | 2.81194 | 2.31710 |
| C | 4.41469 | 2.52837 | 1.34471 |
| H | 4.21260 | 3.41915 | 1.94489 |
| H | 5.48559 | 2.32815 | 1.38786 |
| H | 4.15095 | 2.75517 | 0.30928 |
| C | 3.97504 | 1.09676 | 3.33991 |
| H | 5.03616 | 0.85992 | 3.43678 |
| H | 3.78560 | 1.99708 | 3.93034 |
| H | 3.40461 | 0.27807 | 3.77821 |
| C | 1.46069 | -0.74541 | -2.52874 |
| H | 1.12740 | -0.78831 | -3.56833 |
| H | 0.68418 | -1.23831 | -1.94922 |
| H | 1.51656 | 0.31007 | -2.24736 |
| C | 2.68275 | -2.92583 | -2.68654 |
| H | 2.05976 | -3.40308 | -1.93201 |
| H | 2.22129 | -3.08227 | -3.66525 |
| H | 3.65808 | -3.41871 | -2.69483 |
| C | 3.67912 | -0.80171 | -3.53830 |
| H | 3.82834 | 0.26806 | -3.37276 |
| H | 4.65867 | -1.26935 | -3.63855 |
| H | 3.15823 | -0.92780 | -4.49064 |
| C | 7.96819 | -1.02941 | 1.19607 |
| H | 8.04938 | 0.06052 | 1.19625 |
| H | 7.49930 | -1.34117 | 2.13274 |
| H | 8.98377 | -1.43183 | 1.18370 |
| C | 7.91797 | -1.05644 | -1.28462 |
| H | 7.44900 | -1.44152 | -2.19212 |
| H | 7.91364 | 0.03477 | -1.34092 |
| H | 8.95832 | -1.39288 | -1.27921 |
| C | 7.21965 | -3.07829 | 0.01420 |
| H | 6.72502 | -3.45568 | 0.91238 |
| H | 6.71286 | -3.50801 | -0.85206 |
| H | 8.25088 | -3.44165 | 0.01405 |
| Sn | -1.06475 | -2.62689 | 0.49718 |
| Cl | 1.55488 | -1.31339 | 2.59373 |
| Au | -0.25924 | 2.98585 | -0.43257 |
| Cl | 0.56173 | 5.04523 | -0.92293 |

Coordination through $\pi(\text{C}=\text{P})$ bond**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.69397 | -0.02751 | 1.07102 |
| C | 0.47796 | 0.04697 | -0.63785 |
| P | -1.00172 | -0.24869 | -1.52209 |
| Cl | 1.47464 | -2.66822 | -2.40019 |
| Sn | 1.63533 | -0.28173 | -2.67063 |
| O | -0.61580 | -0.07585 | -2.97531 |
| Au | 0.74848 | 2.08686 | -0.02707 |
| Cl | 1.02455 | 4.31507 | 0.01631 |
| Cl | -2.58743 | 0.88055 | -1.04029 |
| H | 2.11621 | -0.16629 | 1.08513 |
| H | -1.48220 | -1.53593 | -1.23468 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.63132 | 0.01059 | 1.00086 |
| C | 0.43175 | 0.14156 | -0.70334 |
| P | -1.03011 | -0.22644 | -1.60487 |
| Cl | 1.74440 | -2.60194 | -2.23182 |
| Sn | 1.65097 | -0.22086 | -2.67821 |
| O | -0.56620 | -0.21919 | -3.05275 |
| C | 2.42910 | -0.27293 | 1.22622 |
| H | 2.56855 | -1.35621 | 1.30950 |
| H | 3.04038 | 0.10072 | 0.40534 |
| H | 2.75041 | 0.18070 | 2.16590 |
| C | -1.75075 | -1.78916 | -1.12842 |
| H | -2.10733 | -1.74287 | -0.09872 |
| H | -2.57878 | -2.01325 | -1.80275 |
| H | -0.97271 | -2.54935 | -1.23163 |
| Au | 0.62328 | 2.16909 | -0.02732 |
| Cl | 0.84419 | 4.39989 | 0.17251 |
| Cl | -2.52741 | 1.10562 | -1.36145 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.13023 | 0.07913 | 1.17828 |
| C | 0.66672 | 0.11867 | -0.48372 |
| P | -0.92296 | -0.36361 | -1.10381 |
| Cl | 2.19884 | -2.60501 | -2.07320 |
| Sn | 1.57647 | -0.32537 | -2.61341 |
| O | -0.61779 | -0.77310 | -2.53743 |
| Au | 0.81340 | 2.18518 | 0.10373 |
| Cl | 0.93769 | 4.43173 | 0.25829 |
| C | 2.99177 | -0.04797 | 1.30594 |
| C | 3.79307 | 0.30031 | 0.06506 |
| C | 3.37992 | 0.86717 | 2.46954 |
| C | 3.22857 | -1.51304 | 1.69642 |
| H | 3.62915 | -0.42732 | -0.73376 |
| H | 3.57080 | 1.30572 | -0.30079 |
| H | 4.86198 | 0.26418 | 0.30055 |
| H | 2.78426 | 0.66273 | 3.36378 |
| H | 4.43103 | 0.70251 | 2.72529 |
| H | 3.25457 | 1.92177 | 2.21277 |
| H | 4.28963 | -1.65408 | 1.92575 |
| H | 2.66020 | -1.79483 | 2.58758 |
| H | 2.96666 | -2.19333 | 0.88240 |
| C | -1.85930 | -1.67130 | -0.22343 |
| C | -0.92492 | -2.87438 | -0.06865 |
| C | -2.33568 | -1.18132 | 1.14096 |
| C | -3.04771 | -2.04973 | -1.11068 |
| H | -0.51756 | -3.20709 | -1.02426 |
| H | -0.08989 | -2.66204 | 0.60107 |
| H | -1.49971 | -3.69734 | 0.36505 |
| H | -3.03827 | -0.35159 | 1.05383 |
| H | -2.84845 | -2.00622 | 1.64363 |

| | | | |
|----|----------|----------|----------|
| H | -1.50585 | -0.86941 | 1.77916 |
| H | -3.58970 | -2.86684 | -0.62654 |
| H | -3.74105 | -1.21710 | -1.24111 |
| H | -2.72156 | -2.39026 | -2.09441 |
| Cl | -2.18213 | 1.22987 | -1.15035 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.57416 | 0.20074 | 0.95516 |
| C | 0.34351 | 0.18360 | -0.74945 |
| P | -1.15730 | -0.13157 | -1.59978 |
| Cl | 1.76069 | -2.21800 | -2.99602 |
| Sn | 1.45054 | 0.17936 | -2.83226 |
| O | -0.78976 | 0.05514 | -3.06256 |
| Au | 0.60696 | 2.27501 | -0.24636 |
| Cl | 0.89143 | 4.50956 | -0.25203 |
| C | 2.34689 | -0.08358 | 1.20202 |
| C | 2.92111 | 0.46171 | 2.35310 |
| C | 3.12229 | -0.88193 | 0.35974 |
| C | 4.26167 | 0.25418 | 2.62942 |
| H | 2.31734 | 1.06416 | 3.02475 |
| C | 4.45876 | -1.10189 | 0.65110 |
| H | 2.67421 | -1.36134 | -0.50418 |
| C | 5.03129 | -0.52670 | 1.77761 |
| H | 4.70620 | 0.69734 | 3.51289 |
| H | 5.05350 | -1.72937 | -0.00273 |
| H | 6.07867 | -0.69711 | 1.99905 |
| C | -1.81481 | -1.75939 | -1.26937 |
| C | -1.76780 | -2.71449 | -2.28018 |
| C | -2.34436 | -2.07690 | -0.01925 |
| C | -2.25716 | -3.98906 | -2.03672 |
| H | -1.34489 | -2.45921 | -3.24334 |
| C | -2.82557 | -3.35192 | 0.21510 |
| H | -2.38653 | -1.32949 | 0.76570 |
| C | -2.78244 | -4.30662 | -0.79422 |
| H | -2.22191 | -4.73537 | -2.82136 |
| H | -3.23850 | -3.60256 | 1.18502 |
| H | -3.16194 | -5.30473 | -0.60735 |
| Cl | -2.65942 | 1.12736 | -1.09779 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.57337 | 0.26309 | 1.36475 |
| C | 0.20753 | 0.16312 | -0.31739 |
| P | -1.23925 | -0.11515 | -1.28119 |
| Cl | 1.79414 | -1.81933 | -2.94948 |
| Sn | 1.42561 | 0.49403 | -2.31007 |
| O | -0.79184 | 0.38995 | -2.64571 |
| Au | 0.26939 | 2.29793 | 0.13672 |
| Cl | 0.28085 | 4.55574 | 0.07556 |
| C | 2.38418 | 0.03678 | 1.43857 |
| C | 3.21048 | 1.02540 | 1.99836 |
| C | 2.92120 | -1.21997 | 1.09442 |
| C | 4.57549 | 0.78116 | 2.09404 |
| C | 4.29001 | -1.41342 | 1.21566 |
| C | 5.13985 | -0.41902 | 1.68648 |
| H | 5.21341 | 1.55327 | 2.51403 |
| H | 4.70201 | -2.38305 | 0.95219 |
| C | -1.83820 | -1.81018 | -1.28870 |
| C | -2.01022 | -2.50461 | -2.51036 |
| C | -2.16074 | -2.43979 | -0.06918 |
| C | -2.42599 | -3.82832 | -2.45295 |
| C | -2.57365 | -3.76512 | -0.08433 |
| C | -2.69274 | -4.48652 | -1.26086 |
| H | -2.55873 | -4.36112 | -3.38911 |
| H | -2.82312 | -4.23941 | 0.85993 |
| Cl | -2.85426 | 1.01088 | -0.74438 |
| C | 2.67679 | 2.33263 | 2.50227 |

| | | | |
|---|----------|----------|----------|
| H | 2.56988 | 3.06966 | 1.70071 |
| H | 1.69278 | 2.22387 | 2.96733 |
| H | 3.35175 | 2.75569 | 3.24797 |
| C | 2.06189 | -2.37789 | 0.67645 |
| H | 1.19879 | -2.49590 | 1.33909 |
| H | 1.68335 | -2.27346 | -0.34198 |
| H | 2.63540 | -3.30451 | 0.71947 |
| C | 6.61784 | -0.64444 | 1.76276 |
| H | 6.85074 | -1.68184 | 2.01046 |
| H | 7.09032 | -0.42656 | 0.79976 |
| H | 7.08229 | 0.00156 | 2.50945 |
| C | -2.10306 | -1.76787 | 1.26983 |
| H | -1.13165 | -1.91932 | 1.74890 |
| H | -2.28258 | -0.69476 | 1.23007 |
| H | -2.85569 | -2.20097 | 1.93058 |
| C | -1.81072 | -1.92013 | -3.87835 |
| H | -2.33242 | -0.97228 | -4.00531 |
| H | -0.75506 | -1.73576 | -4.08085 |
| H | -2.18312 | -2.62266 | -4.62438 |
| C | -3.10097 | -5.92563 | -1.25148 |
| H | -3.72388 | -6.16822 | -2.11435 |
| H | -2.21904 | -6.57229 | -1.29531 |
| H | -3.65088 | -6.17960 | -0.34412 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.67193 | 0.05456 | 1.16098 |
| C | 0.38782 | 0.09700 | -0.55450 |
| P | -1.04930 | -0.16312 | -1.61903 |
| O | -0.37797 | -0.08056 | -2.98369 |
| Cl | 2.81815 | -1.30318 | -3.25930 |
| Au | 0.34005 | 2.18661 | 0.06258 |
| Cl | 0.13903 | 4.44846 | 0.12150 |
| C | 2.52115 | -0.03001 | 1.25402 |
| C | 3.20877 | -1.16764 | 0.74675 |
| C | 3.28571 | 1.08827 | 1.66626 |
| C | 4.51569 | -1.00057 | 0.31533 |
| C | 4.59406 | 1.18881 | 1.18713 |
| C | 5.20459 | 0.20206 | 0.43410 |
| H | 5.02652 | -1.85249 | -0.11378 |
| H | 5.15619 | 2.07719 | 1.43832 |
| C | 2.91146 | 2.11602 | 2.75549 |
| C | 2.72999 | -2.62457 | 0.90403 |
| C | 6.59366 | 0.35585 | -0.17427 |
| C | 3.88645 | 1.84313 | 3.91994 |
| H | 3.77410 | 0.82225 | 4.29418 |
| H | 4.92714 | 1.97953 | 3.62384 |
| H | 3.67504 | 2.53367 | 4.74096 |
| C | 3.10375 | 3.56180 | 2.29043 |
| H | 2.43884 | 3.81596 | 1.46454 |
| H | 2.87940 | 4.24282 | 3.11598 |
| H | 4.13012 | 3.75910 | 1.97661 |
| C | 1.51444 | 1.97496 | 3.35225 |
| H | 1.44248 | 2.62257 | 4.23022 |
| H | 0.72152 | 2.29192 | 2.67247 |
| H | 1.30969 | 0.95365 | 3.68333 |
| C | 3.05906 | -3.49498 | -0.31116 |
| H | 2.63636 | -3.08439 | -1.22671 |
| H | 4.13403 | -3.60512 | -0.46154 |
| H | 2.65533 | -4.49950 | -0.15769 |
| C | 3.50877 | -3.17033 | 2.11687 |
| H | 4.58622 | -3.12406 | 1.95001 |
| H | 3.28289 | -2.59737 | 3.01987 |
| H | 3.23356 | -4.21425 | 2.29482 |
| C | 1.25178 | -2.80232 | 1.22936 |
| H | 0.95426 | -2.24451 | 2.12381 |
| H | 0.60225 | -2.52404 | 0.40073 |

| | | | |
|----|----------|----------|----------|
| H | 1.06141 | -3.85723 | 1.44696 |
| C | 7.20054 | 1.72734 | 0.10852 |
| H | 6.57553 | 2.53526 | -0.27982 |
| H | 7.35458 | 1.89391 | 1.17795 |
| H | 8.17587 | 1.80111 | -0.37839 |
| C | 6.48383 | 0.17857 | -1.69349 |
| H | 7.47315 | 0.25306 | -2.15379 |
| H | 6.05609 | -0.78964 | -1.96017 |
| H | 5.84690 | 0.95073 | -2.13196 |
| C | 7.53551 | -0.71202 | 0.39436 |
| H | 7.62053 | -0.62193 | 1.48027 |
| H | 7.19261 | -1.72280 | 0.16530 |
| H | 8.53419 | -0.59693 | -0.03584 |
| C | -2.35079 | -1.45978 | -1.66513 |
| C | -2.32345 | -2.35220 | -2.78074 |
| C | -3.58777 | -1.26171 | -0.99346 |
| C | -3.53420 | -2.66407 | -3.37991 |
| C | -1.10124 | -3.13171 | -3.30186 |
| C | -4.75498 | -1.64704 | -1.64453 |
| C | -3.78950 | -0.80781 | 0.46406 |
| C | -4.76520 | -2.25457 | -2.88750 |
| H | -3.51011 | -3.27847 | -4.26998 |
| C | -0.61161 | -2.62921 | -4.66295 |
| C | -1.51731 | -4.60705 | -3.47981 |
| C | 0.02168 | -3.17104 | -2.27397 |
| H | -5.69519 | -1.45402 | -1.14810 |
| C | -2.50507 | -0.46302 | 1.19511 |
| C | -4.38319 | -2.02591 | 1.20044 |
| C | -4.76592 | 0.36497 | 0.59533 |
| C | -6.04338 | -2.55668 | -3.65841 |
| H | 0.19840 | -3.27063 | -5.01979 |
| H | -1.42043 | -2.66914 | -5.39757 |
| H | -0.24395 | -1.60874 | -4.61131 |
| H | -2.19724 | -4.76192 | -4.31812 |
| H | -0.62052 | -5.19756 | -3.68336 |
| H | -1.98807 | -5.00392 | -2.57721 |
| H | 0.45161 | -2.19781 | -2.05010 |
| H | -0.33048 | -3.62827 | -1.34593 |
| H | 0.84503 | -3.77611 | -2.65764 |
| H | -1.76653 | -1.26188 | 1.10197 |
| H | -2.06709 | 0.47597 | 0.85821 |
| H | -2.71154 | -0.33970 | 2.26078 |
| H | -4.52048 | -1.77743 | 2.25633 |
| H | -5.35106 | -2.32366 | 0.79577 |
| H | -3.71199 | -2.88596 | 1.13722 |
| H | -5.74569 | 0.13768 | 0.17220 |
| H | -4.91243 | 0.59617 | 1.65373 |
| H | -4.38375 | 1.26018 | 0.10512 |
| C | -7.28358 | -2.00410 | -2.96121 |
| C | -6.20810 | -4.07377 | -3.80949 |
| C | -5.94370 | -1.91514 | -5.04771 |
| H | -7.44874 | -2.47279 | -1.98769 |
| H | -7.21959 | -0.92263 | -2.81767 |
| H | -8.16552 | -2.20570 | -3.57358 |
| H | -5.37285 | -4.52168 | -4.35126 |
| H | -6.27514 | -4.55988 | -2.83308 |
| H | -7.12346 | -4.29711 | -4.36425 |
| H | -5.83537 | -0.83068 | -4.97126 |
| H | -5.08964 | -2.29760 | -5.61001 |
| H | -6.84772 | -2.12818 | -5.62456 |
| Sn | 1.67250 | 0.67991 | -2.46257 |
| Cl | -2.24781 | 1.50642 | -1.58847 |

[R-P=C(Sn(II)Cl)-P(O)MeR](AuCl)**Coordination through Sn(II) atom****R= H**

| | | | |
|----|----------|----------|----------|
| P | 0.65446 | -0.14382 | 1.17454 |
| C | 0.47593 | -0.20530 | -0.47064 |
| P | -1.01756 | -0.16496 | -1.40760 |
| Cl | 1.76443 | -2.41087 | -2.78958 |
| Sn | 1.65541 | -0.10640 | -2.35730 |
| O | -0.47610 | 0.11022 | -2.81659 |
| C | -2.23516 | 1.03212 | -0.88074 |
| H | -3.08401 | 1.01254 | -1.56703 |
| H | -2.57463 | 0.78647 | 0.12833 |
| H | -1.78500 | 2.02576 | -0.88501 |
| Au | 3.25669 | 1.63528 | -3.17177 |
| Cl | 4.68257 | 3.26666 | -3.84512 |
| H | 2.08186 | -0.13059 | 1.23462 |
| H | -1.67422 | -1.41047 | -1.34120 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.65746 | -0.15984 | 1.16105 |
| C | 0.47511 | -0.21955 | -0.48006 |
| P | -1.03181 | -0.21589 | -1.39842 |
| Cl | 1.80175 | -2.39494 | -2.83167 |
| Sn | 1.61996 | -0.08715 | -2.37299 |
| O | -0.49323 | 0.07479 | -2.81544 |
| C | 2.46731 | -0.14092 | 1.44266 |
| H | 2.76809 | -1.13107 | 1.79975 |
| H | 3.03978 | 0.10830 | 0.54873 |
| H | 2.69752 | 0.57137 | 2.23851 |
| C | -1.86431 | -1.80088 | -1.33394 |
| H | -2.21805 | -2.00261 | -0.32105 |
| H | -2.70851 | -1.79799 | -2.02672 |
| H | -1.15257 | -2.57164 | -1.63445 |
| C | -2.20348 | 1.03763 | -0.88161 |
| H | -3.06804 | 1.02806 | -1.54848 |
| H | -2.52898 | 0.84500 | 0.14277 |
| H | -1.72103 | 2.01435 | -0.93077 |
| Au | 3.22109 | 1.65188 | -3.19917 |
| Cl | 4.66369 | 3.27848 | -3.85908 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.69434 | -0.58428 | 0.94224 |
| C | 0.64333 | -0.20450 | -0.66631 |
| P | -0.81345 | -0.15698 | -1.67744 |
| Cl | 2.72437 | -1.45161 | -3.24688 |
| Sn | 1.84542 | 0.55528 | -2.37253 |
| O | -0.20350 | 0.31816 | -3.01751 |
| Au | 2.90425 | 2.80365 | -2.70643 |
| Cl | 3.81778 | 4.87759 | -2.90795 |
| C | 2.45643 | -0.45577 | 1.55123 |
| C | 2.79761 | -1.85446 | 2.07628 |
| C | 3.47711 | -0.01271 | 0.52190 |
| C | 2.40828 | 0.53274 | 2.72072 |
| H | 2.06012 | -2.20843 | 2.80214 |
| H | 2.85813 | -2.58521 | 1.26603 |
| H | 3.77028 | -1.82685 | 2.57772 |
| H | 3.27251 | 0.99556 | 0.15055 |
| H | 4.47289 | 0.01636 | 0.97630 |
| H | 3.53335 | -0.70796 | -0.32099 |
| H | 3.38246 | 0.55497 | 3.21920 |
| H | 2.18207 | 1.54712 | 2.38309 |
| H | 1.66040 | 0.24595 | 3.46529 |
| C | -1.68487 | -1.75481 | -1.89573 |
| C | -2.72038 | -1.56673 | -3.00797 |
| C | -0.66012 | -2.80717 | -2.31861 |

| | | | |
|---|----------|----------|----------|
| C | -2.36250 | -2.16636 | -0.59049 |
| H | -3.50609 | -0.86116 | -2.72869 |
| H | -2.25575 | -1.22289 | -3.93378 |
| H | -3.20032 | -2.52923 | -3.20607 |
| H | 0.08881 | -2.98007 | -1.54405 |
| H | -1.18266 | -3.75011 | -2.50235 |
| H | -0.13909 | -2.52267 | -3.23387 |
| H | -2.81874 | -3.15097 | -0.72567 |
| H | -1.65083 | -2.24345 | 0.23561 |
| H | -3.15627 | -1.47466 | -0.30024 |
| C | -1.98052 | 1.06381 | -1.06078 |
| H | -2.82229 | 1.16703 | -1.74700 |
| H | -2.33928 | 0.78619 | -0.06881 |
| H | -1.45795 | 2.01941 | -0.99581 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78674 | -0.03528 | 1.22748 |
| C | 0.45782 | -0.31907 | -0.37091 |
| P | -1.11828 | -0.37093 | -1.15832 |
| Cl | 1.75182 | -2.58094 | -2.74963 |
| Sn | 1.45665 | -0.27330 | -2.33896 |
| O | -0.69927 | -0.23298 | -2.63590 |
| Au | 2.86257 | 1.49778 | -3.41843 |
| Cl | 4.12765 | 3.14607 | -4.34320 |
| C | 2.58759 | -0.06714 | 1.35154 |
| C | 3.16308 | 0.73522 | 2.33977 |
| C | 3.41423 | -0.85316 | 0.54390 |
| C | 4.54013 | 0.79534 | 2.47937 |
| H | 2.52675 | 1.32789 | 2.98977 |
| C | 4.78873 | -0.80171 | 0.69578 |
| H | 2.97992 | -1.53967 | -0.17639 |
| C | 5.35252 | 0.03044 | 1.65505 |
| H | 4.98007 | 1.43746 | 3.23343 |
| H | 5.42316 | -1.41569 | 0.06731 |
| H | 6.42978 | 0.07301 | 1.76657 |
| C | -1.99334 | -1.91204 | -0.88818 |
| C | -2.12550 | -2.80645 | -1.94613 |
| C | -2.52280 | -2.22420 | 0.36346 |
| C | -2.79585 | -4.00500 | -1.75187 |
| H | -1.69923 | -2.56088 | -2.91127 |
| C | -3.18912 | -3.42251 | 0.55006 |
| H | -2.40597 | -1.54171 | 1.19932 |
| C | -3.32701 | -4.31151 | -0.50868 |
| H | -2.89795 | -4.70222 | -2.57503 |
| H | -3.59899 | -3.66653 | 1.52307 |
| H | -3.84802 | -5.25029 | -0.35961 |
| C | -2.20820 | 0.96394 | -0.66183 |
| H | -3.12015 | 0.92489 | -1.26022 |
| H | -2.46277 | 0.87119 | 0.39565 |
| H | -1.69744 | 1.91333 | -0.82831 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.91646 | -0.38600 | 1.79074 |
| C | 0.37052 | -0.45591 | 0.22755 |
| P | -1.20876 | -0.36953 | -0.57327 |
| Cl | 1.68233 | -1.99301 | -2.66779 |
| Sn | 1.40202 | 0.11151 | -1.62376 |
| O | -0.74800 | 0.24731 | -1.91270 |
| Au | 2.85711 | 2.09337 | -2.12014 |
| Cl | 4.18757 | 3.91710 | -2.43365 |
| C | 2.71250 | -0.17991 | 1.53551 |
| C | 3.27426 | 1.09837 | 1.68114 |
| C | 3.52140 | -1.28428 | 1.22944 |
| C | 4.63573 | 1.25833 | 1.46946 |
| C | 4.88156 | -1.07418 | 1.03256 |
| C | 5.45529 | 0.18697 | 1.13268 |

| | | | |
|---|----------|----------|----------|
| H | 5.06561 | 2.25166 | 1.55559 |
| H | 5.51170 | -1.92597 | 0.79451 |
| C | -2.04809 | -1.95524 | -0.77946 |
| C | -2.47837 | -2.39489 | -2.05230 |
| C | -2.30689 | -2.74459 | 0.35792 |
| C | -3.13573 | -3.61584 | -2.13666 |
| C | -2.97314 | -3.95390 | 0.20752 |
| C | -3.38819 | -4.41545 | -1.03088 |
| H | -3.46988 | -3.94926 | -3.11413 |
| H | -3.17213 | -4.55001 | 1.09295 |
| C | -2.36415 | 0.78226 | 0.18689 |
| H | -3.19446 | 0.92912 | -0.50725 |
| H | -2.75395 | 0.41319 | 1.13471 |
| H | -1.85238 | 1.73313 | 0.34283 |
| C | -1.87453 | -2.37985 | 1.74760 |
| H | -0.86074 | -2.73979 | 1.94391 |
| H | -1.86915 | -1.30923 | 1.94992 |
| H | -2.53488 | -2.84606 | 2.48014 |
| C | -2.28407 | -1.64059 | -3.33662 |
| H | -2.62856 | -0.60852 | -3.27666 |
| H | -1.23056 | -1.60244 | -3.61783 |
| H | -2.83296 | -2.14065 | -4.13495 |
| C | -4.07355 | -5.73746 | -1.17812 |
| H | -4.52454 | -6.06097 | -0.23895 |
| H | -4.85309 | -5.69833 | -1.94129 |
| H | -3.35833 | -6.50723 | -1.48397 |
| C | 2.95885 | -2.67128 | 1.11511 |
| H | 2.26613 | -2.89444 | 1.93280 |
| H | 2.40932 | -2.80917 | 0.17953 |
| H | 3.75793 | -3.41308 | 1.14328 |
| C | 2.42511 | 2.29024 | 2.00831 |
| H | 1.66182 | 2.05618 | 2.75798 |
| H | 3.03389 | 3.10956 | 2.39191 |
| H | 1.90761 | 2.65953 | 1.11684 |
| C | 6.91401 | 0.39893 | 0.87135 |
| H | 7.05899 | 0.93634 | -0.07031 |
| H | 7.37473 | 0.99941 | 1.65913 |
| H | 7.44997 | -0.54863 | 0.80371 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.19960 | 2.21884 | 1.16953 |
| C | 0.28186 | 0.76791 | 0.52156 |
| P | 1.81173 | -0.13567 | 0.35568 |
| Cl | -1.10312 | 0.28622 | -2.81771 |
| O | 1.40774 | -1.01745 | -0.85605 |
| C | 1.90953 | -1.31567 | 1.72301 |
| H | 2.72595 | -2.00538 | 1.50130 |
| H | 2.05729 | -0.87389 | 2.70275 |
| H | 0.97113 | -1.87543 | 1.71959 |
| C | 3.53281 | 0.43844 | 0.11986 |
| C | 4.09907 | 0.30286 | -1.18111 |
| C | 4.41380 | 0.48814 | 1.23289 |
| C | 5.40413 | -0.16060 | -1.26819 |
| C | 5.71858 | 0.03692 | 1.05788 |
| C | 6.21172 | -0.39257 | -0.16306 |
| H | 5.81245 | -0.33654 | -2.25475 |
| H | 6.37452 | 0.03406 | 1.91725 |
| C | -2.00808 | 2.15867 | 0.83741 |
| C | -2.53714 | 2.89035 | -0.25015 |
| C | -2.84010 | 1.26819 | 1.56285 |
| C | -3.78001 | 2.50475 | -0.74688 |
| C | -4.06054 | 0.92439 | 0.99368 |
| C | -4.52549 | 1.47453 | -0.19413 |
| H | -4.17378 | 3.01954 | -1.60846 |
| H | -4.68411 | 0.20392 | 1.50460 |
| C | -1.85204 | 4.13898 | -0.84075 |

| | | | |
|---|----------|----------|----------|
| C | -2.54384 | 0.76187 | 2.99331 |
| C | -5.83302 | 0.97911 | -0.80317 |
| C | 4.13647 | 1.17501 | 2.58623 |
| C | 3.45132 | 0.76075 | -2.50190 |
| C | 7.59815 | -1.00010 | -0.33555 |
| C | -3.85973 | 0.59006 | 3.76863 |
| H | -3.62898 | 0.39839 | 4.81923 |
| H | -4.48157 | 1.48655 | 3.71414 |
| H | -4.44529 | -0.25974 | 3.41519 |
| C | -1.72383 | 1.78287 | 3.78433 |
| H | -0.69933 | 1.89778 | 3.40998 |
| H | -2.19346 | 2.76926 | 3.77703 |
| H | -1.63018 | 1.45287 | 4.82241 |
| C | -1.82584 | -0.58997 | 3.01720 |
| H | -2.38068 | -1.34676 | 2.45783 |
| H | -0.82443 | -0.51738 | 2.59344 |
| H | -1.73106 | -0.93978 | 4.04952 |
| C | -6.97971 | 1.17974 | 0.19471 |
| H | -7.91872 | 0.82515 | -0.23892 |
| H | -6.81503 | 0.62702 | 1.12162 |
| H | -7.09926 | 2.23635 | 0.44807 |
| C | -6.18617 | 1.71616 | -2.09234 |
| H | -7.11285 | 1.30677 | -2.50131 |
| H | -6.34573 | 2.78454 | -1.92335 |
| H | -5.40958 | 1.59757 | -2.85197 |
| C | -5.69298 | -0.51387 | -1.12506 |
| H | -4.89293 | -0.68466 | -1.84936 |
| H | -5.46744 | -1.10688 | -0.23666 |
| H | -6.62461 | -0.89488 | -1.55234 |
| C | -2.74323 | 4.84283 | -1.86728 |
| H | -3.71188 | 5.12431 | -1.44811 |
| H | -2.24532 | 5.75911 | -2.19258 |
| H | -2.91148 | 4.23008 | -2.75590 |
| C | -1.60052 | 5.14361 | 0.29270 |
| H | -2.53623 | 5.41186 | 0.78915 |
| H | -0.91768 | 4.75232 | 1.05014 |
| H | -1.15412 | 6.05662 | -0.11142 |
| C | -0.53286 | 3.82681 | -1.55153 |
| H | 0.24729 | 3.49214 | -0.86304 |
| H | -0.66121 | 3.05188 | -2.30845 |
| H | -0.15657 | 4.73256 | -2.03624 |
| C | 2.75725 | 1.80966 | 2.70235 |
| H | 2.54906 | 2.46449 | 1.85389 |
| H | 1.94148 | 1.09423 | 2.79172 |
| H | 2.71990 | 2.42783 | 3.60258 |
| C | 5.12995 | 2.35305 | 2.66694 |
| H | 4.95755 | 2.91021 | 3.59181 |
| H | 6.16820 | 2.02081 | 2.66332 |
| H | 4.99116 | 3.03686 | 1.82638 |
| C | 4.39294 | 0.25848 | 3.78663 |
| H | 5.41830 | -0.11494 | 3.79993 |
| H | 4.23534 | 0.81563 | 4.71387 |
| H | 3.73021 | -0.60759 | 3.80167 |
| C | 2.26070 | 1.68656 | -2.27590 |
| H | 1.92603 | 2.08561 | -3.23608 |
| H | 1.39808 | 1.19017 | -1.84265 |
| H | 2.53968 | 2.53150 | -1.64062 |
| C | 3.07215 | -0.41535 | -3.40596 |
| H | 2.31195 | -1.04291 | -2.94732 |
| H | 2.68546 | -0.03823 | -4.35651 |
| H | 3.94670 | -1.03419 | -3.62353 |
| C | 4.48801 | 1.62047 | -3.25381 |
| H | 4.86059 | 2.43541 | -2.62833 |
| H | 5.34301 | 1.04595 | -3.61118 |
| H | 4.00648 | 2.05925 | -4.13115 |
| C | 8.31769 | -1.18741 | 0.99742 |

| | | | |
|----|----------|----------|----------|
| H | 8.51221 | -0.23395 | 1.49528 |
| H | 7.74850 | -1.82395 | 1.67961 |
| H | 9.28368 | -1.66761 | 0.82534 |
| C | 8.45440 | -0.08913 | -1.22345 |
| H | 8.01753 | 0.03930 | -2.21560 |
| H | 8.56778 | 0.90101 | -0.77524 |
| H | 9.45077 | -0.52069 | -1.35169 |
| C | 7.45561 | -2.37268 | -1.00431 |
| H | 6.86100 | -3.04998 | -0.38656 |
| H | 6.97220 | -2.29936 | -1.98038 |
| H | 8.44111 | -2.82271 | -1.15115 |
| Au | -2.13066 | -2.74831 | -0.11761 |
| Cl | -3.40341 | -4.52994 | 0.52715 |
| Sn | -0.74391 | -0.74245 | -0.72355 |

Coordination through O atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.74314 | -0.01583 | 1.04752 |
| C | 0.52740 | -0.12731 | -0.59086 |
| P | -0.98612 | 0.04417 | -1.44087 |
| Cl | 1.20472 | -2.54805 | -2.80579 |
| Sn | 1.78757 | -0.24802 | -2.50362 |
| O | -0.47798 | 0.41083 | -2.86185 |
| C | -2.15471 | 1.23638 | -0.80459 |
| H | -3.04228 | 1.25813 | -1.43993 |
| H | -2.43393 | 0.94830 | 0.21232 |
| H | -1.68962 | 2.22298 | -0.79045 |
| Au | -1.82141 | 0.77923 | -4.43424 |
| Cl | -3.26471 | 1.19392 | -6.07190 |
| H | 2.16624 | -0.17072 | 1.09164 |
| H | -1.67202 | -1.18353 | -1.47584 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.70647 | -0.11544 | 1.03206 |
| C | 0.51283 | -0.15189 | -0.60896 |
| P | -1.02575 | -0.01046 | -1.42374 |
| Cl | 1.44122 | -2.47422 | -2.90967 |
| Sn | 1.73559 | -0.11533 | -2.54645 |
| O | -0.53314 | 0.33854 | -2.86656 |
| C | 2.51186 | -0.30622 | 1.30724 |
| H | 2.70098 | -1.33330 | 1.63513 |
| H | 3.10591 | -0.10390 | 0.41533 |
| H | 2.82575 | 0.35450 | 2.11872 |
| C | -1.94088 | -1.54720 | -1.43385 |
| H | -2.26451 | -1.78973 | -0.41956 |
| H | -2.80908 | -1.45028 | -2.08965 |
| H | -1.28186 | -2.33223 | -1.80887 |
| C | -2.10832 | 1.27628 | -0.80596 |
| H | -3.01234 | 1.32541 | -1.41647 |
| H | -2.37280 | 1.05803 | 0.23136 |
| H | -1.58737 | 2.23317 | -0.85187 |
| Au | -1.87188 | 0.71938 | -4.43402 |
| Cl | -3.31556 | 1.14308 | -6.07120 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.79999 | -0.59565 | 0.86954 |
| C | 0.45339 | -0.11457 | -0.67574 |
| P | -1.18444 | -0.04990 | -1.30768 |
| Cl | 2.00813 | -1.19962 | -3.58395 |
| Sn | 1.40640 | 0.87524 | -2.52245 |
| O | -0.91105 | 0.59155 | -2.71054 |
| C | -2.23262 | 1.04500 | -0.34153 |
| H | -3.21653 | 1.14759 | -0.80127 |
| H | -2.32780 | 0.66336 | 0.67641 |

| | | | |
|----|----------|----------|----------|
| H | -1.75399 | 2.02493 | -0.31037 |
| Au | -2.27433 | 1.68298 | -3.87030 |
| Cl | -3.70819 | 2.86351 | -5.09439 |
| C | 2.65017 | -0.49965 | 1.13636 |
| C | 3.09248 | -1.94491 | 1.38832 |
| C | 3.44154 | 0.10015 | -0.00919 |
| C | 2.84258 | 0.32440 | 2.41215 |
| H | 2.51513 | -2.41202 | 2.19111 |
| H | 2.98844 | -2.55887 | 0.49046 |
| H | 4.14592 | -1.95862 | 1.68671 |
| H | 3.14443 | 1.13522 | -0.20545 |
| H | 4.50803 | 0.11863 | 0.23973 |
| H | 3.33854 | -0.49292 | -0.92305 |
| H | 3.89673 | 0.30743 | 2.70680 |
| H | 2.55142 | 1.36802 | 2.26711 |
| H | 2.25807 | -0.07664 | 3.24470 |
| C | -2.02678 | -1.66985 | -1.49921 |
| C | -3.32658 | -1.46776 | -2.28174 |
| C | -1.09979 | -2.60840 | -2.27088 |
| C | -2.32985 | -2.24295 | -0.11494 |
| H | -4.03435 | -0.82026 | -1.76015 |
| H | -3.14802 | -1.05134 | -3.27467 |
| H | -3.80621 | -2.44262 | -2.40817 |
| H | -0.16686 | -2.79342 | -1.73661 |
| H | -1.61138 | -3.56513 | -2.40819 |
| H | -0.84785 | -2.21314 | -3.25572 |
| H | -2.76526 | -3.23817 | -0.23996 |
| H | -1.42997 | -2.35030 | 0.49571 |
| H | -3.05234 | -1.63608 | 0.43513 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.67819 | 0.16003 | 0.90746 |
| C | 0.51033 | -0.26580 | -0.68483 |
| P | -0.96250 | -0.18680 | -1.61552 |
| Cl | 1.76547 | -2.85136 | -2.65672 |
| Sn | 1.90810 | -0.45531 | -2.47029 |
| O | -0.37141 | -0.14143 | -3.05752 |
| C | -1.96968 | 1.26355 | -1.30108 |
| H | -2.83718 | 1.25984 | -1.96336 |
| H | -2.29853 | 1.26960 | -0.25989 |
| H | -1.36595 | 2.15239 | -1.48975 |
| Au | -1.47828 | 0.29567 | -4.78308 |
| Cl | -2.64428 | 0.77618 | -6.61533 |
| C | 2.43488 | -0.12413 | 1.25086 |
| C | 3.18563 | -1.13274 | 0.63892 |
| C | 3.04723 | 0.69844 | 2.19862 |
| C | 4.52922 | -1.28404 | 0.94124 |
| H | 2.70346 | -1.83381 | -0.03642 |
| C | 4.39446 | 0.55306 | 2.48903 |
| H | 2.46539 | 1.46552 | 2.70053 |
| C | 5.13653 | -0.43537 | 1.85790 |
| H | 5.10109 | -2.07452 | 0.46889 |
| H | 4.86550 | 1.20783 | 3.21309 |
| H | 6.18801 | -0.55566 | 2.09220 |
| C | -2.00035 | -1.63164 | -1.40967 |
| C | -2.79151 | -1.76650 | -0.26891 |
| C | -1.99424 | -2.63129 | -2.37817 |
| C | -3.57960 | -2.89198 | -0.10597 |
| H | -2.79026 | -1.00092 | 0.49993 |
| C | -2.78898 | -3.75453 | -2.20874 |
| H | -1.36949 | -2.53178 | -3.25694 |
| C | -3.57989 | -3.88435 | -1.07784 |
| H | -4.19527 | -2.99577 | 0.77968 |
| H | -2.78713 | -4.52967 | -2.96561 |
| H | -4.20000 | -4.76413 | -0.94973 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.62038 | -0.19467 | 1.26178 |
| C | 0.37012 | -0.34263 | -0.36662 |
| P | -1.03924 | -0.21908 | -1.40278 |
| Cl | 2.08621 | -2.50334 | -2.44748 |
| Sn | 1.94508 | -0.14045 | -1.97704 |
| O | -0.31323 | 0.08192 | -2.75242 |
| Au | -0.99348 | 1.32479 | -4.29898 |
| Cl | -1.68201 | 2.66269 | -5.93828 |
| C | 2.44955 | -0.24704 | 1.36956 |
| C | 3.11444 | -1.48148 | 1.44640 |
| C | 3.16966 | 0.95415 | 1.46244 |
| C | 4.49793 | -1.48498 | 1.57553 |
| C | 4.55188 | 0.89969 | 1.58977 |
| C | 5.23575 | -0.30897 | 1.63994 |
| H | 5.01336 | -2.43901 | 1.63628 |
| H | 5.10897 | 1.82949 | 1.65932 |
| C | -2.05203 | -1.71579 | -1.47668 |
| C | -2.78082 | -2.07599 | -0.32375 |
| C | -2.12140 | -2.53153 | -2.63065 |
| C | -3.54900 | -3.23199 | -0.33780 |
| C | -2.91643 | -3.67078 | -2.58065 |
| C | -3.63624 | -4.04459 | -1.45619 |
| H | -4.09406 | -3.50207 | 0.56149 |
| H | -2.96385 | -4.29570 | -3.46667 |
| C | 2.47618 | 2.28387 | 1.41393 |
| H | 2.12835 | 2.51939 | 0.40301 |
| H | 1.59687 | 2.30605 | 2.06569 |
| H | 3.14661 | 3.08506 | 1.72697 |
| C | 6.72921 | -0.34446 | 1.74751 |
| H | 7.18668 | -0.39810 | 0.75465 |
| H | 7.11529 | 0.55083 | 2.23767 |
| H | 7.06738 | -1.21743 | 2.30863 |
| C | 2.36513 | -2.77923 | 1.39504 |
| H | 1.48795 | -2.76380 | 2.04973 |
| H | 2.00997 | -2.99154 | 0.38254 |
| H | 3.00308 | -3.60672 | 1.70778 |
| C | -2.81317 | -1.26954 | 0.94309 |
| H | -3.59560 | -0.50591 | 0.90007 |
| H | -3.04633 | -1.91705 | 1.78908 |
| H | -1.87070 | -0.77278 | 1.17621 |
| C | -1.40573 | -2.27510 | -3.92406 |
| H | -1.70023 | -1.32559 | -4.37618 |
| H | -0.32405 | -2.25267 | -3.79327 |
| H | -1.64484 | -3.06882 | -4.63167 |
| C | -4.49047 | -5.27299 | -1.46171 |
| H | -4.70631 | -5.61419 | -0.44831 |
| H | -5.44667 | -5.07344 | -1.95514 |
| H | -4.00932 | -6.08777 | -2.00610 |
| C | -2.08280 | 1.20136 | -1.03683 |
| H | -2.90904 | 1.23858 | -1.74929 |
| H | -2.46882 | 1.16445 | -0.02008 |
| H | -1.46880 | 2.09564 | -1.15856 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.87690 | 2.16453 | -0.28398 |
| C | 0.94142 | 0.79737 | -0.31526 |
| P | -0.78709 | 0.51699 | -0.46760 |
| C | 3.56251 | 1.40562 | -0.26017 |
| C | 4.28687 | 1.36512 | 0.96067 |
| C | 4.04861 | 0.69916 | -1.38014 |
| C | 5.29531 | 0.42168 | 1.08299 |
| C | 5.04392 | -0.26024 | -1.16751 |
| C | 5.64254 | -0.45971 | 0.06255 |
| H | 5.82614 | 0.34847 | 2.02081 |
| H | 5.37084 | -0.85378 | -2.00998 |

| | | | |
|---|----------|----------|----------|
| C | 3.68969 | 0.98326 | -2.85608 |
| C | 4.04829 | 2.35865 | 2.11328 |
| C | 6.68788 | -1.54128 | 0.31374 |
| C | 2.69846 | 2.14717 | 2.80385 |
| H | 1.85409 | 2.39560 | 2.15656 |
| H | 2.57352 | 1.11144 | 3.12355 |
| H | 2.62933 | 2.79869 | 3.68002 |
| C | 4.13524 | 3.79031 | 1.56677 |
| H | 5.10843 | 3.97128 | 1.10366 |
| H | 3.36297 | 3.99979 | 0.82366 |
| H | 4.00717 | 4.50728 | 2.38253 |
| C | 5.12016 | 2.23480 | 3.19911 |
| H | 5.07106 | 1.27578 | 3.72002 |
| H | 6.12869 | 2.36608 | 2.79968 |
| H | 4.95511 | 3.01681 | 3.94368 |
| C | 2.92466 | -0.18009 | -3.49075 |
| H | 1.93455 | -0.29080 | -3.04317 |
| H | 2.78787 | -0.00291 | -4.56146 |
| H | 3.45634 | -1.12656 | -3.37266 |
| C | 2.89900 | 2.27173 | -3.07674 |
| H | 1.86179 | 2.19847 | -2.74500 |
| H | 3.36450 | 3.12552 | -2.57748 |
| H | 2.86745 | 2.49308 | -4.14724 |
| C | 5.00871 | 1.17798 | -3.62804 |
| H | 5.60614 | 1.97803 | -3.18454 |
| H | 5.62050 | 0.27645 | -3.65374 |
| H | 4.78665 | 1.45158 | -4.66275 |
| C | 6.91281 | -2.42428 | -0.91073 |
| H | 7.30726 | -1.85716 | -1.75801 |
| H | 7.64225 | -3.20113 | -0.67004 |
| H | 5.99249 | -2.92266 | -1.22596 |
| C | 6.21852 | -2.43295 | 1.46972 |
| H | 6.08075 | -1.86384 | 2.39088 |
| H | 5.26599 | -2.91368 | 1.23572 |
| H | 6.95868 | -3.21391 | 1.66491 |
| C | 8.02315 | -0.88675 | 0.68749 |
| H | 7.93667 | -0.27543 | 1.58797 |
| H | 8.77784 | -1.65492 | 0.87773 |
| H | 8.38540 | -0.24617 | -0.12057 |
| C | -2.23936 | 1.37415 | 0.23292 |
| C | -2.83474 | 0.80386 | 1.39481 |
| C | -3.05340 | 2.17048 | -0.61468 |
| C | -4.21756 | 0.70378 | 1.42315 |
| C | -4.43306 | 2.03078 | -0.51301 |
| C | -5.04087 | 1.21216 | 0.42709 |
| H | -4.67167 | 0.20045 | 2.26716 |
| H | -5.05415 | 2.59424 | -1.19598 |
| C | -2.09368 | 0.43724 | 2.69397 |
| C | -2.15987 | -1.05498 | 3.02525 |
| C | -2.79385 | 1.21290 | 3.82883 |
| H | -1.58359 | -1.64914 | 2.31788 |
| H | -1.74662 | -1.22584 | 4.02298 |
| H | -3.18869 | -1.42167 | 3.01985 |
| H | -2.81787 | 2.28529 | 3.61966 |
| H | -3.81683 | 0.87808 | 4.00244 |
| H | -2.23634 | 1.05940 | 4.75631 |
| C | -2.55811 | 3.32571 | -1.50811 |
| C | -3.22211 | 4.60154 | -0.94912 |
| C | -2.98257 | 3.17975 | -2.97222 |
| H | -2.96745 | 4.74407 | 0.10353 |
| H | -2.86372 | 5.47054 | -1.50785 |
| H | -4.30859 | 4.57404 | -1.03261 |
| H | -2.53603 | 2.30940 | -3.45299 |
| H | -4.06592 | 3.08692 | -3.06749 |
| H | -2.67754 | 4.06646 | -3.53449 |
| C | -6.53857 | 0.94075 | 0.45344 |

| | | | |
|----|----------|----------|----------|
| C | -7.14946 | 1.55210 | 1.72020 |
| C | -6.76341 | -0.57650 | 0.45876 |
| H | -7.00301 | 2.63504 | 1.74560 |
| H | -8.22413 | 1.35280 | 1.74982 |
| H | -6.70847 | 1.13109 | 2.62590 |
| H | -6.32177 | -1.05099 | -0.42013 |
| H | -6.32214 | -1.04958 | 1.33783 |
| H | -7.83519 | -0.79286 | 0.46592 |
| Cl | 2.01435 | -1.56419 | 2.13195 |
| O | -0.83108 | -0.95939 | 0.07800 |
| Au | -2.41969 | -2.24729 | -0.41280 |
| Cl | -4.09432 | -3.61911 | -0.95430 |
| C | -1.05891 | 3.58648 | -1.41379 |
| H | -0.73965 | 3.70133 | -0.37584 |
| H | -0.44005 | 2.81707 | -1.87125 |
| H | -0.82115 | 4.51758 | -1.93405 |
| C | -0.64734 | 0.91286 | 2.70626 |
| H | -0.00075 | 0.34983 | 2.03789 |
| H | -0.57938 | 1.97561 | 2.45900 |
| H | -0.23172 | 0.77461 | 3.70713 |
| C | -7.25177 | 1.53025 | -0.76052 |
| H | -7.19128 | 2.62173 | -0.78409 |
| H | -6.84481 | 1.13916 | -1.69632 |
| H | -8.31061 | 1.26433 | -0.72373 |
| Sn | 1.49530 | -1.42466 | -0.21651 |
| C | -1.11950 | 0.31801 | -2.23760 |
| H | -0.85514 | 1.18392 | -2.83717 |
| H | -0.51253 | -0.53194 | -2.55851 |
| H | -2.17022 | 0.06215 | -2.38107 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.67524 | 0.00286 | 0.91186 |
| C | 0.41429 | -0.23392 | -0.68171 |
| P | -1.09999 | -0.18773 | -1.56555 |
| Cl | 1.17242 | -2.80753 | -2.72867 |
| Sn | 1.54920 | -0.43510 | -2.71759 |
| O | -0.63016 | 0.01623 | -3.00536 |
| C | -2.29149 | 1.03890 | -1.04491 |
| H | -3.16158 | 0.99170 | -1.70300 |
| H | -2.60016 | 0.84089 | -0.01540 |
| H | -1.84145 | 2.03054 | -1.10705 |
| Au | -0.68395 | 0.42402 | 2.59549 |
| Cl | -2.12108 | 0.87669 | 4.27753 |
| H | 2.07052 | -0.08545 | 1.11248 |
| H | -1.74779 | -1.42662 | -1.39148 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.73095 | 0.02971 | 0.87470 |
| C | 0.41248 | -0.18726 | -0.70878 |
| P | -1.15986 | -0.24548 | -1.49477 |
| Cl | 1.34885 | -2.81856 | -2.64833 |
| Sn | 1.43007 | -0.40774 | -2.78954 |
| O | -0.76486 | -0.18296 | -2.97820 |
| C | 2.50742 | -0.00335 | 1.21765 |
| H | 2.71831 | -0.83961 | 1.88880 |
| H | 3.08156 | -0.11391 | 0.29846 |
| H | 2.79013 | 0.91640 | 1.73450 |
| C | -2.01311 | -1.76896 | -1.09770 |
| H | -2.27157 | -1.79156 | -0.03700 |
| H | -2.92076 | -1.84110 | -1.70090 |
| H | -1.34949 | -2.60147 | -1.33745 |
| C | -2.24706 | 1.11272 | -1.06133 |
| H | -3.15790 | 1.04705 | -1.66040 |

| | | | |
|----|----------|---------|----------|
| H | -2.50286 | 1.06939 | -0.00032 |
| H | -1.74423 | 2.05648 | -1.27498 |
| Au | -0.69312 | 0.32792 | 2.54153 |
| Cl | -2.20158 | 0.63318 | 4.20193 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.73088 | 0.09566 | 0.82464 |
| C | 0.45760 | -0.32911 | -0.72948 |
| P | -1.08757 | -0.46456 | -1.57326 |
| Cl | 2.05350 | -2.79744 | -2.69626 |
| Sn | 1.56941 | -0.43296 | -2.77994 |
| O | -0.62337 | -0.57266 | -3.03803 |
| C | -2.08822 | 1.01337 | -1.34703 |
| H | -2.99723 | 0.94901 | -1.94687 |
| H | -2.34501 | 1.15250 | -0.29551 |
| H | -1.50143 | 1.86858 | -1.68545 |
| Au | -0.74698 | 0.66137 | 2.38477 |
| Cl | -2.28602 | 1.27607 | 3.93411 |
| C | 2.51771 | 0.11946 | 1.31177 |
| C | 2.80824 | 1.50212 | 1.89932 |
| C | 2.67349 | -0.94855 | 2.39966 |
| C | 3.44094 | -0.17540 | 0.14175 |
| H | 2.71698 | 2.28958 | 1.14735 |
| H | 2.13555 | 1.74040 | 2.72681 |
| H | 3.83230 | 1.51816 | 2.28400 |
| H | 2.49501 | -1.95249 | 2.00782 |
| H | 3.69605 | -0.91269 | 2.78756 |
| H | 1.99206 | -0.77736 | 3.23671 |
| H | 4.47640 | -0.18385 | 0.49556 |
| H | 3.23707 | -1.15116 | -0.30566 |
| H | 3.37159 | 0.59549 | -0.63071 |
| C | -2.09681 | -1.92990 | -1.11661 |
| C | -1.21165 | -3.17335 | -1.17938 |
| C | -2.69135 | -1.77525 | 0.27968 |
| C | -3.21088 | -2.03948 | -2.16288 |
| H | -0.76215 | -3.30699 | -2.16380 |
| H | -0.40393 | -3.13538 | -0.44656 |
| H | -1.82744 | -4.05050 | -0.96086 |
| H | -3.36546 | -0.92022 | 0.35916 |
| H | -3.27100 | -2.67254 | 0.51444 |
| H | -1.92125 | -1.67543 | 1.04787 |
| H | -3.77973 | -2.95316 | -1.96902 |
| H | -3.91111 | -1.20258 | -2.11282 |
| H | -2.80703 | -2.09824 | -3.17493 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.71616 | 0.21197 | 0.70588 |
| C | 0.49216 | -0.39420 | -0.79412 |
| P | -1.01014 | -0.59388 | -1.68329 |
| Cl | 1.87064 | -3.23439 | -2.25948 |
| Sn | 1.69621 | -0.86514 | -2.71083 |
| O | -0.49210 | -0.87875 | -3.10067 |
| C | -2.05630 | 0.86331 | -1.66063 |
| H | -2.92107 | 0.68915 | -2.30365 |
| H | -2.39271 | 1.08705 | -0.64645 |
| H | -1.48176 | 1.70957 | -2.04007 |
| Au | -0.79368 | 1.08956 | 2.07166 |
| Cl | -2.41280 | 1.96462 | 3.39440 |
| C | 2.43213 | 0.13470 | 1.20049 |
| C | 2.88862 | 1.03725 | 2.16203 |
| C | 3.30667 | -0.81356 | 0.66375 |
| C | 4.21675 | 1.01759 | 2.55362 |
| H | 2.20089 | 1.75558 | 2.59660 |
| C | 4.63012 | -0.83240 | 1.06751 |
| H | 2.94031 | -1.56056 | -0.03284 |
| C | 5.08694 | 0.08645 | 2.00431 |

| | | | |
|---|----------|----------|----------|
| H | 4.57156 | 1.72611 | 3.29270 |
| H | 5.30497 | -1.57531 | 0.65880 |
| H | 6.12437 | 0.06643 | 2.31804 |
| C | -1.97968 | -1.96866 | -1.06338 |
| C | -2.76116 | -1.84245 | 0.08510 |
| C | -1.92409 | -3.18362 | -1.74126 |
| C | -3.48696 | -2.92713 | 0.54634 |
| H | -2.80266 | -0.90571 | 0.63128 |
| C | -2.65547 | -4.26459 | -1.27365 |
| H | -1.30572 | -3.27608 | -2.62565 |
| C | -3.43495 | -4.13687 | -0.13396 |
| H | -4.09286 | -2.82726 | 1.43912 |
| H | -2.61145 | -5.21029 | -1.80091 |
| H | -4.00427 | -4.98466 | 0.22988 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.69432 | 0.33363 | 1.11895 |
| C | 0.32165 | -0.40617 | -0.28917 |
| P | -1.08847 | -0.53284 | -1.34238 |
| Cl | 1.80669 | -3.04799 | -2.01161 |
| Sn | 1.75177 | -0.62532 | -2.07433 |
| O | -0.38279 | -0.43424 | -2.70396 |
| Au | -0.58015 | 1.36398 | 2.61287 |
| Cl | -1.89139 | 2.44340 | 4.11554 |
| C | 2.47976 | 0.26706 | 1.36430 |
| C | 3.23359 | 1.44558 | 1.23466 |
| C | 3.09175 | -0.94805 | 1.71268 |
| C | 4.60446 | 1.37921 | 1.43527 |
| C | 4.46756 | -0.95638 | 1.90757 |
| C | 5.24031 | 0.18981 | 1.77331 |
| H | 5.19322 | 2.28477 | 1.32438 |
| H | 4.94819 | -1.89169 | 2.17755 |
| C | -2.01412 | -2.07715 | -1.14647 |
| C | -2.63024 | -2.36525 | 0.08798 |
| C | -2.14410 | -2.99051 | -2.21946 |
| C | -3.30533 | -3.56747 | 0.25060 |
| C | -2.84537 | -4.16979 | -1.99645 |
| C | -3.41724 | -4.49169 | -0.77479 |
| H | -3.76293 | -3.77785 | 1.21251 |
| H | -2.94297 | -4.86754 | -2.82218 |
| C | 2.59410 | 2.75165 | 0.86992 |
| H | 2.11567 | 2.70499 | -0.11315 |
| H | 1.82128 | 3.03595 | 1.59101 |
| H | 3.33479 | 3.55104 | 0.84097 |
| C | 2.31297 | -2.21800 | 1.88367 |
| H | 1.40630 | -2.05977 | 2.47483 |
| H | 2.00264 | -2.63113 | 0.91975 |
| H | 2.91746 | -2.96934 | 2.39267 |
| C | 6.71687 | 0.15423 | 2.01874 |
| H | 6.94103 | 0.42362 | 3.05563 |
| H | 7.12625 | -0.84157 | 1.84253 |
| H | 7.24412 | 0.86268 | 1.37733 |
| C | -2.65341 | -1.41983 | 1.25114 |
| H | -2.73677 | -1.97010 | 2.18901 |
| H | -1.76667 | -0.79282 | 1.32536 |
| H | -3.52034 | -0.75421 | 1.19525 |
| C | -1.59605 | -2.79607 | -3.60479 |
| H | -1.85459 | -1.82658 | -4.02762 |
| H | -0.50756 | -2.86743 | -3.61105 |
| H | -1.99084 | -3.57567 | -4.25718 |
| C | -4.11696 | -5.79848 | -0.57050 |
| H | -4.62013 | -6.12718 | -1.48161 |
| H | -3.39914 | -6.57764 | -0.29563 |
| H | -4.85579 | -5.73544 | 0.22993 |
| C | -2.23461 | 0.84461 | -1.19070 |
| H | -2.68980 | 0.88749 | -0.20189 |

| | | | |
|---|----------|---------|----------|
| H | -1.68125 | 1.76710 | -1.37340 |
| H | -3.01438 | 0.73379 | -1.94701 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.04304 | 0.95903 | 0.04330 |
| C | -0.19471 | -0.36960 | 0.47801 |
| P | 1.44737 | -0.95275 | 0.77332 |
| Cl | -1.45203 | -3.13709 | -1.58144 |
| O | 1.24827 | -2.44575 | 0.43104 |
| C | 3.08145 | -0.45965 | 0.10646 |
| C | 3.62060 | -1.27891 | -0.92593 |
| C | 3.98275 | 0.29419 | 0.90408 |
| C | 4.96901 | -1.59928 | -0.85787 |
| C | 5.32438 | -0.07662 | 0.90413 |
| C | 5.82976 | -1.08731 | 0.10333 |
| H | 5.36492 | -2.27870 | -1.60175 |
| H | 5.99940 | 0.46577 | 1.55144 |
| C | -2.79730 | 0.45608 | 0.09097 |
| C | -3.47567 | 0.09961 | -1.10445 |
| C | -3.38158 | 0.16927 | 1.34988 |
| C | -4.58291 | -0.73480 | -0.98862 |
| C | -4.47441 | -0.69201 | 1.37117 |
| C | -5.06054 | -1.20400 | 0.22550 |
| H | -5.07813 | -1.05448 | -1.89003 |
| H | -4.89010 | -0.96779 | 2.33177 |
| C | -3.13055 | 0.65338 | -2.50115 |
| C | -3.00298 | 0.78756 | 2.71498 |
| C | -6.20616 | -2.20526 | 0.33185 |
| C | 3.66741 | 1.61334 | 1.63762 |
| C | 2.88166 | -1.73506 | -2.19720 |
| C | 7.27393 | -1.56718 | 0.17905 |
| C | -4.28821 | 1.35483 | 3.34744 |
| H | -4.04033 | 1.84077 | 4.29447 |
| H | -4.74735 | 2.10007 | 2.69377 |
| H | -5.03382 | 0.58923 | 3.56006 |
| C | -2.03537 | 1.96757 | 2.65286 |
| H | -1.00961 | 1.67235 | 2.42880 |
| H | -2.34923 | 2.72219 | 1.92766 |
| H | -2.00588 | 2.45160 | 3.63285 |
| C | -2.41911 | -0.27449 | 3.65061 |
| H | -3.09630 | -1.12181 | 3.77539 |
| H | -1.47142 | -0.65543 | 3.26376 |
| H | -2.23219 | 0.15640 | 4.63842 |
| C | -7.37212 | -1.57717 | 1.10403 |
| H | -8.19591 | -2.29155 | 1.18571 |
| H | -7.08244 | -1.28800 | 2.11634 |
| H | -7.74454 | -0.68558 | 0.59364 |
| C | -6.71897 | -2.64722 | -1.03619 |
| H | -7.51875 | -3.37982 | -0.90443 |
| H | -7.13103 | -1.81134 | -1.60729 |
| H | -5.93277 | -3.11844 | -1.63088 |
| C | -5.70860 | -3.44731 | 1.08144 |
| H | -4.88185 | -3.92060 | 0.54616 |
| H | -5.36173 | -3.20143 | 2.08745 |
| H | -6.51643 | -4.17823 | 1.17591 |
| C | -4.04866 | 0.08413 | -3.58746 |
| H | -5.10053 | 0.31904 | -3.41000 |
| H | -3.77365 | 0.53706 | -4.54227 |
| H | -3.93944 | -0.99807 | -3.69214 |
| C | -3.35936 | 2.17102 | -2.47674 |
| H | -4.39675 | 2.40196 | -2.22174 |
| H | -2.71573 | 2.67583 | -1.75285 |
| H | -3.14530 | 2.59778 | -3.46023 |
| C | -1.70293 | 0.33976 | -2.95481 |
| H | -0.94027 | 0.87087 | -2.38177 |
| H | -1.49384 | -0.72876 | -2.89622 |

| | | | |
|----|----------|----------|----------|
| H | -1.57685 | 0.66618 | -3.99094 |
| C | 2.25046 | 2.12293 | 1.41135 |
| H | 2.03190 | 2.18250 | 0.34321 |
| H | 1.46995 | 1.52920 | 1.88272 |
| H | 2.15686 | 3.13463 | 1.81187 |
| C | 4.57429 | 2.68520 | 0.99563 |
| H | 4.34310 | 3.66049 | 1.43157 |
| H | 5.63380 | 2.48706 | 1.15886 |
| H | 4.40087 | 2.74855 | -0.08064 |
| C | 3.99344 | 1.56236 | 3.13337 |
| H | 5.04054 | 1.30582 | 3.30624 |
| H | 3.81797 | 2.54461 | 3.57997 |
| H | 3.38513 | 0.83647 | 3.67311 |
| C | 1.53607 | -1.04561 | -2.39148 |
| H | 1.16738 | -1.25942 | -3.39743 |
| H | 0.76917 | -1.40505 | -1.71129 |
| H | 1.62776 | 0.03975 | -2.29541 |
| C | 2.71215 | -3.25554 | -2.25017 |
| H | 2.08859 | -3.60847 | -1.43111 |
| H | 2.23872 | -3.54063 | -3.19350 |
| H | 3.67947 | -3.76165 | -2.19525 |
| C | 3.74113 | -1.29671 | -3.40034 |
| H | 3.92245 | -0.21915 | -3.38559 |
| H | 4.70591 | -1.80274 | -3.44433 |
| H | 3.20468 | -1.53737 | -4.32158 |
| C | 8.04796 | -0.89662 | 1.31082 |
| H | 8.13921 | 0.18217 | 1.16097 |
| H | 7.57857 | -1.07185 | 2.28220 |
| H | 9.05983 | -1.30643 | 1.35292 |
| C | 7.98885 | -1.26141 | -1.14256 |
| H | 7.51209 | -1.76181 | -1.98755 |
| H | 7.99238 | -0.18793 | -1.34648 |
| H | 9.02664 | -1.60271 | -1.09527 |
| C | 7.28034 | -3.08129 | 0.42124 |
| H | 6.78888 | -3.32883 | 1.36532 |
| H | 6.76425 | -3.62055 | -0.37540 |
| H | 8.30861 | -3.45053 | 0.46521 |
| Sn | -0.95938 | -2.57224 | 0.71914 |
| Au | -0.38701 | 3.01376 | -0.51611 |
| Cl | 0.27845 | 5.12142 | -1.04749 |
| C | 1.64038 | -0.95342 | 2.57701 |
| H | 2.59153 | -1.43378 | 2.81221 |
| H | 1.58567 | 0.01792 | 3.05644 |
| H | 0.83338 | -1.58271 | 2.96016 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.85188 | -0.12399 | 1.06203 |
| C | 0.54016 | 0.06450 | -0.61974 |
| P | -1.00470 | -0.14556 | -1.45334 |
| Cl | 1.42426 | -2.67790 | -2.33647 |
| Sn | 1.60765 | -0.29712 | -2.68808 |
| O | -0.61191 | -0.05961 | -2.92686 |
| C | -2.33753 | 0.97664 | -1.04299 |
| H | -3.20949 | 0.72686 | -1.65140 |
| H | -2.59015 | 0.87913 | 0.01519 |
| H | -2.03157 | 2.00275 | -1.25240 |
| Au | 0.85145 | 2.06506 | 0.10287 |
| Cl | 1.05635 | 4.30628 | 0.16054 |
| H | 2.27440 | -0.25453 | 1.00043 |
| H | -1.49270 | -1.42334 | -1.11344 |

R = Me

| | | | |
|---|---------|----------|---------|
| P | 0.74859 | -0.12825 | 1.04354 |
|---|---------|----------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.45715 | 0.14730 | -0.62601 |
| P | -1.05794 | -0.16708 | -1.49439 |
| Cl | 1.76719 | -2.55848 | -2.16259 |
| Sn | 1.60738 | -0.18049 | -2.64341 |
| O | -0.58680 | -0.21716 | -2.95472 |
| C | 2.56478 | -0.35760 | 1.16645 |
| H | 2.74798 | -1.43675 | 1.12619 |
| H | 3.12194 | 0.12506 | 0.36383 |
| H | 2.91282 | 0.00941 | 2.13397 |
| C | -1.75027 | -1.73884 | -0.97952 |
| H | -2.06838 | -1.69264 | 0.06396 |
| H | -2.60302 | -1.98354 | -1.61616 |
| H | -0.97917 | -2.50223 | -1.09879 |
| C | -2.34290 | 1.06951 | -1.29189 |
| H | -3.19104 | 0.80288 | -1.92686 |
| H | -2.66673 | 1.11781 | -0.25063 |
| H | -1.96260 | 2.04546 | -1.59611 |
| Au | 0.61400 | 2.11862 | 0.21229 |
| Cl | 0.69219 | 4.35690 | 0.48190 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.06166 | -0.06261 | 1.10549 |
| C | 0.59437 | 0.12266 | -0.53928 |
| P | -1.00593 | -0.28670 | -1.22347 |
| Cl | 2.22238 | -2.37499 | -2.41518 |
| Sn | 1.50396 | -0.07304 | -2.70761 |
| O | -0.65235 | -0.55010 | -2.69796 |
| C | -1.83237 | -1.75838 | -0.49366 |
| Au | 0.68965 | 2.13780 | 0.23311 |
| Cl | 0.65833 | 4.38493 | 0.46010 |
| C | 2.92704 | -0.15099 | 1.23183 |
| C | 3.71915 | 0.33931 | 0.03374 |
| C | 3.28930 | 0.65465 | 2.48098 |
| C | 3.20424 | -1.64014 | 1.47579 |
| H | 3.56978 | -0.30593 | -0.83525 |
| H | 3.47302 | 1.37091 | -0.22991 |
| H | 4.78894 | 0.30445 | 0.26599 |
| H | 2.69985 | 0.34561 | 3.34896 |
| H | 4.34504 | 0.49760 | 2.72240 |
| H | 3.13304 | 1.72565 | 2.32970 |
| H | 4.26806 | -1.77503 | 1.69631 |
| H | 2.64055 | -2.02541 | 2.33058 |
| H | 2.96350 | -2.24201 | 0.59609 |
| C | -2.16355 | 1.09073 | -1.13271 |
| H | -2.39565 | 1.35854 | -0.10197 |
| H | -1.71349 | 1.95173 | -1.62950 |
| H | -3.08021 | 0.82492 | -1.66268 |
| C | -2.37152 | -1.43227 | 0.89821 |
| H | -2.80877 | -2.33873 | 1.32673 |
| H | -1.58346 | -1.09600 | 1.57666 |
| H | -3.15557 | -0.67274 | 0.87038 |
| C | -0.83429 | -2.91302 | -0.42059 |
| H | -0.03157 | -2.71495 | 0.29162 |
| H | -1.36306 | -3.80989 | -0.08516 |
| H | -0.37969 | -3.12468 | -1.38935 |
| C | -2.97846 | -2.14149 | -1.43527 |
| H | -3.45218 | -3.05110 | -1.05518 |
| H | -3.74964 | -1.36977 | -1.48819 |
| H | -2.61608 | -2.34125 | -2.44480 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.61932 | 0.11764 | 0.98191 |
| C | 0.38094 | 0.17599 | -0.71762 |
| P | -1.15098 | -0.08446 | -1.57198 |
| Cl | 1.77909 | -2.23886 | -2.93819 |
| Sn | 1.47604 | 0.16645 | -2.80389 |

| | | | |
|----|----------|----------|----------|
| O | -0.73409 | 0.06027 | -3.04070 |
| C | -2.47604 | 1.06163 | -1.17468 |
| H | -3.34644 | 0.81327 | -1.78547 |
| H | -2.74186 | 0.98857 | -0.11863 |
| H | -2.15107 | 2.07965 | -1.39481 |
| Au | 0.61533 | 2.25076 | -0.12017 |
| Cl | 0.79385 | 4.50050 | -0.12707 |
| C | 2.39925 | -0.13401 | 1.22660 |
| C | 2.96408 | 0.39641 | 2.38883 |
| C | 3.18877 | -0.89792 | 0.36637 |
| C | 4.30891 | 0.20923 | 2.65965 |
| H | 2.34929 | 0.97128 | 3.07462 |
| C | 4.52991 | -1.09799 | 0.65173 |
| H | 2.74892 | -1.36642 | -0.50775 |
| C | 5.09279 | -0.53716 | 1.79012 |
| H | 4.74571 | 0.64128 | 3.55253 |
| H | 5.13581 | -1.69880 | -0.01679 |
| H | 6.14366 | -0.69177 | 2.00677 |
| C | -1.78479 | -1.73117 | -1.23680 |
| C | -1.79273 | -2.67283 | -2.26082 |
| C | -2.27395 | -2.06721 | 0.02508 |
| C | -2.29581 | -3.94327 | -2.02296 |
| H | -1.39558 | -2.40820 | -3.23284 |
| C | -2.77290 | -3.33735 | 0.25632 |
| H | -2.25681 | -1.34480 | 0.83499 |
| C | -2.78513 | -4.27451 | -0.76908 |
| H | -2.29761 | -4.67737 | -2.82003 |
| H | -3.15038 | -3.59858 | 1.23800 |
| H | -3.17457 | -5.26941 | -0.58549 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.56280 | 0.08271 | 1.35659 |
| C | 0.15285 | 0.26884 | -0.30660 |
| P | -1.30610 | -0.00426 | -1.30398 |
| Cl | 2.12016 | -1.37421 | -2.92884 |
| Sn | 1.35962 | 0.82985 | -2.23878 |
| O | -0.78303 | 0.45170 | -2.67383 |
| Au | 0.03934 | 2.27368 | 0.52660 |
| Cl | -0.29775 | 4.50367 | 0.71534 |
| C | 2.38587 | -0.06019 | 1.36795 |
| C | 3.23130 | 0.91860 | 1.91249 |
| C | 2.91103 | -1.30510 | 0.97129 |
| C | 4.59914 | 0.67287 | 1.94952 |
| C | 4.28320 | -1.50225 | 1.03487 |
| C | 5.14867 | -0.51857 | 1.49687 |
| H | 5.25303 | 1.43655 | 2.36048 |
| H | 4.68458 | -2.46280 | 0.72569 |
| C | -1.82827 | -1.73906 | -1.27232 |
| C | -1.78339 | -2.54599 | -2.43282 |
| C | -2.30271 | -2.28701 | -0.06312 |
| C | -2.14822 | -3.88295 | -2.31796 |
| C | -2.64185 | -3.63230 | -0.01119 |
| C | -2.55647 | -4.45532 | -1.12278 |
| H | -2.10979 | -4.49953 | -3.21048 |
| H | -2.99456 | -4.04215 | 0.93055 |
| C | 2.71916 | 2.21363 | 2.46770 |
| H | 2.52578 | 2.95049 | 1.68201 |
| H | 1.78557 | 2.08259 | 3.02193 |
| H | 3.45005 | 2.65140 | 3.14942 |
| C | 2.02927 | -2.43636 | 0.53037 |
| H | 1.16417 | -2.55849 | 1.19114 |
| H | 1.65222 | -2.28496 | -0.48339 |
| H | 2.58541 | -3.37464 | 0.53936 |
| C | 6.62911 | -0.74225 | 1.51225 |
| H | 6.87252 | -1.78488 | 1.72558 |
| H | 7.06515 | -0.49967 | 0.53807 |

| | | | |
|---|----------|----------|----------|
| H | 7.12022 | -0.11404 | 2.25722 |
| C | -2.54643 | -1.48968 | 1.18667 |
| H | -2.42012 | -2.11948 | 2.06823 |
| H | -1.88312 | -0.63523 | 1.31058 |
| H | -3.57601 | -1.11773 | 1.20141 |
| C | -1.39681 | -2.07144 | -3.80401 |
| H | -1.93258 | -1.16945 | -4.09689 |
| H | -0.33237 | -1.84101 | -3.86248 |
| H | -1.61575 | -2.85604 | -4.52907 |
| C | -2.88667 | -5.91237 | -1.03744 |
| H | -3.32346 | -6.27660 | -1.96898 |
| H | -1.98209 | -6.49955 | -0.85064 |
| H | -3.58469 | -6.11737 | -0.22415 |
| C | -2.75107 | 1.01148 | -0.94052 |
| H | -2.47352 | 2.05974 | -1.06506 |
| H | -3.52209 | 0.75746 | -1.67205 |
| H | -3.13909 | 0.85545 | 0.06364 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.68890 | -0.04664 | 1.16220 |
| C | 0.39749 | 0.08040 | -0.54479 |
| P | -1.06162 | -0.12174 | -1.62624 |
| O | -0.33331 | -0.11653 | -2.98440 |
| Cl | 2.84466 | -1.33981 | -3.23497 |
| Au | 0.29580 | 2.13274 | 0.17552 |
| Cl | -0.07742 | 4.37762 | 0.15454 |
| C | 2.54294 | -0.08611 | 1.25979 |
| C | 3.25599 | -1.20772 | 0.75393 |
| C | 3.28302 | 1.05106 | 1.66445 |
| C | 4.55742 | -1.01069 | 0.31720 |
| C | 4.58529 | 1.18368 | 1.17721 |
| C | 5.21677 | 0.20881 | 0.42564 |
| H | 5.08608 | -1.85187 | -0.11186 |
| H | 5.12656 | 2.08695 | 1.42194 |
| C | 2.88996 | 2.07025 | 2.75588 |
| C | 2.80950 | -2.67557 | 0.90451 |
| C | 6.59794 | 0.39440 | -0.19189 |
| C | -2.09684 | 1.36394 | -1.70076 |
| H | -2.61957 | 1.60732 | -0.78132 |
| H | -1.46110 | 2.20433 | -1.98524 |
| H | -2.82193 | 1.18525 | -2.49803 |
| C | 3.89725 | 1.84768 | 3.90347 |
| H | 3.83718 | 0.82470 | 4.28373 |
| H | 4.92542 | 2.02864 | 3.58871 |
| H | 3.67019 | 2.53220 | 4.72540 |
| C | 3.01308 | 3.51958 | 2.27905 |
| H | 2.31671 | 3.74486 | 1.47027 |
| H | 2.78679 | 4.19804 | 3.10623 |
| H | 4.02156 | 3.75200 | 1.93277 |
| C | 1.51324 | 1.87150 | 3.38312 |
| H | 1.43319 | 2.51292 | 4.26490 |
| H | 0.69167 | 2.15688 | 2.72267 |
| H | 1.35692 | 0.84093 | 3.71160 |
| C | 3.12459 | -3.52522 | -0.32853 |
| H | 2.65716 | -3.12190 | -1.22519 |
| H | 4.19656 | -3.59726 | -0.51825 |
| H | 2.75964 | -4.54373 | -0.16944 |
| C | 3.62418 | -3.22275 | 2.09257 |
| H | 4.69677 | -3.16167 | 1.90100 |
| H | 3.41285 | -2.66146 | 3.00638 |
| H | 3.36645 | -4.27179 | 2.26666 |
| C | 1.34221 | -2.88076 | 1.26096 |
| H | 1.06102 | -2.35006 | 2.17603 |
| H | 0.66943 | -2.58908 | 0.45486 |
| H | 1.16870 | -3.94382 | 1.45167 |
| C | 7.17123 | 1.78253 | 0.07971 |

| | | | |
|----|----------|----------|----------|
| H | 6.52331 | 2.57183 | -0.30945 |
| H | 7.32722 | 1.95913 | 1.14729 |
| H | 8.14145 | 1.87849 | -0.41355 |
| C | 6.48393 | 0.20597 | -1.70944 |
| H | 7.46830 | 0.30357 | -2.17610 |
| H | 6.07962 | -0.77432 | -1.96827 |
| H | 5.82399 | 0.95832 | -2.14821 |
| C | 7.57014 | -0.64573 | 0.37693 |
| H | 7.65965 | -0.54703 | 1.46175 |
| H | 7.25114 | -1.66611 | 0.15612 |
| H | 8.56290 | -0.50833 | -0.06045 |
| C | -2.35464 | -1.44373 | -1.65252 |
| C | -2.33248 | -2.35422 | -2.75038 |
| C | -3.60193 | -1.21356 | -1.00947 |
| C | -3.53908 | -2.65589 | -3.36694 |
| C | -1.11488 | -3.15970 | -3.24045 |
| C | -4.76808 | -1.58515 | -1.67264 |
| C | -3.81522 | -0.75060 | 0.44530 |
| C | -4.77062 | -2.21601 | -2.90452 |
| H | -3.50987 | -3.28448 | -4.24722 |
| C | -0.61212 | -2.69905 | -4.61136 |
| C | -1.54699 | -4.63467 | -3.37696 |
| C | 0.00310 | -3.17845 | -2.20698 |
| H | -5.71273 | -1.37084 | -1.19291 |
| C | -2.53452 | -0.42350 | 1.19255 |
| C | -4.42909 | -1.95957 | 1.18057 |
| C | -4.78930 | 0.42579 | 0.56779 |
| C | -6.04220 | -2.51220 | -3.68961 |
| H | 0.19877 | -3.35288 | -4.94301 |
| H | -1.41434 | -2.75699 | -5.35227 |
| H | -0.24061 | -1.67880 | -4.58179 |
| H | -2.23234 | -4.80535 | -4.20786 |
| H | -0.65751 | -5.24072 | -3.56661 |
| H | -2.01889 | -5.00109 | -2.46197 |
| H | 0.44419 | -2.20289 | -2.02094 |
| H | -0.36079 | -3.59495 | -1.26433 |
| H | 0.81691 | -3.81229 | -2.56389 |
| H | -1.81170 | -1.23744 | 1.11551 |
| H | -2.05830 | 0.49910 | 0.86118 |
| H | -2.75383 | -0.28621 | 2.25392 |
| H | -4.57669 | -1.70791 | 2.23445 |
| H | -5.39425 | -2.24931 | 0.76378 |
| H | -3.76472 | -2.82522 | 1.12638 |
| H | -5.77150 | 0.19245 | 0.15391 |
| H | -4.92994 | 0.67298 | 1.62323 |
| H | -4.42509 | 1.32265 | 0.06464 |
| C | -7.28415 | -1.93029 | -3.01985 |
| C | -6.22804 | -4.02882 | -3.81818 |
| C | -5.91451 | -1.89633 | -5.08804 |
| H | -7.46969 | -2.37994 | -2.04102 |
| H | -7.20677 | -0.84747 | -2.89321 |
| H | -8.16039 | -2.12942 | -3.64121 |
| H | -5.39174 | -4.49785 | -4.34001 |
| H | -6.31567 | -4.49728 | -2.83480 |
| H | -7.13865 | -4.24850 | -4.38227 |
| H | -5.79612 | -0.81166 | -5.02883 |
| H | -5.05564 | -2.29731 | -5.62972 |
| H | -6.81144 | -2.10933 | -5.67599 |
| Sn | 1.68048 | 0.64198 | -2.45515 |

[R-P=C(Sn(II)Cl)-P(S)ClR](AuCl)

Coordination through Sn(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.68673 | 0.29534 | 0.99904 |
| C | 0.43878 | -0.11822 | -0.58909 |
| P | -1.11866 | -0.29764 | -1.36007 |
| Cl | 1.62196 | -2.37551 | -2.90618 |
| Sn | 1.63754 | -0.06445 | -2.45401 |
| Au | 3.47472 | 1.53095 | -3.05247 |
| Cl | 5.13893 | 2.99612 | -3.51955 |
| Cl | -2.66537 | 0.51450 | -0.36865 |
| H | 2.11229 | 0.38082 | 0.94678 |
| H | -1.49870 | -1.65074 | -1.36160 |
| S | -0.84999 | 0.42691 | -3.19329 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.66074 | 0.10158 | 1.05053 |
| C | 0.39260 | -0.18564 | -0.56077 |
| P | -1.18176 | -0.26045 | -1.31527 |
| Cl | 1.58887 | -2.38499 | -2.97388 |
| Sn | 1.57508 | -0.08183 | -2.42554 |
| C | 2.48167 | 0.10759 | 1.22498 |
| H | 2.78593 | -0.86745 | 1.61993 |
| H | 3.01607 | 0.29893 | 0.29323 |
| H | 2.76160 | 0.85846 | 1.96714 |
| C | -1.83622 | -1.93050 | -1.33599 |
| H | -2.01141 | -2.26511 | -0.31231 |
| H | -2.76677 | -1.94314 | -1.90496 |
| H | -1.09146 | -2.56480 | -1.82230 |
| Au | 3.49915 | 1.44983 | -2.92009 |
| Cl | 5.25858 | 2.84589 | -3.24640 |
| Cl | -2.60512 | 0.78840 | -0.33606 |
| S | -0.85655 | 0.46460 | -3.15769 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.65693 | -0.39556 | 0.82998 |
| C | 0.65203 | -0.13420 | -0.81147 |
| P | -0.86477 | -0.14934 | -1.71395 |
| Cl | 2.76904 | -1.40805 | -3.33174 |
| Sn | 1.97127 | 0.62456 | -2.42116 |
| Au | 3.34749 | 2.72612 | -2.45361 |
| Cl | 4.58260 | 4.63345 | -2.37692 |
| C | 2.40477 | -0.36366 | 1.47642 |
| C | 2.55698 | -1.70491 | 2.20499 |
| C | 3.50744 | -0.19321 | 0.45015 |
| C | 2.43418 | 0.77908 | 2.49788 |
| H | 1.75893 | -1.86819 | 2.93464 |
| H | 2.56143 | -2.54609 | 1.50723 |
| H | 3.50855 | -1.71269 | 2.74560 |
| H | 3.48242 | 0.79611 | -0.01526 |
| H | 4.48246 | -0.27720 | 0.94119 |
| H | 3.47135 | -0.96219 | -0.32655 |
| H | 3.38966 | 0.76032 | 3.03142 |
| H | 2.33947 | 1.75470 | 2.01559 |
| H | 1.63730 | 0.68432 | 3.24080 |
| C | -1.65410 | -1.81124 | -1.92184 |
| C | -2.85620 | -1.65237 | -2.85103 |
| C | -0.60964 | -2.72808 | -2.55916 |
| C | -2.08810 | -2.36037 | -0.56646 |
| H | -3.62667 | -1.01177 | -2.41895 |
| H | -2.56587 | -1.24771 | -3.82245 |
| H | -3.29342 | -2.64068 | -3.01668 |
| H | 0.26697 | -2.85918 | -1.92302 |
| H | -1.06835 | -3.70881 | -2.71208 |
| H | -0.27267 | -2.35589 | -3.52738 |

| | | | |
|----|----------|----------|----------|
| H | -2.51197 | -3.35614 | -0.72296 |
| H | -1.24856 | -2.46313 | 0.12417 |
| H | -2.85058 | -1.73938 | -0.09510 |
| Cl | -2.28529 | 0.95169 | -0.76563 |
| S | -0.39549 | 0.70012 | -3.47181 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.72934 | 0.24295 | 1.28727 |
| C | 0.30736 | -0.22872 | -0.25120 |
| P | -1.32288 | -0.30300 | -0.87416 |
| Cl | 1.47250 | -2.63777 | -2.54110 |
| Sn | 1.38603 | -0.29935 | -2.16813 |
| Au | 3.18581 | 1.23346 | -3.01349 |
| Cl | 4.84247 | 2.62772 | -3.70620 |
| C | 2.52471 | 0.09298 | 1.31682 |
| C | 3.21595 | 1.01038 | 2.11300 |
| C | 3.24236 | -0.88296 | 0.61726 |
| C | 4.59993 | 0.99043 | 2.16091 |
| H | 2.66518 | 1.75463 | 2.67969 |
| C | 4.62442 | -0.90918 | 0.68177 |
| H | 2.71741 | -1.64888 | 0.05424 |
| C | 5.30331 | 0.03420 | 1.44258 |
| H | 5.13091 | 1.72116 | 2.75942 |
| H | 5.17443 | -1.66721 | 0.13681 |
| H | 6.38622 | 0.01742 | 1.48135 |
| C | -2.11467 | -1.88461 | -0.55233 |
| C | -2.27707 | -2.79998 | -1.58613 |
| C | -2.50525 | -2.20859 | 0.74714 |
| C | -2.84097 | -4.03871 | -1.31926 |
| H | -1.95903 | -2.54503 | -2.58952 |
| C | -3.06488 | -3.44657 | 1.00278 |
| H | -2.37874 | -1.49566 | 1.55418 |
| C | -3.23368 | -4.36095 | -0.03037 |
| H | -2.96893 | -4.75252 | -2.12413 |
| H | -3.37237 | -3.69971 | 2.01046 |
| H | -3.67341 | -5.33024 | 0.17452 |
| Cl | -2.54051 | 1.03603 | 0.03886 |
| S | -1.11376 | 0.10043 | -2.82384 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.80724 | 0.03700 | 1.90088 |
| C | 0.25688 | -0.32355 | 0.37246 |
| P | -1.37427 | -0.25379 | -0.27931 |
| Cl | 1.17200 | -2.24983 | -2.40734 |
| Sn | 1.38471 | -0.06964 | -1.49363 |
| Au | 3.39709 | 1.34374 | -2.01781 |
| Cl | 5.27745 | 2.58849 | -2.36925 |
| C | 2.60907 | 0.04525 | 1.64748 |
| C | 3.26814 | 1.28517 | 1.69312 |
| C | 3.33074 | -1.13888 | 1.42661 |
| C | 4.63274 | 1.32629 | 1.45264 |
| C | 4.69860 | -1.04473 | 1.19844 |
| C | 5.36427 | 0.17504 | 1.18354 |
| H | 5.13546 | 2.28828 | 1.44581 |
| H | 5.26162 | -1.95647 | 1.02292 |
| C | -2.17666 | -1.86914 | -0.42698 |
| C | -2.77264 | -2.32060 | -1.62783 |
| C | -2.17576 | -2.70622 | 0.71277 |
| C | -3.27318 | -3.61565 | -1.66414 |
| C | -2.69696 | -3.98779 | 0.60424 |
| C | -3.22901 | -4.47552 | -0.57780 |
| H | -3.72930 | -3.95806 | -2.58729 |
| H | -2.69340 | -4.61953 | 1.48697 |
| Cl | -2.64332 | 0.85032 | 0.87660 |
| C | -1.65877 | -2.31307 | 2.06439 |
| H | -0.58428 | -2.49630 | 2.14187 |

| | | | |
|---|----------|----------|----------|
| H | -1.83369 | -1.26709 | 2.31171 |
| H | -2.14952 | -2.91550 | 2.82967 |
| C | -3.74207 | -5.87632 | -0.67946 |
| H | -2.95558 | -6.54249 | -1.04764 |
| H | -4.06538 | -6.25528 | 0.29118 |
| H | -4.57912 | -5.94491 | -1.37622 |
| C | -2.94383 | -1.51532 | -2.88194 |
| H | -3.36592 | -0.52819 | -2.69444 |
| H | -1.99462 | -1.36957 | -3.39985 |
| H | -3.61761 | -2.04547 | -3.55549 |
| C | 2.51383 | 2.56068 | 1.92488 |
| H | 2.00693 | 2.89003 | 1.01218 |
| H | 1.74844 | 2.45099 | 2.70038 |
| H | 3.18857 | 3.36132 | 2.22946 |
| C | 2.67799 | -2.49171 | 1.44947 |
| H | 2.01393 | -2.60180 | 2.31227 |
| H | 2.07844 | -2.67888 | 0.55414 |
| H | 3.43277 | -3.27659 | 1.50932 |
| C | 6.82084 | 0.26440 | 0.85716 |
| H | 6.95266 | 0.73804 | -0.12061 |
| H | 7.35448 | 0.87625 | 1.58829 |
| H | 7.28667 | -0.72128 | 0.82579 |
| S | -1.01853 | 0.79255 | -1.96350 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.04048 | 2.03697 | 1.10579 |
| C | 0.32779 | 0.58165 | 0.37476 |
| P | 1.88394 | -0.23138 | 0.17667 |
| Cl | -1.28669 | 0.55868 | -2.81735 |
| C | 3.61181 | 0.37694 | 0.15466 |
| C | 4.22666 | 0.49837 | -1.12857 |
| C | 4.44869 | 0.22310 | 1.29323 |
| C | 5.52764 | 0.03785 | -1.25527 |
| C | 5.74929 | -0.22134 | 1.07664 |
| C | 6.28069 | -0.43025 | -0.18556 |
| H | 5.98074 | 0.06884 | -2.23819 |
| H | 6.37172 | -0.39847 | 1.94250 |
| C | -1.86583 | 2.08226 | 0.92827 |
| C | -2.44842 | 2.93658 | -0.03846 |
| C | -2.68239 | 1.17541 | 1.65144 |
| C | -3.74919 | 2.65792 | -0.44697 |
| C | -3.96423 | 0.94051 | 1.16837 |
| C | -4.50050 | 1.61798 | 0.08117 |
| H | -4.18956 | 3.26912 | -1.21809 |
| H | -4.57827 | 0.20653 | 1.67222 |
| C | -1.75610 | 4.20623 | -0.56968 |
| C | -2.30564 | 0.54808 | 3.01238 |
| C | -5.88569 | 1.25143 | -0.44050 |
| C | 4.14882 | 0.70152 | 2.72977 |
| C | 3.68057 | 1.29575 | -2.33159 |
| C | 7.65623 | -1.03983 | -0.41956 |
| C | -3.54908 | 0.51490 | 3.91728 |
| H | -3.24650 | 0.22293 | 4.92586 |
| H | -4.03207 | 1.49312 | 3.97487 |
| H | -4.28779 | -0.21559 | 3.58615 |
| C | -1.27607 | 1.39482 | 3.75970 |
| H | -0.28522 | 1.38647 | 3.28857 |
| H | -1.59699 | 2.43502 | 3.85377 |
| H | -1.12657 | 0.98875 | 4.76370 |
| C | -1.78891 | -0.88622 | 2.88670 |
| H | -2.50747 | -1.52399 | 2.36714 |
| H | -0.84190 | -0.93101 | 2.34867 |
| H | -1.62569 | -1.30916 | 3.88247 |
| C | -6.92138 | 1.42096 | 0.67754 |
| H | -7.91607 | 1.15942 | 0.30667 |
| H | -6.70812 | 0.77568 | 1.53178 |

| | | | |
|----|----------|----------|----------|
| H | -6.95126 | 2.45440 | 1.03273 |
| C | -6.30819 | 2.12319 | -1.62021 |
| H | -7.29125 | 1.80245 | -1.97254 |
| H | -6.38675 | 3.17835 | -1.34435 |
| H | -5.61257 | 2.03442 | -2.45835 |
| C | -5.86961 | -0.21050 | -0.90260 |
| H | -5.14759 | -0.35788 | -1.70929 |
| H | -5.60754 | -0.89798 | -0.09627 |
| H | -6.85720 | -0.49646 | -1.27479 |
| C | -2.67756 | 5.02123 | -1.48006 |
| H | -3.60165 | 5.31381 | -0.97664 |
| H | -2.15850 | 5.93661 | -1.77336 |
| H | -2.93299 | 4.48221 | -2.39524 |
| C | -1.40087 | 5.10123 | 0.62664 |
| H | -2.29427 | 5.35149 | 1.20372 |
| H | -0.68662 | 4.62437 | 1.30168 |
| H | -0.94958 | 6.03302 | 0.27418 |
| C | -0.49321 | 3.91166 | -1.37882 |
| H | 0.30364 | 3.48414 | -0.76346 |
| H | -0.69134 | 3.21566 | -2.19453 |
| H | -0.09747 | 4.84303 | -1.79474 |
| C | 2.77925 | 1.33992 | 2.91855 |
| H | 2.59409 | 2.11504 | 2.17193 |
| H | 1.96266 | 0.62145 | 2.89614 |
| H | 2.74443 | 1.82318 | 3.89814 |
| C | 5.16530 | 1.83495 | 2.99030 |
| H | 4.98076 | 2.26087 | 3.98012 |
| H | 6.19673 | 1.48296 | 2.96279 |
| H | 5.05995 | 2.63295 | 2.25145 |
| C | 4.36340 | -0.38294 | 3.78871 |
| H | 5.36998 | -0.80261 | 3.74635 |
| H | 4.23230 | 0.05170 | 4.78316 |
| H | 3.65199 | -1.20072 | 3.68204 |
| C | 2.33203 | 1.96090 | -2.09000 |
| H | 2.14195 | 2.67702 | -2.89300 |
| H | 1.49559 | 1.26549 | -2.09626 |
| H | 2.33205 | 2.51802 | -1.14994 |
| C | 3.63006 | 0.48158 | -3.62583 |
| H | 2.90107 | -0.32512 | -3.56114 |
| H | 3.34034 | 1.13442 | -4.45324 |
| H | 4.60088 | 0.04766 | -3.87375 |
| C | 4.68120 | 2.45591 | -2.52740 |
| H | 4.76032 | 3.06330 | -1.62233 |
| H | 5.68074 | 2.10710 | -2.78830 |
| H | 4.32716 | 3.09811 | -3.33801 |
| C | 8.31140 | -1.50351 | 0.87857 |
| H | 8.51304 | -0.67001 | 1.55636 |
| H | 7.69412 | -2.23585 | 1.40474 |
| H | 9.26901 | -1.97830 | 0.65322 |
| C | 8.57446 | -0.00688 | -1.08404 |
| H | 8.18820 | 0.31946 | -2.05161 |
| H | 8.69311 | 0.87699 | -0.45254 |
| H | 9.56400 | -0.44052 | -1.25127 |
| C | 7.50254 | -2.25335 | -1.34473 |
| H | 6.86096 | -3.01286 | -0.89186 |
| H | 7.06537 | -1.97646 | -2.30606 |
| H | 8.48005 | -2.70327 | -1.53758 |
| Au | -2.58543 | -2.54766 | -0.35761 |
| Cl | -4.16914 | -4.09620 | 0.19600 |
| Sn | -0.89205 | -0.76372 | -0.88550 |
| Cl | 1.91463 | -1.60689 | 1.70298 |
| S | 1.55765 | -1.38154 | -1.44588 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.77103 | 0.00051 | 1.10259 |
| C | 0.52617 | -0.17476 | -0.52843 |
| P | -0.94664 | 0.18602 | -1.36251 |
| Cl | 0.76408 | -2.44009 | -3.03691 |
| Sn | 1.88217 | -0.42855 | -2.37252 |
| Au | -1.80117 | 0.85004 | -4.60613 |
| Cl | -3.28554 | 0.50567 | -6.26074 |
| Cl | -2.42106 | 1.07749 | -0.32654 |
| H | -1.55759 | -1.00342 | -1.78103 |
| H | 2.15078 | -0.38235 | 1.13239 |
| S | -0.29310 | 1.25894 | -2.95635 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.78405 | 0.03734 | 1.10351 |
| C | 0.52562 | -0.11062 | -0.52773 |
| P | -1.00583 | 0.18969 | -1.27971 |
| Cl | 1.19346 | -2.41276 | -3.04228 |
| Sn | 1.88094 | -0.20597 | -2.38377 |
| C | 2.53956 | -0.43862 | 1.33965 |
| H | 2.56197 | -1.46419 | 1.72254 |
| H | 3.13693 | -0.39084 | 0.42794 |
| H | 2.98343 | 0.20123 | 2.10571 |
| C | -1.92637 | -1.31476 | -1.58617 |
| H | -2.17379 | -1.76600 | -0.62322 |
| H | -2.83262 | -1.07200 | -2.14263 |
| H | -1.28964 | -1.98350 | -2.16982 |
| Au | -1.92011 | 0.57303 | -4.62329 |
| Cl | -3.38823 | 0.05042 | -6.24858 |
| Cl | -2.29119 | 1.32849 | -0.20401 |
| S | -0.44559 | 1.15247 | -2.99224 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.97982 | -0.06260 | 0.74165 |
| C | 0.69529 | -0.10154 | -0.89682 |
| P | -0.92642 | 0.14620 | -1.49274 |
| Cl | 1.93319 | -2.06831 | -3.60620 |
| Au | -1.89430 | 0.29087 | -4.99227 |
| Cl | -3.16984 | -0.37348 | -6.72787 |
| S | -0.57135 | 1.04559 | -3.30326 |
| C | -2.00509 | -1.36918 | -1.49916 |
| C | -3.40449 | -1.00769 | -1.98982 |
| C | -1.36784 | -2.41706 | -2.40679 |
| C | -2.06957 | -1.88747 | -0.06217 |
| H | -3.90604 | -0.30377 | -1.32529 |
| H | -3.39469 | -0.59667 | -3.00202 |
| H | -3.99425 | -1.92766 | -2.01879 |
| H | -0.36062 | -2.68710 | -2.08837 |
| H | -1.99160 | -3.31436 | -2.36840 |
| H | -1.32159 | -2.08881 | -3.44633 |
| H | -2.71550 | -2.76953 | -0.06056 |
| H | -1.09039 | -2.19208 | 0.30996 |
| H | -2.49775 | -1.15744 | 0.62630 |
| C | 2.80513 | -0.38575 | 1.01378 |
| C | 3.31962 | -1.58457 | 0.22858 |
| C | 3.57555 | 0.88623 | 0.65853 |
| C | 2.94022 | -0.65693 | 2.51426 |
| H | 2.76334 | -2.49420 | 0.46710 |
| H | 3.25825 | -1.44580 | -0.85264 |
| H | 4.37149 | -1.76139 | 0.47689 |
| H | 3.19602 | 1.75788 | 1.19892 |
| H | 4.62912 | 0.76230 | 0.93059 |
| H | 3.53413 | 1.11021 | -0.41037 |
| H | 3.99315 | -0.81018 | 2.76884 |

| | | | |
|----|----------|----------|----------|
| H | 2.56788 | 0.17927 | 3.11189 |
| H | 2.39064 | -1.55328 | 2.81376 |
| Sn | 1.98156 | 0.18785 | -2.78995 |
| Cl | -1.97610 | 1.47040 | -0.35360 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.74541 | 0.49833 | 0.81017 |
| C | 0.53679 | -0.09477 | -0.72924 |
| P | -0.93123 | 0.02774 | -1.64155 |
| Cl | 1.67467 | -2.93408 | -2.48523 |
| Sn | 2.11127 | -0.57285 | -2.30682 |
| Au | -1.73649 | -0.07919 | -5.10257 |
| Cl | -3.19730 | -0.56461 | -6.74908 |
| C | 2.43731 | -0.00676 | 1.21327 |
| C | 3.01355 | -1.20374 | 0.77247 |
| C | 3.18284 | 0.84427 | 2.03275 |
| C | 4.32014 | -1.51737 | 1.11313 |
| H | 2.41962 | -1.91824 | 0.20941 |
| C | 4.49276 | 0.53347 | 2.35980 |
| H | 2.73573 | 1.76141 | 2.40362 |
| C | 5.06275 | -0.64490 | 1.89729 |
| H | 4.75451 | -2.45081 | 0.77427 |
| H | 5.06919 | 1.20851 | 2.98169 |
| H | 6.08440 | -0.89194 | 2.16200 |
| C | -1.93026 | -1.46025 | -1.52381 |
| C | -2.74208 | -1.63998 | -0.40311 |
| C | -1.83878 | -2.45263 | -2.49408 |
| C | -3.46807 | -2.80883 | -0.26723 |
| H | -2.81652 | -0.86817 | 0.35366 |
| C | -2.57416 | -3.61841 | -2.34891 |
| H | -1.19964 | -2.32278 | -3.35722 |
| C | -3.38691 | -3.79604 | -1.24129 |
| H | -4.10568 | -2.94617 | 0.59797 |
| H | -2.51038 | -4.38502 | -3.11135 |
| H | -3.96405 | -4.70735 | -1.13494 |
| Cl | -2.16290 | 1.50656 | -0.99352 |
| S | -0.22307 | 0.46183 | -3.49431 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.59025 | 0.20907 | 1.20622 |
| C | 0.34157 | -0.19060 | -0.38560 |
| P | -1.08163 | -0.04948 | -1.38081 |
| Cl | 1.82373 | -2.69691 | -2.28028 |
| Sn | 2.12255 | -0.35434 | -1.78291 |
| Au | -1.65047 | 1.50611 | -4.58092 |
| Cl | -3.06347 | 2.28514 | -6.15548 |
| C | 2.38856 | -0.10692 | 1.37191 |
| C | 2.87412 | -1.41377 | 1.55398 |
| C | 3.26851 | 0.98910 | 1.40267 |
| C | 4.24306 | -1.59601 | 1.71531 |
| C | 4.62651 | 0.75467 | 1.56682 |
| C | 5.13534 | -0.53089 | 1.71504 |
| H | 4.62074 | -2.60397 | 1.85854 |
| H | 5.30630 | 1.60145 | 1.58510 |
| C | -1.99323 | -1.61301 | -1.49492 |
| C | -2.62131 | -2.07250 | -0.31196 |
| C | -2.04458 | -2.40182 | -2.66992 |
| C | -3.26742 | -3.30125 | -0.33066 |
| C | -2.71921 | -3.61488 | -2.61339 |
| C | -3.33646 | -4.08868 | -1.46696 |
| H | -3.73624 | -3.64697 | 0.58520 |
| H | -2.75312 | -4.21630 | -3.51572 |
| Cl | -2.44108 | 1.32849 | -0.74421 |
| C | 2.76288 | 2.39162 | 1.23910 |
| H | 2.44189 | 2.58625 | 0.21064 |
| H | 1.89900 | 2.58776 | 1.88231 |

| | | | |
|---|----------|----------|----------|
| H | 3.53791 | 3.11771 | 1.48645 |
| C | 6.60771 | -0.76128 | 1.86049 |
| H | 7.08005 | -0.86627 | 0.87878 |
| H | 7.09349 | 0.07388 | 2.36808 |
| H | 6.81485 | -1.67387 | 2.42156 |
| C | 1.95657 | -2.59994 | 1.59734 |
| H | 1.08370 | -2.40922 | 2.22878 |
| H | 1.58476 | -2.85887 | 0.60187 |
| H | 2.47642 | -3.47176 | 1.99605 |
| C | -2.68769 | -1.32157 | 0.98522 |
| H | -3.50464 | -0.59651 | 0.97238 |
| H | -2.87665 | -2.02049 | 1.80068 |
| H | -1.77904 | -0.77286 | 1.23042 |
| C | -1.43851 | -2.05308 | -3.99450 |
| H | -1.88518 | -1.15413 | -4.42409 |
| H | -0.36405 | -1.88844 | -3.92523 |
| H | -1.60650 | -2.87238 | -4.69294 |
| C | -4.06708 | -5.39356 | -1.46817 |
| H | -4.20001 | -5.77836 | -0.45624 |
| H | -5.06049 | -5.27500 | -1.91161 |
| H | -3.53682 | -6.14364 | -2.05803 |
| S | -0.18288 | 0.77478 | -3.00244 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.94434 | 1.98299 | 0.11734 |
| C | 1.05093 | 0.60619 | -0.16265 |
| P | -0.68441 | 0.43096 | -0.23469 |
| C | 3.66125 | 1.33166 | -0.04149 |
| C | 4.44645 | 1.15658 | 1.12855 |
| C | 4.14398 | 0.85469 | -1.28103 |
| C | 5.52129 | 0.28345 | 1.05970 |
| C | 5.21237 | -0.04476 | -1.26195 |
| C | 5.87708 | -0.39642 | -0.10072 |
| H | 6.10048 | 0.10354 | 1.95327 |
| H | 5.54696 | -0.46227 | -2.20046 |
| C | 3.68602 | 1.36176 | -2.66710 |
| C | 4.20704 | 1.94434 | 2.42979 |
| C | 7.00099 | -1.42619 | -0.06685 |
| C | 2.89237 | 1.56740 | 3.11387 |
| H | 2.01968 | 1.86349 | 2.52631 |
| H | 2.82449 | 0.49227 | 3.28498 |
| H | 2.81521 | 2.08690 | 4.07366 |
| C | 4.21418 | 3.44577 | 2.10922 |
| H | 5.16123 | 3.74084 | 1.65075 |
| H | 3.40731 | 3.73000 | 1.43043 |
| H | 4.08655 | 4.02252 | 3.02950 |
| C | 5.31881 | 1.70432 | 3.45392 |
| H | 5.33494 | 0.67157 | 3.80974 |
| H | 6.30581 | 1.95518 | 3.05819 |
| H | 5.13883 | 2.34404 | 4.32081 |
| C | 2.75861 | 0.37279 | -3.37662 |
| H | 1.79799 | 0.28435 | -2.86760 |
| H | 2.56131 | 0.71165 | -4.39797 |
| H | 3.21099 | -0.62009 | -3.43640 |
| C | 3.01115 | 2.73027 | -2.59357 |
| H | 2.03648 | 2.70571 | -2.09660 |
| H | 3.63902 | 3.46047 | -2.07749 |
| H | 2.82168 | 3.09910 | -3.60526 |
| C | 4.92536 | 1.56576 | -3.55728 |
| H | 5.67345 | 2.18942 | -3.06262 |
| H | 5.39967 | 0.62662 | -3.84379 |
| H | 4.62247 | 2.06436 | -4.48133 |
| C | 7.22362 | -2.08413 | -1.42593 |
| H | 7.54258 | -1.36306 | -2.18314 |
| H | 8.01004 | -2.83766 | -1.34090 |
| H | 6.32211 | -2.58712 | -1.78508 |

| | | | |
|----|----------|----------|----------|
| C | 6.64337 | -2.52142 | 0.94530 |
| H | 6.51789 | -2.11792 | 1.95168 |
| H | 5.71027 | -3.02006 | 0.67376 |
| H | 7.43768 | -3.27216 | 0.98081 |
| C | 8.30764 | -0.74705 | 0.36026 |
| H | 8.22477 | -0.29558 | 1.35091 |
| H | 9.11788 | -1.48056 | 0.39551 |
| H | 8.59009 | 0.03851 | -0.34518 |
| C | -2.10758 | 1.43852 | 0.29756 |
| C | -2.75530 | 1.02765 | 1.49650 |
| C | -2.85713 | 2.18338 | -0.66075 |
| C | -4.14521 | 0.98768 | 1.48917 |
| C | -4.23667 | 2.10511 | -0.58525 |
| C | -4.90963 | 1.40738 | 0.41321 |
| H | -4.64386 | 0.60704 | 2.36944 |
| H | -4.81827 | 2.62280 | -1.33775 |
| C | -2.08637 | 0.82286 | 2.87033 |
| C | -2.43706 | -0.51324 | 3.52871 |
| C | -2.65341 | 1.95888 | 3.75011 |
| H | -2.01588 | -1.35421 | 2.97938 |
| H | -2.02870 | -0.53322 | 4.54256 |
| H | -3.51513 | -0.66413 | 3.60485 |
| H | -2.43278 | 2.93806 | 3.31779 |
| H | -3.73327 | 1.88190 | 3.87959 |
| H | -2.18976 | 1.91018 | 4.73899 |
| C | -2.29521 | 3.24099 | -1.63351 |
| C | -2.86718 | 4.58494 | -1.13420 |
| C | -2.75240 | 3.03507 | -3.07978 |
| H | -2.57159 | 4.77561 | -0.09974 |
| H | -2.47737 | 5.39605 | -1.75539 |
| H | -3.95590 | 4.61446 | -1.18458 |
| H | -2.35865 | 2.11146 | -3.50241 |
| H | -3.83995 | 3.00614 | -3.16432 |
| H | -2.39837 | 3.86721 | -3.69423 |
| C | -6.41778 | 1.22087 | 0.34131 |
| C | -7.10672 | 2.58957 | 0.40284 |
| C | -6.94353 | 0.35482 | 1.48293 |
| H | -6.80503 | 3.23457 | -0.42537 |
| H | -8.19102 | 2.46201 | 0.34618 |
| H | -6.87386 | 3.10741 | 1.33692 |
| H | -6.46938 | -0.62947 | 1.48888 |
| H | -6.79466 | 0.82474 | 2.45893 |
| H | -8.01797 | 0.20379 | 1.35648 |
| Cl | 2.49112 | -1.92982 | 1.83995 |
| Cl | -1.02926 | 0.15617 | -2.23898 |
| Au | -2.85606 | -2.30467 | -0.26097 |
| Cl | -4.86191 | -3.12452 | -0.91635 |
| C | -0.78083 | 3.40394 | -1.59567 |
| H | -0.41678 | 3.53900 | -0.57462 |
| H | -0.25047 | 2.57206 | -2.05448 |
| H | -0.50663 | 4.30023 | -2.15787 |
| C | -0.57487 | 1.01368 | 2.88054 |
| H | -0.02595 | 0.19139 | 2.42351 |
| H | -0.29176 | 1.94992 | 2.39225 |
| H | -0.23504 | 1.07140 | 3.91751 |
| C | -6.76408 | 0.52905 | -0.98365 |
| H | -6.44759 | 1.12175 | -1.84480 |
| H | -6.28847 | -0.45218 | -1.05227 |
| H | -7.84640 | 0.39122 | -1.05461 |
| Sn | 1.73187 | -1.58176 | -0.42918 |
| S | -0.87936 | -1.47260 | 0.50658 |

Coordination through P(sp²) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.59381 | -0.01685 | 0.91664 |
| C | 0.34979 | -0.34024 | -0.66914 |
| P | -1.12799 | -0.28357 | -1.57513 |
| Cl | 1.14536 | -2.79782 | -2.86026 |
| Sn | 1.75828 | -0.49683 | -2.50527 |
| Au | -0.70667 | 0.54308 | 2.59522 |
| Cl | -2.02028 | 1.11462 | 4.33555 |
| Cl | -2.68630 | 0.63378 | -0.68835 |
| H | -1.61963 | -1.59470 | -1.67692 |
| H | 1.98811 | -0.14867 | 1.10242 |
| S | -0.62930 | 0.49814 | -3.32481 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.67670 | 0.08945 | 0.89451 |
| C | 0.35579 | -0.23323 | -0.67708 |
| P | -1.19756 | -0.26362 | -1.45867 |
| Cl | 1.34677 | -2.86718 | -2.62477 |
| Sn | 1.65376 | -0.46628 | -2.57272 |
| C | 2.45039 | -0.04392 | 1.22374 |
| H | 2.60646 | -0.85503 | 1.93967 |
| H | 3.01992 | -0.24110 | 0.31589 |
| H | 2.79386 | 0.88096 | 1.69234 |
| C | -1.97259 | -1.86773 | -1.25355 |
| H | -2.18910 | -2.03394 | -0.19694 |
| H | -2.89372 | -1.88992 | -1.83756 |
| H | -1.27046 | -2.61748 | -1.62582 |
| Au | -0.66883 | 0.57942 | 2.56957 |
| Cl | -2.02643 | 1.04571 | 4.31453 |
| Cl | -2.55204 | 1.01624 | -0.66124 |
| S | -0.81329 | 0.18852 | -3.36127 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.71399 | 0.19567 | 0.67452 |
| C | 0.50456 | -0.33114 | -0.86806 |
| P | -1.05030 | -0.48030 | -1.66250 |
| Cl | 2.22251 | -2.90264 | -2.58075 |
| Sn | 1.87187 | -0.51340 | -2.73860 |
| Au | -0.78868 | 0.93964 | 2.12312 |
| Cl | -2.29829 | 1.69665 | 3.63271 |
| C | 2.45932 | 0.12592 | 1.29031 |
| C | 2.80978 | 1.52574 | 1.80119 |
| C | 2.43707 | -0.86181 | 2.46336 |
| C | 3.45717 | -0.32904 | 0.23952 |
| H | 2.83981 | 2.25800 | 0.99092 |
| H | 2.09632 | 1.87440 | 2.55152 |
| H | 3.79926 | 1.49484 | 2.26684 |
| H | 2.21467 | -1.87861 | 2.13160 |
| H | 3.42475 | -0.86757 | 2.93422 |
| H | 1.70569 | -0.57616 | 3.22323 |
| H | 4.44736 | -0.40763 | 0.69877 |
| H | 3.20854 | -1.31096 | -0.17055 |
| H | 3.54334 | 0.39415 | -0.57606 |
| C | -2.02929 | -1.97418 | -1.15992 |
| C | -1.17486 | -3.20522 | -1.45695 |
| C | -2.37358 | -1.91394 | 0.32383 |
| C | -3.30107 | -1.99959 | -2.00679 |
| H | -0.91783 | -3.28076 | -2.51395 |
| H | -0.24595 | -3.21249 | -0.88523 |
| H | -1.75257 | -4.09174 | -1.18061 |
| H | -2.96541 | -1.03494 | 0.58242 |
| H | -2.96468 | -2.80028 | 0.57102 |
| H | -1.48186 | -1.93097 | 0.95279 |
| H | -3.84479 | -2.91888 | -1.77306 |

| | | | |
|----|----------|----------|----------|
| H | -3.95669 | -1.15551 | -1.78848 |
| H | -3.07630 | -2.00538 | -3.07506 |
| Cl | -2.27590 | 1.08169 | -1.20736 |
| S | -0.64613 | -0.46486 | -3.61848 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.67022 | 0.31288 | 0.52966 |
| C | 0.47944 | -0.41105 | -0.93036 |
| P | -1.00228 | -0.63546 | -1.81322 |
| Cl | 1.97098 | -3.34386 | -2.10085 |
| Sn | 1.97771 | -0.96599 | -2.58022 |
| Au | -0.78713 | 1.38888 | 1.79421 |
| Cl | -2.28773 | 2.45621 | 3.10871 |
| C | 2.35926 | 0.15286 | 1.08805 |
| C | 2.87478 | 1.14603 | 1.92347 |
| C | 3.15537 | -0.93908 | 0.72951 |
| C | 4.18607 | 1.06911 | 2.36036 |
| H | 2.24637 | 1.97804 | 2.22397 |
| C | 4.46248 | -1.01232 | 1.17965 |
| H | 2.74031 | -1.75256 | 0.14286 |
| C | 4.97978 | -0.00647 | 1.98568 |
| H | 4.58739 | 1.84645 | 2.99965 |
| H | 5.07464 | -1.86470 | 0.90959 |
| H | 6.00362 | -0.06921 | 2.33614 |
| C | -1.93767 | -2.02894 | -1.16620 |
| C | -2.71892 | -1.88198 | -0.02015 |
| C | -1.81316 | -3.27076 | -1.78136 |
| C | -3.37907 | -2.98069 | 0.50019 |
| H | -2.82060 | -0.91561 | 0.46028 |
| C | -2.47947 | -4.36473 | -1.25114 |
| H | -1.19474 | -3.37877 | -2.66382 |
| C | -3.26019 | -4.22061 | -0.11499 |
| H | -3.99100 | -2.86666 | 1.38706 |
| H | -2.38395 | -5.33203 | -1.72976 |
| H | -3.78106 | -5.07807 | 0.29557 |
| Cl | -2.26792 | 0.93951 | -1.61063 |
| S | -0.45100 | -0.85587 | -3.71333 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.62123 | 0.44562 | 1.09944 |
| C | 0.26730 | -0.37507 | -0.27488 |
| P | -1.15431 | -0.46735 | -1.28030 |
| Cl | 1.46354 | -3.17165 | -1.96139 |
| Sn | 1.89036 | -0.78715 | -1.84984 |
| Au | -0.64524 | 1.60402 | 2.49358 |
| Cl | -1.90782 | 2.78476 | 3.95578 |
| C | 2.39633 | 0.31282 | 1.39392 |
| C | 3.20199 | 1.44609 | 1.19156 |
| C | 2.94930 | -0.89457 | 1.85122 |
| C | 4.56412 | 1.33976 | 1.43154 |
| C | 4.31869 | -0.94427 | 2.07954 |
| C | 5.14195 | 0.15614 | 1.87630 |
| H | 5.19280 | 2.20919 | 1.26519 |
| H | 4.75365 | -1.87418 | 2.43264 |
| C | -2.01382 | -2.05639 | -1.13772 |
| C | -2.35397 | -2.50571 | 0.15879 |
| C | -2.35132 | -2.84411 | -2.26261 |
| C | -2.96489 | -3.74351 | 0.30244 |
| C | -2.96148 | -4.07284 | -2.04334 |
| C | -3.26206 | -4.55493 | -0.77962 |
| H | -3.22484 | -4.07377 | 1.30323 |
| H | -3.21932 | -4.67297 | -2.90989 |
| Cl | -2.58282 | 0.92027 | -0.81554 |
| C | 2.62490 | 2.74374 | 0.71196 |
| H | 2.13552 | 2.63440 | -0.26069 |
| H | 1.87267 | 3.12886 | 1.40762 |

| | | | |
|---|----------|----------|----------|
| H | 3.40342 | 3.49985 | 0.60928 |
| C | 2.11194 | -2.11254 | 2.10667 |
| H | 1.24128 | -1.87502 | 2.72560 |
| H | 1.74103 | -2.55493 | 1.17767 |
| H | 2.69320 | -2.87237 | 2.62957 |
| C | 6.60987 | 0.08019 | 2.16023 |
| H | 6.82197 | 0.41923 | 3.17903 |
| H | 6.98107 | -0.94176 | 2.07047 |
| H | 7.18006 | 0.71583 | 1.48053 |
| C | -2.10899 | -1.73681 | 1.42184 |
| H | -2.77587 | -2.09660 | 2.20572 |
| H | -1.08433 | -1.87729 | 1.77347 |
| H | -2.27939 | -0.66577 | 1.31968 |
| C | -2.12654 | -2.47313 | -3.69861 |
| H | -2.50687 | -1.48154 | -3.94251 |
| H | -1.06552 | -2.48541 | -3.95229 |
| H | -2.63590 | -3.19603 | -4.33644 |
| C | -3.88281 | -5.90269 | -0.59293 |
| H | -4.52829 | -6.16425 | -1.43307 |
| H | -3.10742 | -6.67216 | -0.52460 |
| H | -4.47141 | -5.94774 | 0.32469 |
| S | -0.36018 | 0.04660 | -3.04315 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -1.00028 | 0.88860 | 0.13338 |
| C | -0.34166 | -0.60568 | 0.32149 |
| P | 1.29256 | -1.23212 | 0.37080 |
| Cl | -2.25143 | -2.57919 | -2.08331 |
| C | 2.93506 | -0.48508 | 0.06989 |
| C | 3.52591 | -0.77735 | -1.19781 |
| C | 3.78481 | -0.11468 | 1.14865 |
| C | 4.87799 | -1.08058 | -1.21400 |
| C | 5.13225 | -0.44826 | 1.04109 |
| C | 5.68771 | -1.02646 | -0.08720 |
| H | 5.32295 | -1.35457 | -2.16201 |
| H | 5.77326 | -0.22453 | 1.88177 |
| C | -2.80503 | 0.65709 | 0.18757 |
| C | -3.57688 | 0.66087 | -1.00401 |
| C | -3.38011 | 0.20413 | 1.40295 |
| C | -4.79103 | -0.01758 | -0.98070 |
| C | -4.58129 | -0.49136 | 1.32512 |
| C | -5.27830 | -0.67051 | 0.14055 |
| H | -5.36567 | -0.06617 | -1.89032 |
| H | -4.99746 | -0.89748 | 2.23773 |
| C | -3.20765 | 1.44217 | -2.27915 |
| C | -2.86591 | 0.50706 | 2.82758 |
| C | -6.54646 | -1.51669 | 0.11806 |
| C | 3.44540 | 0.80539 | 2.34285 |
| C | 2.87956 | -0.58808 | -2.58753 |
| C | 7.13563 | -1.49358 | -0.15627 |
| C | -4.05274 | 1.01580 | 3.66764 |
| H | -3.68933 | 1.31975 | 4.65236 |
| H | -4.52544 | 1.88142 | 3.19785 |
| H | -4.81879 | 0.25738 | 3.82806 |
| C | -1.82387 | 1.62165 | 2.89080 |
| H | -0.84471 | 1.32020 | 2.51558 |
| H | -2.14667 | 2.51593 | 2.35215 |
| H | -1.66559 | 1.90461 | 3.93492 |
| C | -2.30122 | -0.74960 | 3.49451 |
| H | -3.03046 | -1.56293 | 3.49428 |
| H | -1.40079 | -1.09931 | 2.98643 |
| H | -2.03708 | -0.53531 | 4.53410 |
| C | -7.58525 | -0.91908 | 1.07416 |
| H | -8.49572 | -1.52448 | 1.06391 |
| H | -7.22124 | -0.88518 | 2.10307 |
| H | -7.85061 | 0.09874 | 0.77781 |

| | | | |
|----|----------|----------|----------|
| C | -7.16457 | -1.59743 | -1.27517 |
| H | -8.05045 | -2.23603 | -1.24237 |
| H | -7.48127 | -0.61668 | -1.63920 |
| H | -6.47102 | -2.02910 | -2.00071 |
| C | -6.19529 | -2.93966 | 0.57005 |
| H | -5.46001 | -3.39064 | -0.10074 |
| H | -5.78286 | -2.95330 | 1.58128 |
| H | -7.09115 | -3.56662 | 0.56631 |
| C | -4.26566 | 1.28635 | -3.37572 |
| H | -5.24971 | 1.63868 | -3.05842 |
| H | -3.96487 | 1.89322 | -4.23235 |
| H | -4.35269 | 0.25276 | -3.71906 |
| C | -3.15654 | 2.93405 | -1.92175 |
| H | -4.12129 | 3.27221 | -1.53520 |
| H | -2.39766 | 3.15481 | -1.16777 |
| H | -2.91740 | 3.52439 | -2.81015 |
| C | -1.88464 | 0.99964 | -2.90612 |
| H | -1.01748 | 1.23323 | -2.28620 |
| H | -1.87981 | -0.07175 | -3.10882 |
| H | -1.73380 | 1.53864 | -3.84571 |
| C | 2.00647 | 1.29977 | 2.40734 |
| H | 1.68444 | 1.69479 | 1.44081 |
| H | 1.30067 | 0.54366 | 2.74001 |
| H | 1.94957 | 2.12757 | 3.11806 |
| C | 4.29401 | 2.07656 | 2.11422 |
| H | 4.09566 | 2.78773 | 2.92032 |
| H | 5.36382 | 1.86682 | 2.10478 |
| H | 4.03052 | 2.55841 | 1.16993 |
| C | 3.83598 | 0.19981 | 3.69410 |
| H | 4.89803 | -0.04636 | 3.74484 |
| H | 3.63206 | 0.92540 | 4.48591 |
| H | 3.26867 | -0.70517 | 3.91062 |
| C | 1.43700 | -0.09960 | -2.57385 |
| H | 1.16542 | 0.21288 | -3.58506 |
| H | 0.72173 | -0.86584 | -2.28082 |
| H | 1.32291 | 0.77493 | -1.92725 |
| C | 2.97928 | -1.83823 | -3.46483 |
| H | 2.39534 | -2.66015 | -3.05107 |
| H | 2.58973 | -1.61254 | -4.46097 |
| H | 4.01040 | -2.17628 | -3.58494 |
| C | 3.68832 | 0.54696 | -3.25292 |
| H | 3.63855 | 1.46323 | -2.65981 |
| H | 4.73860 | 0.28764 | -3.38973 |
| H | 3.26282 | 0.75774 | -4.23753 |
| C | 7.84716 | -1.37308 | 1.18866 |
| H | 7.92893 | -0.33378 | 1.51690 |
| H | 7.33694 | -1.94298 | 1.96920 |
| H | 8.86217 | -1.76717 | 1.09969 |
| C | 7.90082 | -0.65354 | -1.18600 |
| H | 7.47325 | -0.74674 | -2.18617 |
| H | 7.89215 | 0.40457 | -0.91358 |
| H | 8.94199 | -0.98338 | -1.23770 |
| C | 7.15695 | -2.96606 | -0.58422 |
| H | 6.62755 | -3.59159 | 0.13841 |
| H | 6.68692 | -3.11077 | -1.55893 |
| H | 8.18861 | -3.32158 | -0.65270 |
| Sn | -1.41172 | -2.68182 | 0.19175 |
| Cl | 1.42440 | -1.88252 | 2.33001 |
| Au | 0.05845 | 2.82386 | -0.19869 |
| Cl | 1.18131 | 4.77063 | -0.52557 |
| S | 1.12760 | -2.95358 | -0.63341 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.62401 | 0.05020 | 1.09973 |
| C | 0.46791 | 0.01424 | -0.61979 |
| P | -1.01128 | -0.22261 | -1.51751 |
| Cl | 1.35983 | -2.73231 | -2.41030 |
| Sn | 1.84102 | -0.36422 | -2.47846 |
| Au | 0.77309 | 2.08405 | -0.12569 |
| Cl | 1.10571 | 4.30391 | -0.20219 |
| Cl | -2.68857 | 0.59476 | -0.73606 |
| H | 2.03874 | -0.14338 | 1.16367 |
| H | -1.32860 | -1.58731 | -1.42915 |
| S | -0.62152 | 0.36211 | -3.36729 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.58559 | 0.12859 | 1.04171 |
| C | 0.40415 | 0.09801 | -0.67203 |
| P | -1.09927 | -0.17934 | -1.52653 |
| Cl | 1.68782 | -2.66959 | -2.30531 |
| Sn | 1.79377 | -0.24993 | -2.51662 |
| C | 2.35887 | -0.25382 | 1.31113 |
| H | 2.42366 | -1.32609 | 1.52438 |
| H | 2.99702 | -0.02396 | 0.45767 |
| H | 2.71196 | 0.28540 | 2.19235 |
| C | -1.67319 | -1.85170 | -1.21899 |
| H | -1.92733 | -1.96132 | -0.16344 |
| H | -2.55101 | -2.03639 | -1.83940 |
| H | -0.86634 | -2.53446 | -1.49587 |
| Au | 0.71098 | 2.17393 | -0.18644 |
| Cl | 1.06242 | 4.39592 | -0.19583 |
| Cl | -2.66339 | 0.95439 | -0.88367 |
| S | -0.68542 | 0.16775 | -3.44253 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 1.05103 | 0.38920 | 1.16301 |
| C | 0.64255 | 0.10069 | -0.49036 |
| P | -1.01626 | -0.21940 | -1.00987 |
| Cl | 2.16078 | -2.58166 | -2.36507 |
| Sn | 1.69214 | -0.20687 | -2.56920 |
| Au | 1.01795 | 2.23934 | -0.34656 |
| Cl | 1.42175 | 4.43340 | -0.65650 |
| C | 2.86962 | 0.04345 | 1.42755 |
| C | 3.75812 | 0.04043 | 0.19755 |
| C | 3.34240 | 1.09661 | 2.43138 |
| C | 2.87676 | -1.34223 | 2.08611 |
| H | 3.49853 | -0.77317 | -0.48493 |
| H | 3.72354 | 0.99445 | -0.33491 |
| H | 4.79766 | -0.12565 | 0.49984 |
| H | 2.69690 | 1.13713 | 3.31327 |
| H | 4.35343 | 0.84954 | 2.76915 |
| H | 3.36935 | 2.09374 | 1.98541 |
| H | 3.89507 | -1.57851 | 2.41074 |
| H | 2.23312 | -1.38112 | 2.96979 |
| H | 2.55961 | -2.12096 | 1.38794 |
| C | -1.76619 | -1.75162 | -0.27334 |
| C | -0.83282 | -2.92368 | -0.56634 |
| C | -1.95820 | -1.58862 | 1.23139 |
| C | -3.11440 | -1.97716 | -0.95770 |
| H | -0.66615 | -3.06031 | -1.63502 |
| H | 0.14153 | -2.80835 | -0.09002 |
| H | -1.29700 | -3.83294 | -0.17385 |
| H | -2.64627 | -0.77866 | 1.47468 |
| H | -2.37982 | -2.51957 | 1.62091 |
| H | -1.01662 | -1.40886 | 1.75381 |
| H | -3.54467 | -2.90112 | -0.56175 |

| | | | |
|----|----------|----------|----------|
| H | -3.81688 | -1.16618 | -0.75914 |
| H | -3.00497 | -2.09148 | -2.03734 |
| Cl | -2.31071 | 1.24706 | -0.40842 |
| S | -0.95013 | -0.27852 | -3.00273 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.52468 | 0.33572 | 0.96693 |
| C | 0.30236 | 0.20980 | -0.73874 |
| P | -1.22865 | -0.04922 | -1.54817 |
| Cl | 1.67097 | -2.35885 | -2.82472 |
| Sn | 1.64637 | 0.06559 | -2.64839 |
| Au | 0.63862 | 2.32150 | -0.36122 |
| Cl | 1.00198 | 4.54059 | -0.49289 |
| C | 2.28079 | -0.03244 | 1.22766 |
| C | 2.92988 | 0.62900 | 2.27305 |
| C | 2.96727 | -1.00492 | 0.49824 |
| C | 4.25859 | 0.35785 | 2.55054 |
| H | 2.39595 | 1.37087 | 2.85861 |
| C | 4.29299 | -1.28415 | 0.79213 |
| H | 2.46011 | -1.57025 | -0.27699 |
| C | 4.94124 | -0.59774 | 1.80914 |
| H | 4.76247 | 0.88956 | 3.34925 |
| H | 4.81804 | -2.04405 | 0.22493 |
| H | 5.97942 | -0.81507 | 2.03262 |
| C | -1.79232 | -1.73847 | -1.29329 |
| C | -1.85377 | -2.62229 | -2.36355 |
| C | -2.14926 | -2.15585 | -0.01117 |
| C | -2.27785 | -3.92543 | -2.15060 |
| H | -1.56207 | -2.29192 | -3.35253 |
| C | -2.56707 | -3.45810 | 0.19240 |
| H | -2.10947 | -1.46482 | 0.82391 |
| C | -2.63212 | -4.34238 | -0.87788 |
| H | -2.32389 | -4.61585 | -2.98423 |
| H | -2.84554 | -3.78448 | 1.18743 |
| H | -2.96055 | -5.36248 | -0.71473 |
| Cl | -2.74673 | 1.06289 | -0.76109 |
| S | -0.90479 | 0.41835 | -3.45300 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.50200 | 0.36222 | 1.39401 |
| C | 0.15317 | 0.19637 | -0.29419 |
| P | -1.30029 | -0.01765 | -1.25737 |
| Cl | 1.65696 | -2.02000 | -2.76453 |
| Sn | 1.69079 | 0.31241 | -2.06105 |
| Au | 0.28913 | 2.34014 | 0.07289 |
| Cl | 0.38778 | 4.59783 | -0.02264 |
| C | 2.30462 | 0.05665 | 1.46548 |
| C | 3.18259 | 1.03894 | 1.95435 |
| C | 2.78742 | -1.23628 | 1.17218 |
| C | 4.54053 | 0.74865 | 2.02255 |
| C | 4.15264 | -1.47159 | 1.25763 |
| C | 5.05097 | -0.48712 | 1.65321 |
| H | 5.21730 | 1.51588 | 2.38693 |
| H | 4.52229 | -2.46640 | 1.02801 |
| C | -1.83113 | -1.75185 | -1.32546 |
| C | -1.99713 | -2.45560 | -2.54358 |
| C | -2.08963 | -2.40862 | -0.10134 |
| C | -2.33425 | -3.80100 | -2.48207 |
| C | -2.42538 | -3.75675 | -0.11655 |
| C | -2.53101 | -4.48146 | -1.28996 |
| H | -2.45777 | -4.33550 | -3.41832 |
| H | -2.62376 | -4.24623 | 0.83212 |
| Cl | -2.96873 | 0.97253 | -0.56580 |
| C | 2.71494 | 2.38724 | 2.41333 |
| H | 2.61651 | 3.09337 | 1.58344 |
| H | 1.74021 | 2.34030 | 2.90626 |

| | | | |
|---|----------|----------|----------|
| H | 3.42705 | 2.81218 | 3.12251 |
| C | 1.87584 | -2.39047 | 0.86881 |
| H | 1.14486 | -2.52759 | 1.67236 |
| H | 1.32600 | -2.27185 | -0.06575 |
| H | 2.45128 | -3.31306 | 0.79036 |
| C | 6.52226 | -0.76007 | 1.69157 |
| H | 6.72902 | -1.79299 | 1.97800 |
| H | 6.96825 | -0.60107 | 0.70474 |
| H | 7.03295 | -0.09817 | 2.39272 |
| C | -2.05037 | -1.76737 | 1.25458 |
| H | -1.08308 | -1.92979 | 1.73758 |
| H | -2.23960 | -0.69736 | 1.24986 |
| H | -2.80621 | -2.22784 | 1.89305 |
| C | -1.86909 | -1.87630 | -3.92120 |
| H | -2.47226 | -0.97852 | -4.05388 |
| H | -0.83575 | -1.61465 | -4.15084 |
| H | -2.20045 | -2.61712 | -4.64944 |
| C | -2.85322 | -5.94191 | -1.27975 |
| H | -3.52327 | -6.20686 | -2.09990 |
| H | -1.94108 | -6.53412 | -1.40205 |
| H | -3.31936 | -6.24240 | -0.34041 |
| S | -0.76761 | 0.91291 | -2.94687 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.66143 | 0.18855 | 1.11861 |
| C | 0.40591 | 0.08804 | -0.60119 |
| P | -1.09520 | -0.09580 | -1.57733 |
| Cl | 2.90877 | -1.40482 | -3.30886 |
| Au | 0.45175 | 2.24297 | -0.14653 |
| Cl | 0.37464 | 4.50963 | -0.23726 |
| C | 2.50311 | 0.05104 | 1.23777 |
| C | 3.16932 | -1.11145 | 0.75615 |
| C | 3.28844 | 1.16191 | 1.63273 |
| C | 4.48249 | -0.98209 | 0.32989 |
| C | 4.60564 | 1.21839 | 1.17021 |
| C | 5.19986 | 0.20517 | 0.44004 |
| H | 4.97581 | -1.85236 | -0.08238 |
| H | 5.18588 | 2.09822 | 1.40902 |
| C | 2.92116 | 2.23722 | 2.67736 |
| C | 2.65929 | -2.55299 | 0.94983 |
| C | 6.59726 | 0.31708 | -0.15800 |
| C | 3.85706 | 1.97231 | 3.87486 |
| H | 3.69752 | 0.97103 | 4.28341 |
| H | 4.90888 | 2.05916 | 3.59986 |
| H | 3.65246 | 2.70040 | 4.66452 |
| C | 3.17257 | 3.65894 | 2.16709 |
| H | 2.54052 | 3.90150 | 1.31222 |
| H | 2.94427 | 4.37497 | 2.96130 |
| H | 4.21308 | 3.81609 | 1.87861 |
| C | 1.50449 | 2.16969 | 3.23944 |
| H | 1.43413 | 2.85517 | 4.08831 |
| H | 0.74372 | 2.48637 | 2.52386 |
| H | 1.25215 | 1.17153 | 3.60592 |
| C | 2.98426 | -3.46471 | -0.23570 |
| H | 2.58796 | -3.06908 | -1.16968 |
| H | 4.05809 | -3.60749 | -0.36496 |
| H | 2.55138 | -4.45358 | -0.06184 |
| C | 3.41496 | -3.07571 | 2.18741 |
| H | 4.49483 | -3.05263 | 2.03179 |
| H | 3.18870 | -2.47301 | 3.07077 |
| H | 3.11960 | -4.10913 | 2.39203 |
| C | 1.17481 | -2.69195 | 1.26290 |
| H | 0.87294 | -2.08687 | 2.12541 |
| H | 0.54354 | -2.44036 | 0.41263 |
| H | 0.96463 | -3.73185 | 1.52854 |
| C | 7.23976 | 1.67271 | 0.12256 |

| | | | |
|----|----------|----------|----------|
| H | 6.64253 | 2.49539 | -0.27822 |
| H | 7.38717 | 1.84207 | 1.19254 |
| H | 8.22182 | 1.71518 | -0.35435 |
| C | 6.49220 | 0.13524 | -1.67715 |
| H | 7.48630 | 0.17989 | -2.13091 |
| H | 6.03916 | -0.82170 | -1.94296 |
| H | 5.88051 | 0.92344 | -2.12315 |
| C | 7.50515 | -0.77345 | 0.42266 |
| H | 7.58409 | -0.68127 | 1.50889 |
| H | 7.13798 | -1.77578 | 0.19423 |
| H | 8.50982 | -0.68644 | 0.00007 |
| C | -2.33647 | -1.47602 | -1.65964 |
| C | -2.31372 | -2.31380 | -2.81639 |
| C | -3.56765 | -1.35349 | -0.95825 |
| C | -3.52220 | -2.56862 | -3.44521 |
| C | -1.12055 | -3.16179 | -3.29610 |
| C | -4.73736 | -1.67671 | -1.63892 |
| C | -3.74118 | -1.09764 | 0.55092 |
| C | -4.75022 | -2.17242 | -2.93214 |
| H | -3.49792 | -3.13784 | -4.36620 |
| C | -0.67046 | -2.86163 | -4.72705 |
| C | -1.60091 | -4.62921 | -3.25629 |
| C | 0.05219 | -3.10220 | -2.33280 |
| H | -5.67591 | -1.53089 | -1.12307 |
| C | -2.45091 | -0.79007 | 1.29138 |
| C | -4.24998 | -2.43947 | 1.11925 |
| C | -4.77289 | -0.01459 | 0.87670 |
| C | -6.02800 | -2.38509 | -3.73205 |
| H | 0.04533 | -3.62278 | -5.04799 |
| H | -1.51405 | -2.88210 | -5.42123 |
| H | -0.18539 | -1.89149 | -4.80399 |
| H | -2.35754 | -4.84577 | -4.01112 |
| H | -0.74587 | -5.28281 | -3.44849 |
| H | -2.01292 | -4.88584 | -2.27735 |
| H | 0.49809 | -2.11347 | -2.25427 |
| H | -0.25307 | -3.44098 | -1.34022 |
| H | 0.84750 | -3.76116 | -2.68564 |
| H | -1.67298 | -1.52063 | 1.05884 |
| H | -2.07600 | 0.21076 | 1.08738 |
| H | -2.62873 | -0.83950 | 2.36842 |
| H | -4.36949 | -2.35032 | 2.20255 |
| H | -5.21210 | -2.72743 | 0.69395 |
| H | -3.53790 | -3.24401 | 0.91954 |
| H | -5.75612 | -0.23825 | 0.45986 |
| H | -4.88868 | 0.05671 | 1.96140 |
| H | -4.46091 | 0.96169 | 0.50685 |
| C | -7.26224 | -1.86958 | -2.99691 |
| C | -6.22130 | -3.87987 | -4.01451 |
| C | -5.90410 | -1.62885 | -5.06045 |
| H | -7.44564 | -2.41895 | -2.06991 |
| H | -7.17608 | -0.80685 | -2.75747 |
| H | -8.14306 | -1.99691 | -3.63048 |
| H | -5.39417 | -4.29521 | -4.59342 |
| H | -6.30038 | -4.44798 | -3.08437 |
| H | -7.13932 | -4.03598 | -4.58753 |
| H | -5.77674 | -0.55718 | -4.89057 |
| H | -5.05112 | -1.97792 | -5.64573 |
| H | -6.80628 | -1.77489 | -5.66061 |
| Sn | 1.97249 | 0.62369 | -2.30798 |
| Cl | -2.41017 | 1.45207 | -1.17589 |
| S | -0.43424 | 0.33185 | -3.41829 |

[R-P=C(Sn(II)Cl)-P(S)MeR](AuCl)

Coordination through Sn(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.70147 | 0.42588 | 0.92033 |
| C | 0.47567 | 0.01864 | -0.67262 |
| P | -1.09851 | -0.09488 | -1.46136 |
| Cl | 1.62089 | -2.37247 | -2.85110 |
| Sn | 1.72065 | -0.04128 | -2.49715 |
| C | -2.45270 | 0.78026 | -0.66791 |
| H | -3.36789 | 0.62501 | -1.24189 |
| H | -2.58722 | 0.39806 | 0.34667 |
| H | -2.21706 | 1.84443 | -0.63563 |
| Au | 3.66871 | 1.41962 | -3.09088 |
| Cl | 5.42494 | 2.78467 | -3.54438 |
| H | 2.12918 | 0.47845 | 0.91646 |
| H | -1.49529 | -1.44709 | -1.44295 |
| S | -0.69990 | 0.52727 | -3.32842 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.45410 | 0.60323 | 0.29595 |
| C | 0.14044 | 0.33319 | -1.30886 |
| P | -1.47626 | 0.02823 | -1.94769 |
| Cl | 1.57006 | -1.66999 | -3.75170 |
| Sn | 1.18277 | 0.61112 | -3.23028 |
| S | -1.32650 | 0.73461 | -3.83830 |
| C | 2.25316 | 0.92572 | 0.38765 |
| H | 2.74099 | 0.02598 | 0.77610 |
| H | 2.69943 | 1.19090 | -0.57190 |
| H | 2.43316 | 1.72732 | 1.10763 |
| C | -1.83022 | -1.73673 | -1.92943 |
| H | -1.89535 | -2.08862 | -0.89752 |
| H | -2.77107 | -1.92452 | -2.45011 |
| H | -1.01859 | -2.25187 | -2.44575 |
| C | -2.80392 | 0.83420 | -1.03612 |
| H | -3.75875 | 0.61860 | -1.51920 |
| H | -2.82118 | 0.46448 | -0.00849 |
| H | -2.63184 | 1.91040 | -1.03590 |
| Au | 2.79738 | 2.42712 | -3.85504 |
| Cl | 4.26766 | 4.10210 | -4.30482 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.65225 | -0.41375 | 0.81051 |
| C | 0.64018 | -0.12469 | -0.82441 |
| P | -0.90739 | -0.10636 | -1.70453 |
| Cl | 2.78357 | -1.39772 | -3.33912 |
| Sn | 1.95142 | 0.62927 | -2.43878 |
| Au | 3.31105 | 2.74343 | -2.43981 |
| Cl | 4.50820 | 4.67723 | -2.32583 |
| C | 2.39699 | -0.37400 | 1.47065 |
| C | 2.56383 | -1.72019 | 2.18537 |
| C | 3.49755 | -0.18175 | 0.44583 |
| C | 2.41527 | 0.75842 | 2.50287 |
| H | 1.76759 | -1.89871 | 2.91346 |
| H | 2.57505 | -2.55383 | 1.47872 |
| H | 3.51595 | -1.72529 | 2.72515 |
| H | 3.45912 | 0.80969 | -0.01378 |
| H | 4.47352 | -0.25745 | 0.93652 |
| H | 3.47028 | -0.94504 | -0.33670 |
| H | 3.36923 | 0.74308 | 3.03932 |
| H | 2.31406 | 1.73768 | 2.02925 |
| H | 1.61711 | 0.64992 | 3.24272 |
| C | -1.66430 | -1.78413 | -1.92609 |
| C | -2.82614 | -1.65323 | -2.91126 |
| C | -0.60390 | -2.72305 | -2.49507 |

| | | | |
|---|----------|----------|----------|
| C | -2.16620 | -2.30353 | -0.58042 |
| H | -3.62612 | -1.01382 | -2.53123 |
| H | -2.49510 | -1.26441 | -3.87601 |
| H | -3.25282 | -2.64617 | -3.07809 |
| H | 0.23438 | -2.85582 | -1.80957 |
| H | -1.06127 | -3.70131 | -2.66751 |
| H | -0.20693 | -2.36106 | -3.44467 |
| H | -2.54400 | -3.32023 | -0.72038 |
| H | -1.37181 | -2.34718 | 0.16818 |
| H | -2.98524 | -1.70144 | -0.18195 |
| C | -2.12068 | 0.94010 | -0.87005 |
| H | -3.04342 | 0.98611 | -1.44958 |
| H | -2.32376 | 0.55629 | 0.13086 |
| H | -1.69688 | 1.94172 | -0.79472 |
| S | -0.39620 | 0.70662 | -3.49115 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.69305 | 0.16473 | 1.08386 |
| C | 0.37887 | -0.23995 | -0.49701 |
| P | -1.24158 | -0.28530 | -1.19168 |
| Cl | 1.69136 | -2.62623 | -2.71661 |
| Sn | 1.55204 | -0.28668 | -2.35412 |
| Au | 3.38058 | 1.26559 | -3.09714 |
| Cl | 5.04647 | 2.69681 | -3.69687 |
| C | 2.48658 | 0.05763 | 1.24014 |
| C | 3.10069 | 0.95581 | 2.11642 |
| C | 3.27113 | -0.87599 | 0.55637 |
| C | 4.47811 | 0.95930 | 2.26165 |
| H | 2.49622 | 1.66706 | 2.67069 |
| C | 4.64598 | -0.87843 | 0.71614 |
| H | 2.80305 | -1.62731 | -0.07249 |
| C | 5.25029 | 0.04567 | 1.55864 |
| H | 4.95033 | 1.67533 | 2.92393 |
| H | 5.24834 | -1.60318 | 0.18131 |
| H | 6.32801 | 0.04740 | 1.67292 |
| C | -2.00513 | -1.90242 | -0.94347 |
| C | -2.28554 | -2.73222 | -2.02211 |
| C | -2.30417 | -2.31692 | 0.35446 |
| C | -2.87740 | -3.96769 | -1.80391 |
| H | -2.03063 | -2.41253 | -3.02563 |
| C | -2.89444 | -3.55042 | 0.56495 |
| H | -2.06310 | -1.68786 | 1.20553 |
| C | -3.18318 | -4.37502 | -0.51521 |
| H | -3.09238 | -4.61487 | -2.64590 |
| H | -3.12425 | -3.87264 | 1.57375 |
| H | -3.64194 | -5.34266 | -0.34758 |
| C | -2.36913 | 0.91946 | -0.46421 |
| H | -3.33100 | 0.86068 | -0.97595 |
| H | -2.50826 | 0.70778 | 0.59766 |
| H | -1.94348 | 1.91552 | -0.58765 |
| S | -0.89584 | 0.11262 | -3.14086 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.77635 | 0.04693 | 1.52346 |
| C | 0.50252 | -0.57054 | 0.00099 |
| P | -1.07366 | -0.55135 | -0.81922 |
| Cl | 1.81368 | -2.90783 | -2.21147 |
| Sn | 1.85890 | -0.58303 | -1.71322 |
| Au | 3.93220 | 0.76847 | -2.15450 |
| Cl | 5.83941 | 2.00320 | -2.40703 |
| C | 2.59097 | 0.18370 | 1.57382 |
| C | 3.14697 | 1.47152 | 1.48317 |
| C | 3.41983 | -0.93959 | 1.70241 |
| C | 4.52595 | 1.60465 | 1.46123 |
| C | 4.79755 | -0.75347 | 1.68380 |
| C | 5.37109 | 0.50293 | 1.54041 |

| | | | |
|---|----------|----------|----------|
| H | 4.95545 | 2.59529 | 1.34969 |
| H | 5.44237 | -1.62229 | 1.77732 |
| C | -2.02646 | -2.09598 | -0.94333 |
| C | -3.10822 | -2.11946 | -1.85079 |
| C | -1.75652 | -3.22982 | -0.14995 |
| C | -3.89059 | -3.26490 | -1.93084 |
| C | -2.57151 | -4.34645 | -0.28455 |
| C | -3.64086 | -4.39229 | -1.16571 |
| H | -4.72282 | -3.27069 | -2.62795 |
| H | -2.35623 | -5.21434 | 0.33058 |
| C | -2.16679 | 0.62558 | 0.01439 |
| H | -3.15672 | 0.63989 | -0.43806 |
| H | -2.25977 | 0.31394 | 1.05784 |
| H | -1.71744 | 1.61779 | -0.02989 |
| C | -0.63552 | -3.32422 | 0.83948 |
| H | 0.33148 | -3.16481 | 0.36114 |
| H | -0.72964 | -2.59151 | 1.64338 |
| H | -0.62820 | -4.31620 | 1.29152 |
| C | -3.46684 | -1.00678 | -2.79472 |
| H | -3.34082 | -0.00553 | -2.38511 |
| H | -2.84444 | -1.05241 | -3.69190 |
| H | -4.50839 | -1.10808 | -3.10222 |
| C | -4.47664 | -5.62551 | -1.30391 |
| H | -4.56688 | -6.15411 | -0.35335 |
| H | -5.47856 | -5.39040 | -1.66617 |
| H | -4.02172 | -6.31708 | -2.01979 |
| C | 2.86852 | -2.32743 | 1.85456 |
| H | 1.95686 | -2.34210 | 2.45800 |
| H | 2.62390 | -2.77385 | 0.88567 |
| H | 3.59985 | -2.97821 | 2.33609 |
| C | 2.28189 | 2.68907 | 1.34207 |
| H | 1.41648 | 2.65834 | 2.01232 |
| H | 2.84754 | 3.59422 | 1.56559 |
| H | 1.90110 | 2.78544 | 0.32013 |
| C | 6.85249 | 0.67726 | 1.43620 |
| H | 7.11979 | 0.94880 | 0.41009 |
| H | 7.20525 | 1.48021 | 2.08766 |
| H | 7.38400 | -0.23875 | 1.69724 |
| S | -0.44548 | 0.12023 | -2.63956 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.04215 | 1.99054 | 1.13930 |
| C | 0.34632 | 0.55679 | 0.38481 |
| P | 1.90813 | -0.29273 | 0.23956 |
| Cl | -1.26433 | 0.55788 | -2.85119 |
| C | 3.63342 | 0.34685 | 0.21195 |
| C | 4.26994 | 0.50118 | -1.05422 |
| C | 4.45813 | 0.15984 | 1.35472 |
| C | 5.57625 | 0.04967 | -1.17491 |
| C | 5.76302 | -0.27899 | 1.14979 |
| C | 6.31614 | -0.44662 | -0.10967 |
| H | 6.04169 | 0.10664 | -2.15097 |
| H | 6.37279 | -0.47946 | 2.01992 |
| C | -1.86885 | 2.03723 | 0.94097 |
| C | -2.44320 | 2.89005 | -0.03055 |
| C | -2.69474 | 1.13844 | 1.66597 |
| C | -3.74236 | 2.61383 | -0.44835 |
| C | -3.97663 | 0.91204 | 1.17993 |
| C | -4.50165 | 1.58239 | 0.08240 |
| H | -4.17401 | 3.22134 | -1.22730 |
| H | -4.60029 | 0.18824 | 1.68548 |
| C | -1.74942 | 4.16322 | -0.55369 |
| C | -2.32177 | 0.51465 | 3.03145 |
| C | -5.88347 | 1.21466 | -0.44729 |
| C | 4.13052 | 0.59882 | 2.79869 |
| C | 3.73362 | 1.31524 | -2.24904 |

| | | | |
|---|----------|----------|----------|
| C | 7.69940 | -1.04086 | -0.34066 |
| C | -3.58636 | 0.32131 | 3.88292 |
| H | -3.28958 | 0.04467 | 4.89749 |
| H | -4.18128 | 1.23575 | 3.93932 |
| H | -4.22104 | -0.48383 | 3.51005 |
| C | -1.41972 | 1.45532 | 3.83350 |
| H | -0.42466 | 1.58358 | 3.39029 |
| H | -1.86591 | 2.44717 | 3.93735 |
| H | -1.25585 | 1.04380 | 4.83312 |
| C | -1.65020 | -0.85553 | 2.91354 |
| H | -2.27280 | -1.55600 | 2.35211 |
| H | -0.68312 | -0.78642 | 2.41740 |
| H | -1.49069 | -1.27443 | 3.91176 |
| C | -6.92866 | 1.39566 | 0.65994 |
| H | -7.92066 | 1.13211 | 0.28315 |
| H | -6.72347 | 0.75813 | 1.52199 |
| H | -6.95995 | 2.43242 | 1.00525 |
| C | -6.29390 | 2.07677 | -1.63826 |
| H | -7.27459 | 1.75520 | -1.99659 |
| H | -6.37224 | 3.13445 | -1.37220 |
| H | -5.59087 | 1.97937 | -2.46921 |
| C | -5.86609 | -0.25138 | -0.89661 |
| H | -5.13692 | -0.40661 | -1.69536 |
| H | -5.61135 | -0.93134 | -0.08156 |
| H | -6.85088 | -0.53922 | -1.27492 |
| C | -2.66635 | 4.97810 | -1.46895 |
| H | -3.59606 | 5.26534 | -0.97280 |
| H | -2.14812 | 5.89647 | -1.75437 |
| H | -2.91149 | 4.44148 | -2.38839 |
| C | -1.40915 | 5.05542 | 0.64917 |
| H | -2.30877 | 5.29986 | 1.21913 |
| H | -0.69926 | 4.57822 | 1.32860 |
| H | -0.95839 | 5.99035 | 0.30414 |
| C | -0.47718 | 3.88023 | -1.35234 |
| H | 0.31727 | 3.45748 | -0.73206 |
| H | -0.66301 | 3.18549 | -2.17198 |
| H | -0.08690 | 4.81632 | -1.76294 |
| C | 2.78003 | 1.28711 | 2.95968 |
| H | 2.66898 | 2.10937 | 2.25030 |
| H | 1.91892 | 0.63118 | 2.85072 |
| H | 2.71386 | 1.71304 | 3.96385 |
| C | 5.16932 | 1.68943 | 3.14035 |
| H | 4.95665 | 2.09045 | 4.13499 |
| H | 6.18940 | 1.30543 | 3.14500 |
| H | 5.12040 | 2.51244 | 2.42382 |
| C | 4.28548 | -0.52725 | 3.82545 |
| H | 5.28947 | -0.95498 | 3.80372 |
| H | 4.12045 | -0.13116 | 4.83082 |
| H | 3.57955 | -1.34280 | 3.66926 |
| C | 2.37399 | 1.95776 | -2.01215 |
| H | 2.18024 | 2.68165 | -2.80722 |
| H | 1.55105 | 1.24684 | -2.03463 |
| H | 2.35625 | 2.50002 | -1.06383 |
| C | 3.71010 | 0.52382 | -3.55840 |
| H | 2.99510 | -0.29653 | -3.51408 |
| H | 3.41642 | 1.18658 | -4.37655 |
| H | 4.69129 | 0.11266 | -3.80494 |
| C | 4.72333 | 2.48954 | -2.40979 |
| H | 4.78134 | 3.08266 | -1.49363 |
| H | 5.73104 | 2.15700 | -2.66111 |
| H | 4.37425 | 3.14133 | -3.21491 |
| C | 8.33939 | -1.53591 | 0.95350 |
| H | 8.52398 | -0.72032 | 1.65748 |
| H | 7.72077 | -2.28789 | 1.44979 |
| H | 9.30415 | -1.99669 | 0.72952 |
| C | 8.62010 | 0.01607 | -0.96249 |

| | | | |
|----|----------|----------|----------|
| H | 8.24468 | 0.36739 | -1.92551 |
| H | 8.72366 | 0.88246 | -0.30467 |
| H | 9.61494 | -0.40599 | -1.12822 |
| C | 7.56902 | -2.22910 | -1.30133 |
| H | 6.92845 | -3.00681 | -0.87866 |
| H | 7.14162 | -1.92891 | -2.26000 |
| H | 8.55272 | -2.66549 | -1.49398 |
| Au | -2.50876 | -2.55562 | -0.33077 |
| Cl | -4.04006 | -4.12382 | 0.31892 |
| Sn | -0.84199 | -0.76653 | -0.92935 |
| S | 1.58945 | -1.38827 | -1.45899 |
| C | 1.90298 | -1.60064 | 1.50240 |
| H | 1.91695 | -1.23809 | 2.52485 |
| H | 0.99252 | -2.17906 | 1.33818 |
| H | 2.76210 | -2.24646 | 1.31691 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.77450 | 0.12330 | 1.02189 |
| C | 0.56886 | -0.13178 | -0.60453 |
| P | -0.89834 | 0.26313 | -1.47287 |
| Cl | 0.71544 | -2.60267 | -2.87551 |
| Sn | 1.94787 | -0.60742 | -2.36739 |
| C | -2.16664 | 1.24107 | -0.65944 |
| H | -2.99204 | 1.39412 | -1.35769 |
| H | -2.52426 | 0.70521 | 0.22293 |
| H | -1.75006 | 2.20465 | -0.36508 |
| Au | -1.76181 | 0.81817 | -4.68579 |
| Cl | -3.42797 | 0.55280 | -6.17844 |
| H | 2.14177 | -0.28979 | 1.13009 |
| H | -1.51513 | -0.94637 | -1.83133 |
| S | -0.12067 | 1.15198 | -3.13956 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.40962 | 0.40797 | 0.47164 |
| C | 0.28981 | 0.34377 | -1.18022 |
| P | -1.26506 | 0.43831 | -1.98335 |
| Cl | 1.47670 | -1.77838 | -3.62132 |
| Sn | 1.74622 | 0.51567 | -2.93829 |
| S | -0.74068 | 1.48309 | -3.67436 |
| C | 2.20318 | 0.26240 | 0.83185 |
| H | 2.39498 | -0.74754 | 1.20763 |
| H | 2.83793 | 0.44272 | -0.03700 |
| H | 2.46679 | 0.95925 | 1.63101 |
| C | -1.88384 | -1.20358 | -2.36498 |
| H | -2.10556 | -1.71658 | -1.42584 |
| H | -2.78429 | -1.11914 | -2.97615 |
| H | -1.11389 | -1.74934 | -2.91211 |
| C | -2.57685 | 1.29832 | -1.09849 |
| H | -3.46200 | 1.34366 | -1.73640 |
| H | -2.81370 | 0.76014 | -0.17796 |
| H | -2.24825 | 2.30913 | -0.85776 |
| Au | -2.17409 | 0.80922 | -5.31216 |
| Cl | -3.64838 | 0.19166 | -6.90246 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.96941 | -0.12090 | 0.71306 |
| C | 0.72903 | -0.13629 | -0.93177 |
| P | -0.91088 | 0.13626 | -1.52676 |
| Cl | 2.01880 | -2.22253 | -3.48604 |
| C | -1.80142 | 1.40117 | -0.59112 |
| H | -2.72087 | 1.66579 | -1.11413 |
| H | -2.02993 | 1.04600 | 0.41500 |
| H | -1.15939 | 2.27944 | -0.52541 |
| Au | -1.98723 | 0.37473 | -4.99439 |

| | | | |
|----|----------|----------|----------|
| Cl | -3.47093 | -0.11120 | -6.62346 |
| S | -0.48743 | 0.94333 | -3.37964 |
| C | -1.97850 | -1.38703 | -1.53772 |
| C | -3.40005 | -0.99858 | -1.94452 |
| C | -1.41016 | -2.41963 | -2.50349 |
| C | -1.98754 | -1.95755 | -0.11812 |
| H | -3.88410 | -0.35802 | -1.20490 |
| H | -3.43422 | -0.50745 | -2.92054 |
| H | -3.99131 | -1.91452 | -2.02508 |
| H | -0.38651 | -2.70069 | -2.25393 |
| H | -2.03460 | -3.31593 | -2.45193 |
| H | -1.42301 | -2.06347 | -3.53491 |
| H | -2.66192 | -2.81831 | -0.10973 |
| H | -1.00062 | -2.30330 | 0.19065 |
| H | -2.35604 | -1.24739 | 0.62551 |
| C | 2.79798 | -0.37570 | 1.04297 |
| C | 3.34198 | -1.60363 | 0.32408 |
| C | 3.55908 | 0.88627 | 0.64056 |
| C | 2.90945 | -0.57405 | 2.55622 |
| H | 2.80098 | -2.51020 | 0.60620 |
| H | 3.28357 | -1.52183 | -0.76310 |
| H | 4.39507 | -1.74738 | 0.58854 |
| H | 3.15814 | 1.77774 | 1.13081 |
| H | 4.60934 | 0.79063 | 0.93631 |
| H | 3.53451 | 1.05784 | -0.43844 |
| H | 3.95924 | -0.70138 | 2.83706 |
| H | 2.51613 | 0.28461 | 3.10695 |
| H | 2.36477 | -1.46197 | 2.88792 |
| Sn | 2.05027 | 0.08391 | -2.79976 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.71796 | 0.44160 | 0.81322 |
| C | 0.54994 | -0.14135 | -0.73370 |
| P | -0.93882 | 0.00746 | -1.64603 |
| Cl | 1.62181 | -3.03602 | -2.36635 |
| Sn | 2.13275 | -0.68339 | -2.26928 |
| C | -2.03777 | 1.34219 | -1.13535 |
| H | -2.89299 | 1.36511 | -1.81335 |
| H | -2.38423 | 1.18394 | -0.11281 |
| H | -1.49268 | 2.28438 | -1.19560 |
| Au | -1.85326 | 0.15483 | -5.03594 |
| Cl | -3.50873 | -0.00445 | -6.56112 |
| C | 2.41502 | -0.02361 | 1.25217 |
| C | 3.00886 | -1.22005 | 0.83598 |
| C | 3.14270 | 0.84883 | 2.06378 |
| C | 4.31673 | -1.51239 | 1.19187 |
| H | 2.42767 | -1.95026 | 0.27932 |
| C | 4.45336 | 0.55876 | 2.40746 |
| H | 2.68216 | 1.76686 | 2.41558 |
| C | 5.04214 | -0.61937 | 1.96850 |
| H | 4.76511 | -2.44552 | 0.87074 |
| H | 5.01616 | 1.25068 | 3.02341 |
| H | 6.06450 | -0.84945 | 2.24543 |
| C | -1.88814 | -1.51999 | -1.52467 |
| C | -2.54737 | -1.78323 | -0.32295 |
| C | -1.94757 | -2.43735 | -2.56638 |
| C | -3.27623 | -2.95002 | -0.17761 |
| H | -2.48621 | -1.08819 | 0.50782 |
| C | -2.68162 | -3.60358 | -2.41397 |
| H | -1.42261 | -2.24499 | -3.49323 |
| C | -3.34663 | -3.85859 | -1.22570 |
| H | -3.78976 | -3.15091 | 0.75523 |
| H | -2.73057 | -4.31257 | -3.23146 |
| H | -3.92047 | -4.77100 | -1.11137 |
| S | -0.18263 | 0.38942 | -3.50244 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.60530 | 0.12280 | 1.19018 |
| C | 0.38145 | -0.23221 | -0.41678 |
| P | -1.08393 | -0.06680 | -1.38489 |
| Cl | 1.93294 | -2.70243 | -2.27697 |
| Sn | 2.17180 | -0.34723 | -1.78704 |
| Au | -1.72619 | 1.51715 | -4.49645 |
| Cl | -3.27661 | 2.37342 | -5.89562 |
| C | 2.41336 | -0.13241 | 1.36963 |
| C | 2.93383 | -1.42534 | 1.55443 |
| C | 3.26371 | 0.98641 | 1.40843 |
| C | 4.30602 | -1.57103 | 1.72559 |
| C | 4.62621 | 0.78901 | 1.58372 |
| C | 5.16894 | -0.48234 | 1.73395 |
| H | 4.70981 | -2.56888 | 1.86863 |
| H | 5.28264 | 1.65393 | 1.60806 |
| C | -1.99241 | -1.64698 | -1.50076 |
| C | -2.65466 | -2.08546 | -0.33126 |
| C | -2.04604 | -2.44886 | -2.66690 |
| C | -3.35412 | -3.28585 | -0.35398 |
| C | -2.77274 | -3.63240 | -2.62039 |
| C | -3.43758 | -4.07380 | -1.48758 |
| H | -3.84721 | -3.61009 | 0.55733 |
| H | -2.80819 | -4.23882 | -3.51951 |
| C | 2.72337 | 2.37570 | 1.24306 |
| H | 2.40120 | 2.56090 | 0.21318 |
| H | 1.85317 | 2.54952 | 1.88397 |
| H | 3.47945 | 3.12100 | 1.49218 |
| C | 6.64607 | -0.67275 | 1.88939 |
| H | 7.12823 | -0.76113 | 0.91081 |
| H | 7.10511 | 0.17351 | 2.40354 |
| H | 6.87413 | -1.58140 | 2.44881 |
| C | 2.04894 | -2.63621 | 1.58621 |
| H | 1.16788 | -2.47240 | 2.21395 |
| H | 1.68968 | -2.89800 | 0.58687 |
| H | 2.59012 | -3.49615 | 1.98247 |
| C | -2.69127 | -1.34815 | 0.97802 |
| H | -3.54875 | -0.67026 | 1.02231 |
| H | -2.81056 | -2.06223 | 1.79381 |
| H | -1.79303 | -0.77092 | 1.19340 |
| C | -1.38357 | -2.14523 | -3.97690 |
| H | -1.78349 | -1.24108 | -4.43914 |
| H | -0.30751 | -2.01476 | -3.87105 |
| H | -1.55453 | -2.97329 | -4.66462 |
| C | -4.21973 | -5.34885 | -1.49964 |
| H | -4.45391 | -5.68396 | -0.48843 |
| H | -5.16495 | -5.21477 | -2.03417 |
| H | -3.67109 | -6.14396 | -2.00881 |
| S | -0.16834 | 0.68722 | -3.05030 |
| C | -2.23934 | 1.22071 | -0.85458 |
| H | -1.69710 | 2.16633 | -0.87842 |
| H | -3.05707 | 1.26129 | -1.57713 |
| H | -2.63288 | 1.04427 | 0.14298 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -1.91086 | 1.98071 | 0.32669 |
| C | -1.00269 | 0.58948 | 0.27742 |
| P | 0.74944 | 0.40607 | 0.36837 |
| C | -3.62798 | 1.30050 | 0.34908 |
| C | -4.41567 | 1.37061 | -0.83025 |
| C | -4.11438 | 0.58458 | 1.46700 |
| C | -5.48970 | 0.50057 | -0.94297 |
| C | -5.19098 | -0.28271 | 1.26783 |
| C | -5.85163 | -0.39505 | 0.05744 |
| H | -6.06692 | 0.50543 | -1.85573 |
| H | -5.53303 | -0.87672 | 2.10214 |

| | | | |
|---|----------|----------|----------|
| C | -3.63748 | 0.78430 | 2.92454 |
| C | -4.19050 | 2.42083 | -1.93498 |
| C | -6.97761 | -1.39447 | -0.18482 |
| C | -2.88045 | 2.21547 | -2.69639 |
| H | -2.00427 | 2.38835 | -2.06791 |
| H | -2.80450 | 1.20327 | -3.09557 |
| H | -2.82177 | 2.92953 | -3.52332 |
| C | -4.20583 | 3.81751 | -1.29722 |
| H | -5.15036 | 3.99762 | -0.77783 |
| H | -3.39397 | 3.95513 | -0.57999 |
| H | -4.09197 | 4.58052 | -2.07236 |
| C | -5.31073 | 2.39887 | -2.97786 |
| H | -5.32391 | 1.46748 | -3.54872 |
| H | -6.29566 | 2.55046 | -2.52986 |
| H | -5.14235 | 3.21218 | -3.68732 |
| C | -2.61543 | -0.26867 | 3.35900 |
| H | -1.68395 | -0.16919 | 2.80199 |
| H | -2.38740 | -0.15345 | 4.42294 |
| H | -3.00085 | -1.27964 | 3.20633 |
| C | -3.05791 | 2.18103 | 3.15191 |
| H | -2.11237 | 2.34870 | 2.62683 |
| H | -3.75727 | 2.95932 | 2.83801 |
| H | -2.84599 | 2.32050 | 4.21548 |
| C | -4.83974 | 0.67989 | 3.87877 |
| H | -5.65880 | 1.33079 | 3.56491 |
| H | -5.22416 | -0.33721 | 3.96524 |
| H | -4.52610 | 0.98554 | 4.87988 |
| C | -7.21682 | -2.30049 | 1.01998 |
| H | -7.53997 | -1.73649 | 1.89895 |
| H | -8.00572 | -3.01860 | 0.78427 |
| H | -6.32128 | -2.86894 | 1.28371 |
| C | -6.61053 | -2.27628 | -1.38460 |
| H | -6.46529 | -1.68667 | -2.29159 |
| H | -5.68562 | -2.82741 | -1.20004 |
| H | -7.40852 | -2.99886 | -1.57698 |
| C | -8.27885 | -0.64196 | -0.48719 |
| H | -8.18602 | -0.01098 | -1.37333 |
| H | -9.09023 | -1.35241 | -0.66824 |
| H | -8.56639 | -0.00353 | 0.35200 |
| C | 2.15151 | 1.50093 | -0.07980 |
| C | 2.77181 | 1.30109 | -1.34724 |
| C | 2.92960 | 2.07219 | 0.96351 |
| C | 4.15743 | 1.27489 | -1.38491 |
| C | 4.31372 | 2.00651 | 0.84946 |
| C | 4.95650 | 1.50424 | -0.27199 |
| H | 4.63495 | 1.06424 | -2.33355 |
| H | 4.91021 | 2.37650 | 1.67225 |
| C | 2.06187 | 1.31872 | -2.71507 |
| C | 2.40920 | 0.11676 | -3.59643 |
| C | 2.58152 | 2.59524 | -3.41088 |
| H | 2.03891 | -0.81367 | -3.16814 |
| H | 1.94779 | 0.24483 | -4.57915 |
| H | 3.48529 | 0.01707 | -3.74977 |
| H | 2.35597 | 3.48508 | -2.81768 |
| H | 3.65862 | 2.56582 | -3.57927 |
| H | 2.09010 | 2.69943 | -4.38197 |
| C | 2.39216 | 2.94542 | 2.11684 |
| C | 3.02336 | 4.33843 | 1.90559 |
| C | 2.81448 | 2.45026 | 3.50322 |
| H | 2.77729 | 4.73240 | 0.91695 |
| H | 2.63092 | 5.02998 | 2.65623 |
| H | 4.10894 | 4.32006 | 2.00142 |
| H | 2.38617 | 1.48028 | 3.75405 |
| H | 3.89917 | 2.35884 | 3.58224 |
| H | 2.48892 | 3.16589 | 4.26293 |
| C | 6.46243 | 1.29724 | -0.34742 |

| | | | |
|----|----------|----------|----------|
| C | 7.06312 | 2.26566 | -1.37362 |
| C | 6.73908 | -0.14736 | -0.78343 |
| H | 6.87950 | 3.30532 | -1.09026 |
| H | 8.14427 | 2.11627 | -1.43809 |
| H | 6.64676 | 2.10905 | -2.37087 |
| H | 6.31196 | -0.86821 | -0.08238 |
| H | 6.32079 | -0.35882 | -1.76958 |
| H | 7.81784 | -0.31750 | -0.83651 |
| Cl | -2.36015 | -1.45985 | -2.28385 |
| Au | 2.78132 | -2.41283 | 0.12108 |
| Cl | 4.64540 | -3.42208 | 0.91687 |
| C | 0.88718 | 3.18729 | 2.07048 |
| H | 0.57745 | 3.57222 | 1.09682 |
| H | 0.28180 | 2.31011 | 2.28919 |
| H | 0.62240 | 3.93759 | 2.81971 |
| C | 0.54929 | 1.47674 | -2.64209 |
| H | 0.02998 | 0.57919 | -2.30897 |
| H | 0.27183 | 2.31191 | -1.99429 |
| H | 0.16890 | 1.69761 | -3.64234 |
| C | 7.14300 | 1.53221 | 0.99845 |
| H | 7.04713 | 2.56862 | 1.33363 |
| H | 6.73949 | 0.87560 | 1.77305 |
| H | 8.21022 | 1.31820 | 0.90713 |
| Sn | -1.68112 | -1.59762 | 0.03152 |
| S | 0.95369 | -1.34835 | -0.73174 |
| C | 1.07955 | -0.16941 | 2.06140 |
| H | 2.14105 | -0.39903 | 2.15766 |
| H | 0.76879 | 0.54673 | 2.81670 |
| H | 0.51487 | -1.09380 | 2.19120 |

Coordination through P(sp²) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.66385 | 0.00714 | 0.86972 |
| C | 0.41970 | -0.30207 | -0.71760 |
| P | -1.07088 | -0.12119 | -1.62534 |
| Cl | 1.00017 | -2.87711 | -2.79038 |
| Sn | 1.82604 | -0.62515 | -2.52304 |
| C | -2.37513 | 0.87993 | -0.89998 |
| H | -3.22093 | 0.89751 | -1.59053 |
| H | -2.68922 | 0.45276 | 0.05510 |
| H | -2.01012 | 1.89597 | -0.74740 |
| Au | -0.66610 | 0.64530 | 2.50730 |
| Cl | -2.06347 | 1.30233 | 4.15420 |
| H | 2.04348 | -0.19790 | 1.09508 |
| H | -1.62210 | -1.41387 | -1.71370 |
| S | -0.44377 | 0.53983 | -3.40494 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.42905 | 0.51839 | 0.37757 |
| C | 0.16658 | 0.28785 | -1.21833 |
| P | -1.39866 | 0.08188 | -1.99503 |
| Cl | 1.57291 | -2.14879 | -3.10767 |
| Sn | 1.49442 | 0.27637 | -3.09933 |
| S | -1.02196 | 0.51826 | -3.92313 |
| C | 2.19543 | 0.65698 | 0.74455 |
| H | 2.48315 | -0.17881 | 1.38717 |
| H | 2.79420 | 0.64298 | -0.16607 |
| H | 2.37387 | 1.58064 | 1.29920 |
| C | -1.93434 | -1.62288 | -1.78306 |
| H | -2.13472 | -1.81722 | -0.72697 |
| H | -2.83766 | -1.78911 | -2.37318 |
| H | -1.13612 | -2.27556 | -2.14029 |
| C | -2.71330 | 1.12467 | -1.34020 |
| H | -3.61168 | 0.96946 | -1.94145 |
| H | -2.91891 | 0.87006 | -0.29794 |

| | | | |
|----|----------|---------|----------|
| H | -2.41012 | 2.16920 | -1.41120 |
| Au | -1.02705 | 0.63371 | 2.03829 |
| Cl | -2.55742 | 0.73179 | 3.70220 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.71391 | 0.16228 | 0.70744 |
| C | 0.48545 | -0.31807 | -0.84500 |
| P | -1.10258 | -0.42462 | -1.62312 |
| Cl | 2.22040 | -2.86669 | -2.56591 |
| Sn | 1.83378 | -0.47781 | -2.72778 |
| C | -2.14917 | 1.00314 | -1.26100 |
| H | -3.03804 | 0.96408 | -1.89182 |
| H | -2.43537 | 1.03325 | -0.20828 |
| H | -1.58228 | 1.90149 | -1.50638 |
| Au | -0.80008 | 0.85759 | 2.18068 |
| Cl | -2.37010 | 1.58982 | 3.64484 |
| C | 2.46604 | 0.12379 | 1.30931 |
| C | 2.79171 | 1.52428 | 1.83356 |
| C | 2.48071 | -0.87862 | 2.46919 |
| C | 3.45933 | -0.29572 | 0.23964 |
| H | 2.79935 | 2.26582 | 1.03123 |
| H | 2.07782 | 1.84964 | 2.59413 |
| H | 3.78557 | 1.50965 | 2.29072 |
| H | 2.27647 | -1.89551 | 2.12632 |
| H | 3.47355 | -0.86910 | 2.92904 |
| H | 1.75192 | -0.61964 | 3.24116 |
| H | 4.45703 | -0.35907 | 0.68499 |
| H | 3.22524 | -1.27685 | -0.18060 |
| H | 3.51792 | 0.43839 | -0.56834 |
| C | -2.04245 | -1.95214 | -1.13843 |
| C | -1.19435 | -3.17672 | -1.46691 |
| C | -2.37392 | -1.92968 | 0.35042 |
| C | -3.32969 | -1.97346 | -1.96495 |
| H | -0.94586 | -3.22683 | -2.52761 |
| H | -0.25858 | -3.19120 | -0.90640 |
| H | -1.76408 | -4.07275 | -1.20446 |
| H | -2.98332 | -1.07167 | 0.64052 |
| H | -2.94586 | -2.83125 | 0.58849 |
| H | -1.47630 | -1.94091 | 0.97080 |
| H | -3.84754 | -2.91652 | -1.76981 |
| H | -4.01083 | -1.16413 | -1.69409 |
| H | -3.12463 | -1.92092 | -3.03628 |
| S | -0.67128 | -0.44625 | -3.59520 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.68136 | 0.24878 | 0.63034 |
| C | 0.47082 | -0.35971 | -0.87615 |
| P | -1.06502 | -0.51262 | -1.72364 |
| Cl | 1.96475 | -3.22637 | -2.15984 |
| Sn | 1.91882 | -0.83437 | -2.58945 |
| C | -2.14968 | 0.91526 | -1.53576 |
| H | -3.04508 | 0.75005 | -2.13774 |
| H | -2.42831 | 1.07083 | -0.49201 |
| H | -1.62030 | 1.79476 | -1.90316 |
| Au | -0.80929 | 1.17740 | 1.98303 |
| Cl | -2.39751 | 2.09800 | 3.31083 |
| C | 2.38466 | 0.11458 | 1.15505 |
| C | 2.88137 | 1.06660 | 2.04711 |
| C | 3.20912 | -0.92290 | 0.71139 |
| C | 4.20186 | 1.00527 | 2.45835 |
| H | 2.23155 | 1.85515 | 2.41250 |
| C | 4.52589 | -0.98114 | 1.13547 |
| H | 2.81081 | -1.70759 | 0.07595 |
| C | 5.02403 | -0.01503 | 1.99981 |
| H | 4.58841 | 1.75122 | 3.14265 |
| H | 5.16102 | -1.79182 | 0.79830 |

| | | | |
|---|----------|----------|----------|
| H | 6.05539 | -0.06621 | 2.32956 |
| C | -1.96825 | -1.94478 | -1.09839 |
| C | -2.72894 | -1.83569 | 0.06623 |
| C | -1.86827 | -3.16774 | -1.75368 |
| C | -3.39322 | -2.94508 | 0.56093 |
| H | -2.80399 | -0.89447 | 0.59962 |
| C | -2.53457 | -4.27425 | -1.25041 |
| H | -1.26547 | -3.24875 | -2.65025 |
| C | -3.29708 | -4.16359 | -0.09776 |
| H | -3.98571 | -2.85597 | 1.46382 |
| H | -2.45321 | -5.22612 | -1.76173 |
| H | -3.81784 | -5.03050 | 0.29264 |
| S | -0.52603 | -0.73078 | -3.64869 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.66980 | 0.45275 | 1.00433 |
| C | 0.30384 | -0.34776 | -0.37903 |
| P | -1.16474 | -0.40753 | -1.35746 |
| Cl | 1.59752 | -3.11710 | -2.03531 |
| Sn | 1.92584 | -0.70923 | -1.95544 |
| Au | -0.61052 | 1.62899 | 2.38241 |
| Cl | -1.93365 | 2.83651 | 3.77217 |
| C | 2.43845 | 0.29611 | 1.31995 |
| C | 3.26569 | 1.42140 | 1.16189 |
| C | 2.96391 | -0.93209 | 1.75380 |
| C | 4.62077 | 1.28766 | 1.42282 |
| C | 4.32877 | -1.00884 | 2.00486 |
| C | 5.17199 | 0.08278 | 1.84575 |
| H | 5.26608 | 2.15081 | 1.29051 |
| H | 4.74308 | -1.95467 | 2.34001 |
| C | -1.99391 | -2.02997 | -1.20076 |
| C | -2.48714 | -2.38509 | 0.07413 |
| C | -2.16411 | -2.93149 | -2.27960 |
| C | -3.08111 | -3.62826 | 0.25672 |
| C | -2.77997 | -4.15169 | -2.02988 |
| C | -3.23143 | -4.53451 | -0.77647 |
| H | -3.44223 | -3.88381 | 1.24832 |
| H | -2.90471 | -4.83562 | -2.86321 |
| C | 2.71796 | 2.73920 | 0.70360 |
| H | 2.25672 | 2.66108 | -0.28570 |
| H | 1.95044 | 3.11458 | 1.38770 |
| H | 3.50813 | 3.48786 | 0.64391 |
| C | 2.10703 | -2.14651 | 1.95552 |
| H | 1.19217 | -1.90798 | 2.50553 |
| H | 1.80349 | -2.59025 | 1.00286 |
| H | 2.64992 | -2.90488 | 2.52041 |
| C | 6.63408 | -0.02281 | 2.14997 |
| H | 6.84800 | 0.36491 | 3.15081 |
| H | 6.97443 | -1.05862 | 2.11761 |
| H | 7.22964 | 0.55817 | 1.44313 |
| C | -2.47556 | -1.49604 | 1.28319 |
| H | -2.37997 | -2.09713 | 2.18846 |
| H | -1.67073 | -0.76653 | 1.29896 |
| H | -3.41802 | -0.94590 | 1.36694 |
| C | -1.74737 | -2.69840 | -3.70274 |
| H | -2.14494 | -1.77012 | -4.11136 |
| H | -0.66214 | -2.65784 | -3.79876 |
| H | -2.11071 | -3.52218 | -4.31797 |
| C | -3.84208 | -5.88181 | -0.55314 |
| H | -4.47407 | -6.17555 | -1.39356 |
| H | -3.06239 | -6.64301 | -0.45194 |
| H | -4.44431 | -5.90217 | 0.35623 |
| C | -2.40136 | 0.86072 | -0.99592 |
| H | -2.85824 | 0.73280 | -0.01650 |
| H | -1.91490 | 1.83500 | -1.05207 |
| H | -3.17074 | 0.79749 | -1.76859 |

| | | | |
|---|----------|---------|----------|
| S | -0.34654 | 0.06771 | -3.14111 |
|---|----------|---------|----------|

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.99035 | 0.88573 | 0.09493 |
| C | -0.29310 | -0.56216 | 0.42994 |
| P | 1.35813 | -1.15223 | 0.66227 |
| Cl | -2.02718 | -2.82644 | -1.86806 |
| C | 2.99760 | -0.47362 | 0.16553 |
| C | 3.56141 | -0.95411 | -1.05310 |
| C | 3.88224 | 0.02856 | 1.15982 |
| C | 4.91068 | -1.27609 | -1.05531 |
| C | 5.22149 | -0.34512 | 1.08443 |
| C | 5.74608 | -1.08208 | 0.03614 |
| H | 5.32918 | -1.69006 | -1.96397 |
| H | 5.88157 | -0.02005 | 1.87640 |
| C | -2.79232 | 0.61131 | 0.14447 |
| C | -3.53920 | 0.46243 | -1.05393 |
| C | -3.38370 | 0.28314 | 1.39142 |
| C | -4.73471 | -0.24499 | -0.97862 |
| C | -4.56758 | -0.44604 | 1.36964 |
| C | -5.23201 | -0.77848 | 0.19998 |
| H | -5.28649 | -0.41297 | -1.88815 |
| H | -4.99417 | -0.75969 | 2.31334 |
| C | -3.17152 | 1.11992 | -2.39828 |
| C | -2.90590 | 0.74357 | 2.78724 |
| C | -6.47872 | -1.65514 | 0.24903 |
| C | 3.56915 | 1.11168 | 2.21614 |
| C | 2.88083 | -0.97046 | -2.43696 |
| C | 7.18606 | -1.57782 | 0.00361 |
| C | -4.11864 | 1.31529 | 3.54597 |
| H | -3.78392 | 1.71801 | 4.50513 |
| H | -4.58732 | 2.12534 | 2.98251 |
| H | -4.88152 | 0.56717 | 3.75980 |
| C | -1.88070 | 1.87600 | 2.76531 |
| H | -0.88628 | 1.55322 | 2.45480 |
| H | -2.19406 | 2.70164 | 2.12198 |
| H | -1.76648 | 2.27268 | 3.77770 |
| C | -2.33839 | -0.42935 | 3.59045 |
| H | -3.05756 | -1.24772 | 3.66707 |
| H | -1.43205 | -0.81998 | 3.12420 |
| H | -2.08654 | -0.10459 | 4.60427 |
| C | -7.55412 | -0.97812 | 1.10665 |
| H | -8.45004 | -1.60368 | 1.14731 |
| H | -7.21583 | -0.81607 | 2.13218 |
| H | -7.83524 | -0.00844 | 0.68846 |
| C | -7.06100 | -1.91271 | -1.13824 |
| H | -7.93100 | -2.56781 | -1.05049 |
| H | -7.39350 | -0.98955 | -1.61983 |
| H | -6.33951 | -2.40521 | -1.79451 |
| C | -6.10645 | -3.00679 | 0.87075 |
| H | -5.34662 | -3.51482 | 0.27202 |
| H | -5.71588 | -2.89276 | 1.88429 |
| H | -6.98797 | -3.65176 | 0.92273 |
| C | -4.19223 | 0.79748 | -3.49399 |
| H | -5.19865 | 1.13813 | -3.24040 |
| H | -3.89420 | 1.31962 | -4.40563 |
| H | -4.22583 | -0.27058 | -3.72207 |
| C | -3.19961 | 2.64182 | -2.19814 |
| H | -4.18745 | 2.97059 | -1.86541 |
| H | -2.46797 | 2.97570 | -1.45886 |
| H | -2.96924 | 3.14755 | -3.13956 |
| C | -1.81305 | 0.68460 | -2.94932 |
| H | -0.97393 | 1.03235 | -2.34479 |
| H | -1.74708 | -0.40029 | -3.03412 |
| H | -1.66986 | 1.12602 | -3.93969 |
| C | 2.18443 | 1.73395 | 2.08142 |

| | | | |
|----|----------|----------|----------|
| H | 2.06365 | 2.18178 | 1.09313 |
| H | 1.35219 | 1.05276 | 2.23968 |
| H | 2.07668 | 2.53813 | 2.81321 |
| C | 4.53660 | 2.28097 | 1.92569 |
| H | 4.29039 | 3.11911 | 2.58286 |
| H | 5.57923 | 2.01564 | 2.10107 |
| H | 4.43762 | 2.62311 | 0.89368 |
| C | 3.83213 | 0.64975 | 3.65345 |
| H | 4.85457 | 0.28540 | 3.77243 |
| H | 3.70322 | 1.49361 | 4.33635 |
| H | 3.16142 | -0.14508 | 3.97730 |
| C | 1.43819 | -0.48627 | -2.44915 |
| H | 1.12850 | -0.33536 | -3.48605 |
| H | 0.74222 | -1.20307 | -2.01669 |
| H | 1.33930 | 0.47524 | -1.93848 |
| C | 2.95675 | -2.33696 | -3.12266 |
| H | 2.38612 | -3.08528 | -2.57334 |
| H | 2.53641 | -2.25923 | -4.12879 |
| H | 3.98450 | -2.69171 | -3.22338 |
| C | 3.66954 | 0.05070 | -3.28446 |
| H | 3.63483 | 1.04514 | -2.83291 |
| H | 4.71643 | -0.22894 | -3.40869 |
| H | 3.21796 | 0.11413 | -4.27799 |
| C | 7.92959 | -1.28065 | 1.30303 |
| H | 8.02917 | -0.20691 | 1.48128 |
| H | 7.43183 | -1.72963 | 2.16634 |
| H | 8.93829 | -1.69667 | 1.24878 |
| C | 7.93863 | -0.90297 | -1.14945 |
| H | 7.48603 | -1.12779 | -2.11712 |
| H | 7.95040 | 0.18284 | -1.02785 |
| H | 8.97384 | -1.25396 | -1.17700 |
| C | 7.18033 | -3.09586 | -0.21320 |
| H | 6.66073 | -3.60599 | 0.60149 |
| H | 6.68543 | -3.36885 | -1.14719 |
| H | 8.20574 | -3.47336 | -0.25325 |
| Sn | -1.34689 | -2.65030 | 0.45557 |
| Au | -0.02540 | 2.83790 | -0.38721 |
| Cl | 0.98764 | 4.81737 | -0.86105 |
| S | 1.21884 | -3.03760 | -0.08420 |
| C | 1.46062 | -1.48367 | 2.45047 |
| H | 0.65329 | -2.18529 | 2.66642 |
| H | 2.40904 | -1.98636 | 2.64263 |
| H | 1.35504 | -0.61109 | 3.08662 |

Coordination through $\pi(C=P)$ bond

| | | | |
|-------------|----------|----------|----------|
| R= H | | | |
| P | 0.68588 | 0.03286 | 1.07565 |
| C | 0.54022 | 0.05431 | -0.64286 |
| P | -0.98495 | -0.05900 | -1.53265 |
| Cl | 1.26184 | -2.76197 | -2.30204 |
| Sn | 1.90102 | -0.42931 | -2.46601 |
| C | -2.39630 | 0.86457 | -0.90205 |
| H | -3.27111 | 0.63202 | -1.51267 |
| H | -2.58652 | 0.57809 | 0.13506 |
| H | -2.18630 | 1.93318 | -0.95956 |
| Au | 0.92260 | 2.10222 | -0.08201 |
| Cl | 1.28854 | 4.32101 | -0.16498 |
| H | 2.09270 | -0.20866 | 1.15804 |
| H | -1.37370 | -1.40709 | -1.41178 |
| S | -0.49241 | 0.40299 | -3.41113 |

| | | | |
|---------------|----------|----------|----------|
| R = Me | | | |
| P | 0.65646 | 0.03055 | 1.02380 |
| C | 0.46822 | 0.12009 | -0.68445 |
| P | -1.07992 | -0.11080 | -1.52111 |

| | | | |
|----|----------|----------|----------|
| Cl | 1.75346 | -2.66386 | -2.15708 |
| Sn | 1.85038 | -0.25254 | -2.51241 |
| C | 2.43786 | -0.32763 | 1.27316 |
| H | 2.52893 | -1.41210 | 1.39518 |
| H | 3.07023 | -0.01239 | 0.44281 |
| H | 2.77650 | 0.14632 | 2.19651 |
| C | -1.67235 | -1.76892 | -1.14197 |
| H | -1.93549 | -1.83656 | -0.08392 |
| H | -2.54647 | -1.98275 | -1.75965 |
| H | -0.87641 | -2.47783 | -1.37697 |
| C | -2.40935 | 1.01022 | -1.03972 |
| H | -3.30850 | 0.75241 | -1.60369 |
| H | -2.60731 | 0.91302 | 0.03015 |
| H | -2.12335 | 2.03688 | -1.26864 |
| Au | 0.74444 | 2.16600 | -0.05766 |
| Cl | 1.00001 | 4.40468 | -0.00129 |
| S | -0.61699 | 0.08606 | -3.46598 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.99470 | 0.14204 | 1.01469 |
| C | 0.61181 | 0.10737 | -0.66658 |
| P | -1.05585 | -0.21541 | -1.24216 |
| Cl | 2.31444 | -2.39985 | -2.51025 |
| Sn | 1.71861 | -0.04457 | -2.71814 |
| C | -1.76787 | -1.79127 | -0.55537 |
| Au | 0.85816 | 2.21351 | -0.17643 |
| Cl | 1.04559 | 4.46137 | -0.23300 |
| C | 2.83087 | -0.10518 | 1.27272 |
| C | 3.74479 | 0.21046 | 0.10274 |
| C | 3.18667 | 0.76425 | 2.48021 |
| C | 2.94664 | -1.58869 | 1.64572 |
| H | 3.59161 | -0.48569 | -0.72542 |
| H | 3.62283 | 1.23688 | -0.25196 |
| H | 4.78788 | 0.09379 | 0.41620 |
| H | 2.52254 | 0.57485 | 3.32822 |
| H | 4.20889 | 0.54123 | 2.80060 |
| H | 3.13357 | 1.82891 | 2.23932 |
| H | 3.97269 | -1.79816 | 1.96480 |
| H | 2.28473 | -1.85695 | 2.47462 |
| H | 2.72209 | -2.23377 | 0.79268 |
| C | -2.22574 | 1.09576 | -0.80622 |
| H | -2.25005 | 1.25116 | 0.27316 |
| H | -1.91220 | 2.01595 | -1.29942 |
| H | -3.22063 | 0.82703 | -1.16582 |
| C | -2.17655 | -1.59090 | 0.90351 |
| H | -2.52746 | -2.54903 | 1.29771 |
| H | -1.34337 | -1.26293 | 1.52904 |
| H | -2.99347 | -0.87458 | 1.00995 |
| C | -0.73488 | -2.90738 | -0.67044 |
| H | 0.13971 | -2.72525 | -0.04441 |
| H | -1.19565 | -3.84293 | -0.34036 |
| H | -0.38722 | -3.04029 | -1.69567 |
| C | -2.99694 | -2.14927 | -1.39280 |
| H | -3.42091 | -3.07733 | -0.99897 |
| H | -3.77714 | -1.38636 | -1.34141 |
| H | -2.73752 | -2.31115 | -2.43978 |
| S | -0.86846 | -0.31621 | -3.24660 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.57579 | 0.26509 | 0.93364 |
| C | 0.37614 | 0.19330 | -0.77567 |
| P | -1.19556 | -0.01612 | -1.57213 |
| Cl | 1.73769 | -2.38245 | -2.79953 |
| Sn | 1.71719 | 0.05115 | -2.67501 |
| C | -2.52526 | 1.03161 | -0.94147 |
| H | -3.44203 | 0.79097 | -1.48302 |

| | | | |
|----|----------|----------|----------|
| H | -2.67506 | 0.85224 | 0.12501 |
| H | -2.26481 | 2.07784 | -1.10479 |
| Au | 0.68576 | 2.30160 | -0.32021 |
| Cl | 0.97128 | 4.53599 | -0.44245 |
| C | 2.33411 | -0.07252 | 1.22524 |
| C | 2.95126 | 0.57853 | 2.29585 |
| C | 3.05153 | -1.01589 | 0.48816 |
| C | 4.27968 | 0.32638 | 2.59243 |
| H | 2.39257 | 1.29744 | 2.88703 |
| C | 4.37697 | -1.27623 | 0.80063 |
| H | 2.56908 | -1.57266 | -0.30882 |
| C | 4.99370 | -0.60018 | 1.84376 |
| H | 4.75884 | 0.85015 | 3.41140 |
| H | 4.92667 | -2.01340 | 0.22679 |
| H | 6.03171 | -0.80275 | 2.08161 |
| C | -1.75886 | -1.71222 | -1.30107 |
| C | -1.84695 | -2.60659 | -2.36052 |
| C | -2.11620 | -2.11753 | -0.01494 |
| C | -2.29986 | -3.89821 | -2.13646 |
| H | -1.54913 | -2.29033 | -3.35280 |
| C | -2.56587 | -3.40824 | 0.20265 |
| H | -2.03492 | -1.43388 | 0.82404 |
| C | -2.65955 | -4.29838 | -0.85951 |
| H | -2.36241 | -4.59464 | -2.96418 |
| H | -2.84075 | -3.72143 | 1.20306 |
| H | -3.00947 | -5.30973 | -0.68680 |
| S | -0.81646 | 0.37826 | -3.50163 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.51924 | 0.34083 | 1.35444 |
| C | 0.15410 | 0.26475 | -0.33557 |
| P | -1.35775 | 0.05896 | -1.26228 |
| Cl | 1.82119 | -1.82057 | -2.78882 |
| Sn | 1.66923 | 0.51311 | -2.08213 |
| Au | 0.20234 | 2.39189 | 0.17476 |
| Cl | 0.09796 | 4.65355 | 0.13284 |
| C | 2.32376 | 0.04960 | 1.40397 |
| C | 3.23620 | 1.02039 | 1.84897 |
| C | 2.76222 | -1.26359 | 1.14060 |
| C | 4.58395 | 0.68812 | 1.91529 |
| C | 4.11924 | -1.54338 | 1.22665 |
| C | 5.05046 | -0.57738 | 1.58666 |
| H | 5.28941 | 1.44403 | 2.24761 |
| H | 4.45448 | -2.55561 | 1.02118 |
| C | -1.81603 | -1.71123 | -1.33218 |
| C | -1.84856 | -2.46637 | -2.52964 |
| C | -2.15258 | -2.34435 | -0.11455 |
| C | -2.13717 | -3.82365 | -2.44826 |
| C | -2.41968 | -3.70810 | -0.10289 |
| C | -2.39983 | -4.47521 | -1.25383 |
| H | -2.15397 | -4.39363 | -3.37158 |
| H | -2.66243 | -4.17674 | 0.84611 |
| C | 2.81383 | 2.39739 | 2.26370 |
| H | 2.67742 | 3.06119 | 1.40451 |
| H | 1.86881 | 2.38977 | 2.81338 |
| H | 3.57015 | 2.84904 | 2.90749 |
| C | 1.80811 | -2.37998 | 0.82921 |
| H | 0.94018 | -2.36698 | 1.49649 |
| H | 1.43661 | -2.33126 | -0.19698 |
| H | 2.30452 | -3.34325 | 0.95318 |
| C | 6.51275 | -0.89588 | 1.62710 |
| H | 6.68698 | -1.93446 | 1.91438 |
| H | 6.96488 | -0.75081 | 0.64090 |
| H | 7.04297 | -0.24973 | 2.32868 |
| C | -2.32969 | -1.64862 | 1.20572 |
| H | -2.07783 | -2.32709 | 2.02214 |

| | | | |
|---|----------|----------|----------|
| H | -1.72435 | -0.75528 | 1.33918 |
| H | -3.37787 | -1.36296 | 1.34158 |
| C | -1.62885 | -1.93281 | -3.91513 |
| H | -2.26159 | -1.07373 | -4.13574 |
| H | -0.59472 | -1.62449 | -4.06773 |
| H | -1.85804 | -2.71713 | -4.63741 |
| C | -2.64784 | -5.94999 | -1.21502 |
| H | -3.21473 | -6.28068 | -2.08738 |
| H | -1.70002 | -6.49708 | -1.21764 |
| H | -3.19433 | -6.24056 | -0.31655 |
| C | -2.83399 | 0.94145 | -0.68525 |
| H | -2.61549 | 2.01007 | -0.68058 |
| H | -3.62958 | 0.74267 | -1.40728 |
| H | -3.15628 | 0.62310 | 0.30362 |
| S | -0.81117 | 0.97284 | -2.97681 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.68894 | 0.00840 | 1.07969 |
| C | 0.43223 | 0.09078 | -0.64221 |
| P | -1.10127 | -0.05758 | -1.63281 |
| Cl | 3.01878 | -1.30238 | -3.25498 |
| Au | 0.38417 | 2.17451 | 0.03600 |
| Cl | 0.08130 | 4.42929 | -0.00271 |
| C | 2.53884 | -0.04968 | 1.21392 |
| C | 3.25575 | -1.17719 | 0.72719 |
| C | 3.27933 | 1.08349 | 1.63372 |
| C | 4.56655 | -0.99012 | 0.31380 |
| C | 4.59326 | 1.20318 | 1.17632 |
| C | 5.23287 | 0.22399 | 0.43672 |
| H | 5.09612 | -1.83592 | -0.10527 |
| H | 5.13738 | 2.10088 | 1.43416 |
| C | 2.87293 | 2.10642 | 2.71696 |
| C | 2.79832 | -2.64102 | 0.87909 |
| C | 6.62687 | 0.40107 | -0.15357 |
| C | 3.83897 | 1.85463 | 3.89367 |
| H | 3.74151 | 0.83242 | 4.26832 |
| H | 4.88026 | 2.01010 | 3.60970 |
| H | 3.60478 | 2.54238 | 4.71090 |
| C | 3.04355 | 3.55506 | 2.25241 |
| H | 2.38393 | 3.79739 | 1.41833 |
| H | 2.79851 | 4.23343 | 3.07428 |
| H | 4.06900 | 3.77012 | 1.94762 |
| C | 1.47265 | 1.93899 | 3.29952 |
| H | 1.38027 | 2.58179 | 4.17911 |
| H | 0.67998 | 2.24400 | 2.61316 |
| H | 1.28176 | 0.91257 | 3.62253 |
| C | 3.08018 | -3.48635 | -0.36391 |
| H | 2.59246 | -3.07904 | -1.24736 |
| H | 4.14689 | -3.55484 | -0.58204 |
| H | 2.71951 | -4.50570 | -0.19970 |
| C | 3.62907 | -3.20338 | 2.04903 |
| H | 4.69829 | -3.16138 | 1.83569 |
| H | 3.44661 | -2.64031 | 2.96796 |
| H | 3.35679 | -4.24808 | 2.22678 |
| C | 1.33720 | -2.82689 | 1.26921 |
| H | 1.08578 | -2.29291 | 2.19085 |
| H | 0.65046 | -2.52174 | 0.47986 |
| H | 1.15125 | -3.88783 | 1.45940 |
| C | 7.21136 | 1.77860 | 0.14672 |
| H | 6.58136 | 2.58054 | -0.24589 |
| H | 7.34810 | 1.94031 | 1.21936 |
| H | 8.19227 | 1.86820 | -0.32610 |
| C | 6.53556 | 0.23424 | -1.67523 |
| H | 7.52901 | 0.32460 | -2.12382 |
| H | 6.12137 | -0.73626 | -1.95441 |
| H | 5.89329 | 1.00155 | -2.11434 |

| | | | |
|----|----------|----------|----------|
| C | 7.57723 | -0.65780 | 0.41743 |
| H | 7.64842 | -0.57607 | 1.50506 |
| H | 7.25245 | -1.67146 | 0.17531 |
| H | 8.57897 | -0.52431 | -0.00013 |
| C | -2.35366 | -1.43971 | -1.67148 |
| C | -2.33468 | -2.33760 | -2.77864 |
| C | -3.59751 | -1.24557 | -1.00823 |
| C | -3.54007 | -2.61291 | -3.40956 |
| C | -1.14755 | -3.21734 | -3.21230 |
| C | -4.76476 | -1.58081 | -1.68840 |
| C | -3.79267 | -0.89299 | 0.48014 |
| C | -4.76804 | -2.16421 | -2.94508 |
| H | -3.51141 | -3.23438 | -4.29607 |
| C | -0.74261 | -3.03584 | -4.67653 |
| C | -1.62487 | -4.67482 | -3.02998 |
| C | 0.06054 | -3.07441 | -2.30351 |
| H | -5.70881 | -1.38247 | -1.20010 |
| C | -2.50175 | -0.61783 | 1.23321 |
| C | -4.37981 | -2.16880 | 1.12038 |
| C | -4.78373 | 0.25061 | 0.71807 |
| C | -6.03812 | -2.41140 | -3.74851 |
| H | 0.00162 | -3.79129 | -4.94161 |
| H | -1.59559 | -3.16081 | -5.34776 |
| H | -0.30595 | -2.05514 | -4.85290 |
| H | -2.42664 | -4.94440 | -3.71841 |
| H | -0.78388 | -5.34739 | -3.21874 |
| H | -1.97888 | -4.85037 | -2.01102 |
| H | 0.53259 | -2.09689 | -2.36406 |
| H | -0.21396 | -3.28733 | -1.26825 |
| H | 0.82234 | -3.79741 | -2.60164 |
| H | -1.77277 | -1.41429 | 1.07247 |
| H | -2.03492 | 0.33280 | 0.98007 |
| H | -2.70525 | -0.57688 | 2.30587 |
| H | -4.51269 | -2.00822 | 2.19389 |
| H | -5.34808 | -2.43380 | 0.69453 |
| H | -3.70652 | -3.01815 | 0.98302 |
| H | -5.76943 | 0.03197 | 0.30433 |
| H | -4.90904 | 0.40379 | 1.79307 |
| H | -4.44832 | 1.19437 | 0.28664 |
| C | -7.27435 | -1.82863 | -3.06898 |
| C | -6.25136 | -3.91907 | -3.92970 |
| C | -5.88600 | -1.75155 | -5.12428 |
| H | -7.47864 | -2.30954 | -2.10889 |
| H | -7.17590 | -0.75300 | -2.90235 |
| H | -8.14844 | -1.98697 | -3.70488 |
| H | -5.42207 | -4.38551 | -4.46489 |
| H | -6.35259 | -4.41962 | -2.96360 |
| H | -7.16315 | -4.10182 | -4.50488 |
| H | -5.74830 | -0.67191 | -5.02786 |
| H | -5.02892 | -2.14981 | -5.67076 |
| H | -6.78098 | -1.92848 | -5.72695 |
| Sn | 1.95611 | 0.70522 | -2.34199 |
| S | -0.36306 | 0.21921 | -3.50186 |
| C | -2.21365 | 1.37887 | -1.47033 |
| H | -2.63111 | 1.51366 | -0.47759 |
| H | -1.65384 | 2.26836 | -1.75803 |
| H | -3.01723 | 1.22274 | -2.19246 |

[R-P=C(Pb(II)Cl)-P(O)ClR](AuCl)**Coordination through Pb(II) atom****R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.82625 | 0.08960 | 0.83597 |
| C | 0.43990 | -0.10123 | -0.76223 |
| P | -1.16184 | -0.22556 | -1.46941 |
| O | -0.95473 | 0.03880 | -2.93819 |
| Pb | 1.44180 | -0.06541 | -2.84078 |
| Cl | 1.50836 | -2.49219 | -3.08066 |
| Au | 2.75524 | 1.61751 | -4.31006 |
| Cl | 3.91132 | 3.11928 | -5.52527 |
| Cl | -2.48653 | 1.01556 | -0.62389 |
| H | 2.24762 | 0.15470 | 0.69822 |
| H | -1.75848 | -1.47008 | -1.21022 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.84400 | 0.02204 | 0.83673 |
| C | 0.46128 | -0.10713 | -0.76451 |
| P | -1.13906 | -0.27436 | -1.47205 |
| O | -0.91374 | 0.00518 | -2.94371 |
| Pb | 1.44169 | -0.01375 | -2.84028 |
| Cl | 1.60115 | -2.45129 | -3.09808 |
| C | -1.88510 | -1.86885 | -1.17571 |
| H | -2.05252 | -2.01780 | -0.10861 |
| H | -2.83154 | -1.92299 | -1.71622 |
| H | -1.19551 | -2.62412 | -1.56024 |
| C | 2.67101 | 0.14324 | 0.88877 |
| H | 3.13274 | 0.27682 | -0.08960 |
| H | 2.95051 | 0.97191 | 1.54459 |
| H | 3.05852 | -0.77162 | 1.34815 |
| Au | 2.72699 | 1.63737 | -4.36937 |
| Cl | 3.86819 | 3.11996 | -5.62653 |
| Cl | -2.44286 | 1.04065 | -0.67473 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.82212 | -0.24810 | 0.72314 |
| C | 0.53661 | -0.16788 | -0.90234 |
| P | -1.00883 | -0.44383 | -1.71200 |
| O | -0.68185 | -0.23893 | -3.17908 |
| Pb | 1.59593 | 0.28947 | -2.89329 |
| Cl | 2.46217 | -1.97849 | -3.28547 |
| Au | 2.49053 | 2.31568 | -4.24284 |
| Cl | 3.27945 | 4.12839 | -5.33147 |
| C | 2.62801 | 0.11121 | 1.05047 |
| C | 3.17182 | -1.16160 | 1.70846 |
| C | 3.46602 | 0.47936 | -0.15763 |
| C | 2.62455 | 1.25577 | 2.06918 |
| H | 2.56996 | -1.46264 | 2.57039 |
| H | 3.20445 | -1.99656 | 1.00447 |
| H | 4.19112 | -0.97952 | 2.06365 |
| H | 3.10147 | 1.38960 | -0.64422 |
| H | 4.49551 | 0.68481 | 0.15315 |
| H | 3.51644 | -0.34121 | -0.88026 |
| H | 3.64571 | 1.43346 | 2.42067 |
| H | 2.25313 | 2.18604 | 1.63219 |
| H | 2.00855 | 1.02075 | 2.94139 |
| C | -1.85092 | -2.04196 | -1.41587 |
| C | -3.07380 | -2.09258 | -2.33400 |
| C | -0.85383 | -3.13618 | -1.80924 |
| C | -2.26060 | -2.18827 | 0.04547 |
| H | -3.81332 | -1.33496 | -2.06930 |
| H | -2.79530 | -1.95835 | -3.38042 |
| H | -3.54356 | -3.07433 | -2.22817 |
| H | 0.03707 | -3.12664 | -1.17908 |

| | | | |
|----|----------|----------|----------|
| H | -1.34484 | -4.10549 | -1.68710 |
| H | -0.53492 | -3.04383 | -2.84825 |
| H | -2.72276 | -3.17032 | 0.17883 |
| H | -1.40384 | -2.13098 | 0.72079 |
| H | -2.98701 | -1.43090 | 0.34376 |
| Cl | -2.31985 | 0.97532 | -1.09350 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.91582 | 0.11942 | 0.80099 |
| C | 0.47807 | -0.20490 | -0.76216 |
| P | -1.12129 | -0.37905 | -1.46430 |
| O | -0.88138 | -0.19743 | -2.94673 |
| Pb | 1.49701 | -0.09849 | -2.80078 |
| Cl | 1.80334 | -2.51563 | -3.16241 |
| Au | 2.70888 | 1.60997 | -4.32884 |
| Cl | 3.78527 | 3.12890 | -5.60381 |
| C | 2.72328 | 0.16468 | 0.74668 |
| C | 3.36125 | 1.06982 | 1.59760 |
| C | 3.49671 | -0.66614 | -0.07082 |
| C | 4.74200 | 1.18719 | 1.58582 |
| H | 2.77073 | 1.69709 | 2.25811 |
| C | 4.87728 | -0.55671 | -0.06696 |
| H | 3.02198 | -1.43502 | -0.67365 |
| C | 5.49931 | 0.37800 | 0.75116 |
| H | 5.22827 | 1.90889 | 2.23168 |
| H | 5.47012 | -1.20890 | -0.69772 |
| H | 6.57959 | 0.46522 | 0.74725 |
| C | -1.92836 | -1.92661 | -1.08886 |
| C | -1.90979 | -2.91792 | -2.06716 |
| C | -2.50948 | -2.17049 | 0.15449 |
| C | -2.48143 | -4.15203 | -1.79788 |
| H | -1.45016 | -2.71983 | -3.02752 |
| C | -3.07410 | -3.40608 | 0.41378 |
| H | -2.52867 | -1.39592 | 0.91283 |
| C | -3.06041 | -4.39536 | -0.56219 |
| H | -2.47135 | -4.92423 | -2.55779 |
| H | -3.53033 | -3.59836 | 1.37762 |
| H | -3.50620 | -5.36162 | -0.35555 |
| Cl | -2.35581 | 1.04233 | -0.73137 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.03272 | -0.17782 | 1.32694 |
| C | 0.45747 | -0.35234 | -0.21494 |
| P | -1.09670 | -0.39443 | -1.05173 |
| O | -0.71804 | 0.10809 | -2.42694 |
| Pb | 1.66105 | 0.08948 | -2.08274 |
| Cl | 1.95330 | -2.22874 | -2.87377 |
| Au | 3.10342 | 1.98894 | -3.10187 |
| Cl | 4.41427 | 3.66972 | -3.85500 |
| C | 2.81298 | 0.06606 | 0.97679 |
| C | 3.32090 | 1.37633 | 0.94656 |
| C | 3.65523 | -1.03387 | 0.75465 |
| C | 4.66046 | 1.56394 | 0.63812 |
| C | 4.99152 | -0.79246 | 0.45157 |
| C | 5.50989 | 0.49383 | 0.37450 |
| H | 5.05047 | 2.57631 | 0.59344 |
| H | 5.64658 | -1.63996 | 0.27398 |
| C | -1.95461 | -1.96969 | -1.03585 |
| C | -2.22006 | -2.64981 | -2.24739 |
| C | -2.33819 | -2.54137 | 0.19727 |
| C | -2.83239 | -3.89570 | -2.17242 |
| C | -2.93664 | -3.79200 | 0.19891 |
| C | -3.18689 | -4.49206 | -0.97232 |
| H | -3.03787 | -4.41859 | -3.10085 |
| H | -3.22312 | -4.22727 | 1.15115 |
| Cl | -2.36113 | 0.95815 | -0.21372 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 2.43853 | 2.56179 | 1.20586 | H | -7.72214 | 0.98192 | -0.14096 |
| H | 1.76797 | 2.39318 | 2.05464 | H | -6.58610 | 0.80906 | 1.19576 |
| H | 3.03439 | 3.44965 | 1.41896 | H | -6.89878 | 2.40781 | 0.50952 |
| H | 1.80848 | 2.79212 | 0.34072 | C | -6.04068 | 1.86212 | -2.04620 |
| C | 3.14887 | -2.44362 | 0.83637 | H | -6.97310 | 1.43970 | -2.42768 |
| H | 2.47622 | -2.58207 | 1.68838 | H | -6.20588 | 2.93118 | -1.88755 |
| H | 2.59471 | -2.72331 | -0.06456 | H | -5.28081 | 1.73917 | -2.82177 |
| H | 3.97763 | -3.14398 | 0.94630 | C | -5.50638 | -0.35032 | -1.06261 |
| C | 6.94152 | 0.73398 | 0.00931 | H | -4.71955 | -0.52296 | -1.80103 |
| H | 7.01190 | 1.20237 | -0.97661 | H | -5.26307 | -0.93144 | -0.17065 |
| H | 7.42307 | 1.40845 | 0.72124 | H | -6.44268 | -0.74388 | -1.46724 |
| H | 7.50845 | -0.19714 | -0.01872 | C | -2.59916 | 4.99255 | -1.98809 |
| C | -2.18099 | -1.85610 | 1.52065 | H | -3.54550 | 5.30519 | -1.54057 |
| H | -1.21014 | -1.37482 | 1.64658 | H | -2.09962 | 5.88834 | -2.36375 |
| H | -2.94018 | -1.08141 | 1.65231 | H | -2.81249 | 4.35375 | -2.84810 |
| H | -2.29470 | -2.57702 | 2.33055 | C | -1.35262 | 5.34940 | 0.10499 |
| C | -1.90057 | -2.13728 | -3.62152 | H | -2.25839 | 5.66334 | 0.62947 |
| H | -2.30530 | -1.14163 | -3.79784 | H | -0.64625 | 4.97264 | 0.84787 |
| H | -0.82318 | -2.07558 | -3.78342 | H | -0.90196 | 6.23269 | -0.35593 |
| H | -2.31663 | -2.81899 | -4.36352 | C | -0.40335 | 3.92494 | -1.72903 |
| C | -3.80352 | -5.85458 | -0.94018 | H | 0.39883 | 3.60135 | -1.05969 |
| H | -3.02790 | -6.62207 | -0.85395 | H | -0.58783 | 3.11671 | -2.43825 |
| H | -4.47328 | -5.96965 | -0.08633 | H | -0.02542 | 4.79508 | -2.27375 |
| H | -4.36548 | -6.05932 | -1.85267 | C | 2.96811 | 1.99357 | 2.57219 |

R = Mes*

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| P | 0.01610 | 2.43878 | 1.03925 | H | 2.74197 | 2.59739 | 1.69064 |
| C | 0.41548 | 0.91920 | 0.50664 | H | 2.15456 | 1.29150 | 2.74400 |
| P | 1.88761 | -0.03836 | 0.29832 | H | 2.98365 | 2.67128 | 3.42940 |
| Cl | -1.27139 | 0.34757 | -2.71795 | C | 5.35771 | 2.46053 | 2.42540 |
| O | 1.46525 | -1.02443 | -0.77082 | H | 5.23094 | 3.07594 | 3.32017 |
| C | 3.62361 | 0.44237 | 0.04506 | H | 6.38465 | 2.09491 | 2.41279 |
| C | 4.13921 | 0.20461 | -1.26465 | H | 5.21570 | 3.09910 | 1.55019 |
| C | 4.53529 | 0.54255 | 1.12853 | C | 4.58135 | 0.45560 | 3.68736 |
| C | 5.42723 | -0.29869 | -1.35892 | H | 5.58335 | 0.02296 | 3.68436 |
| C | 5.81969 | 0.04192 | 0.94047 | H | 4.49467 | 1.07581 | 4.58361 |
| C | 6.26101 | -0.48074 | -0.26331 | H | 3.86219 | -0.35890 | 3.76831 |
| H | 5.80007 | -0.55147 | -2.34275 | C | 2.27520 | 1.53223 | -2.41236 |
| H | 6.50039 | 0.07021 | 1.77948 | H | 1.96855 | 1.91531 | -3.38838 |
| C | -1.80421 | 2.39584 | 0.78169 | H | 1.39460 | 1.05053 | -1.99730 |
| C | -2.36301 | 3.09700 | -0.31136 | H | 2.54575 | 2.38940 | -1.78981 |
| C | -2.61044 | 1.51243 | 1.54164 | C | 3.05732 | -0.63561 | -3.41770 |
| C | -3.61631 | 2.69470 | -0.76507 | H | 2.30551 | -1.22829 | -2.90116 |
| C | -3.83305 | 1.12819 | 0.99736 | H | 2.64770 | -0.31382 | -4.37893 |
| C | -4.33552 | 1.66031 | -0.18355 | H | 3.92192 | -1.27304 | -3.61975 |
| H | -4.03449 | 3.18930 | -1.62678 | C | 4.49054 | 1.39919 | -3.41256 |
| H | -4.43148 | 0.40361 | 1.53495 | H | 4.85931 | 2.25975 | -2.84885 |
| C | -1.67948 | 4.30781 | -0.97410 | H | 5.34905 | 0.80629 | -3.72832 |
| C | -2.31642 | 1.06465 | 2.99128 | H | 4.00367 | 1.76991 | -4.31785 |
| C | -5.65195 | 1.14505 | -0.75600 | C | 8.37636 | -1.26553 | 0.88669 |
| C | 4.32416 | 1.31491 | 2.44633 | H | 8.61574 | -0.28806 | 1.31336 |
| C | 3.46211 | 0.59049 | -2.59506 | H | 7.80911 | -1.83625 | 1.62616 |
| C | 7.62169 | -1.14356 | -0.43438 | H | 9.32108 | -1.78774 | 0.71888 |
| C | -3.59325 | 1.28169 | 3.82411 | C | 8.47752 | -0.32296 | -1.40679 |
| H | -3.37630 | 1.07542 | 4.87510 | H | 8.01461 | -0.24758 | -2.39258 |
| H | -3.94744 | 2.31211 | 3.74409 | H | 8.63548 | 0.69084 | -1.03073 |
| H | -4.40664 | 0.61917 | 3.52847 | H | 9.45553 | -0.79502 | -1.53367 |
| C | -1.23546 | 1.90054 | 3.67494 | C | 7.41406 | -2.55228 | -1.00388 |
| H | -0.23046 | 1.69984 | 3.29241 | H | 6.81534 | -3.16474 | -0.32562 |
| H | -1.43503 | 2.97193 | 3.59141 | H | 6.90498 | -2.52791 | -1.96931 |
| H | -1.20500 | 1.64897 | 4.73849 | H | 8.37970 | -3.04484 | -1.14618 |
| C | -1.93352 | -0.41415 | 3.07910 | Au | -2.32491 | -2.77951 | -0.02340 |
| H | -2.67500 | -1.05407 | 2.59505 | Cl | -3.60760 | -4.57959 | 0.46413 |
| H | -0.95989 | -0.60464 | 2.62234 | Pb | -0.89832 | -0.66033 | -0.49528 |
| H | -1.86531 | -0.72165 | 4.12645 | Cl | 1.96322 | -1.16355 | 2.01623 |
| C | -6.77637 | 1.34924 | 0.26625 | | | | |

Coordination through O atom**R= H**

| | | | |
|----|----------|----------|----------|
| P | 0.84877 | 0.08847 | 1.00871 |
| C | 0.57903 | -0.13388 | -0.61043 |
| P | -0.96185 | -0.01132 | -1.38567 |
| O | -0.62575 | 0.43645 | -2.81132 |
| Pb | 1.81260 | -0.29252 | -2.66548 |
| Cl | 1.17284 | -2.66380 | -2.94281 |
| Au | -2.00955 | 0.70978 | -4.37607 |
| Cl | -3.44059 | 1.00763 | -6.04838 |
| Cl | -2.28292 | 1.21647 | -0.52203 |
| H | 2.26833 | -0.10522 | 1.01343 |
| H | -1.65778 | -1.22878 | -1.38987 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.84716 | 0.02016 | 1.00575 |
| C | 0.58394 | -0.13384 | -0.61882 |
| P | -0.97649 | -0.02727 | -1.36347 |
| O | -0.64266 | 0.39300 | -2.80946 |
| Pb | 1.77533 | -0.17715 | -2.70163 |
| Cl | 1.35674 | -2.60755 | -3.02204 |
| C | -1.90450 | -1.54937 | -1.32721 |
| H | -2.15733 | -1.80215 | -0.29686 |
| H | -2.81207 | -1.42902 | -1.92186 |
| H | -1.27040 | -2.32525 | -1.76397 |
| C | 2.65425 | -0.21871 | 1.22192 |
| H | 3.20386 | -0.29483 | 0.28362 |
| H | 3.05227 | 0.60510 | 1.82079 |
| H | 2.80889 | -1.13441 | 1.80138 |
| Au | -2.02981 | 0.63261 | -4.37012 |
| Cl | -3.47511 | 0.89014 | -6.03896 |
| Cl | -2.20008 | 1.34283 | -0.53878 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.91268 | -0.55250 | 0.93666 |
| C | 0.48729 | -0.09767 | -0.59635 |
| P | -1.15988 | -0.10107 | -1.16404 |
| O | -1.05556 | 0.61215 | -2.52671 |
| Pb | 1.42041 | 0.94688 | -2.54784 |
| Cl | 2.05271 | -1.20915 | -3.62991 |
| Au | -2.48630 | 1.50736 | -3.77270 |
| Cl | -3.95035 | 2.48857 | -5.12824 |
| C | 2.77285 | -0.41805 | 1.10038 |
| C | 3.25659 | -1.85566 | 1.31933 |
| C | 3.49496 | 0.20394 | -0.07876 |
| C | 3.01314 | 0.40312 | 2.37018 |
| H | 2.72922 | -2.33879 | 2.14659 |
| H | 3.12068 | -2.46640 | 0.42358 |
| H | 4.32332 | -1.84955 | 1.56620 |
| H | 3.16255 | 1.23358 | -0.25200 |
| H | 4.57078 | 0.25217 | 0.12033 |
| H | 3.36807 | -0.39384 | -0.98701 |
| H | 4.08120 | 0.40820 | 2.60996 |
| H | 2.69066 | 1.44061 | 2.24893 |
| H | 2.48128 | -0.01614 | 3.22842 |
| C | -1.99430 | -1.72658 | -1.31818 |
| C | -3.39039 | -1.52820 | -1.90962 |
| C | -1.13490 | -2.56975 | -2.26489 |
| C | -2.08903 | -2.38941 | 0.05342 |
| H | -4.03252 | -0.93519 | -1.25683 |
| H | -3.35900 | -1.04957 | -2.89036 |
| H | -3.84976 | -2.51314 | -2.03121 |
| H | -0.12344 | -2.72065 | -1.88438 |
| H | -1.60889 | -3.54928 | -2.37151 |
| H | -1.05906 | -2.12119 | -3.25627 |

| | | | |
|----|----------|----------|----------|
| H | -2.55973 | -3.36826 | -0.07194 |
| H | -1.10735 | -2.54784 | 0.50462 |
| H | -2.69985 | -1.80930 | 0.74722 |
| Cl | -2.35032 | 1.00683 | 0.04170 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.81997 | 0.26792 | 0.92298 |
| C | 0.54382 | -0.22435 | -0.63333 |
| P | -0.94397 | -0.18155 | -1.50909 |
| O | -0.48059 | -0.04563 | -2.96840 |
| Pb | 1.99889 | -0.39168 | -2.50378 |
| Cl | 1.87995 | -2.87108 | -2.74566 |
| Au | -1.67552 | 0.18293 | -4.67973 |
| Cl | -2.89248 | 0.42846 | -6.52532 |
| C | 2.59667 | -0.04494 | 1.13219 |
| C | 3.27280 | -1.10288 | 0.51381 |
| C | 3.30638 | 0.81317 | 1.97419 |
| C | 4.63609 | -1.26723 | 0.70275 |
| H | 2.71920 | -1.83240 | -0.07127 |
| C | 4.67232 | 0.65407 | 2.15009 |
| H | 2.78583 | 1.61872 | 2.48301 |
| C | 5.33824 | -0.38256 | 1.51168 |
| H | 5.14817 | -2.09743 | 0.22970 |
| H | 5.21765 | 1.33686 | 2.79139 |
| H | 6.40429 | -0.51284 | 1.65809 |
| C | -1.98225 | -1.61394 | -1.27846 |
| C | -2.86396 | -1.70227 | -0.20221 |
| C | -1.84333 | -2.67829 | -2.16744 |
| C | -3.60958 | -2.85321 | -0.02285 |
| H | -2.97632 | -0.87165 | 0.48476 |
| C | -2.59784 | -3.82526 | -1.97949 |
| H | -1.15138 | -2.61285 | -2.99778 |
| C | -3.47754 | -3.91262 | -0.91176 |
| H | -4.30147 | -2.92185 | 0.80814 |
| H | -2.49715 | -4.65005 | -2.67450 |
| H | -4.06826 | -4.81056 | -0.77115 |
| Cl | -2.09597 | 1.40062 | -1.01427 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.71383 | -0.01967 | 1.36234 |
| C | 0.37362 | -0.34172 | -0.22212 |
| P | -1.03561 | -0.25823 | -1.22640 |
| O | -0.43168 | 0.14269 | -2.57936 |
| Pb | 2.05115 | -0.19630 | -1.87612 |
| Cl | 2.11440 | -2.63997 | -2.39790 |
| Au | -1.08856 | 1.41592 | -4.11456 |
| Cl | -1.69973 | 2.77214 | -5.76897 |
| C | 2.54781 | -0.13683 | 1.33487 |
| C | 3.19179 | -1.38608 | 1.37003 |
| C | 3.30029 | 1.05017 | 1.33478 |
| C | 4.58163 | -1.41752 | 1.35828 |
| C | 4.68736 | 0.96574 | 1.32094 |
| C | 5.34715 | -0.25762 | 1.32422 |
| H | 5.08049 | -2.38164 | 1.38881 |
| H | 5.26813 | 1.88348 | 1.31848 |
| C | -2.01966 | -1.75827 | -1.27481 |
| C | -2.66777 | -2.17360 | -0.08961 |
| C | -2.11645 | -2.54334 | -2.44829 |
| C | -3.38012 | -3.36359 | -0.09686 |
| C | -2.85499 | -3.71879 | -2.38525 |
| C | -3.49178 | -4.15126 | -1.23222 |
| H | -3.86614 | -3.68001 | 0.82070 |
| H | -2.92553 | -4.32321 | -3.28365 |
| Cl | -2.28609 | 1.25013 | -0.69296 |
| C | 2.63240 | 2.39458 | 1.34267 |
| H | 2.14789 | 2.61658 | 0.38653 |

| | | | |
|---|----------|----------|----------|
| H | 1.85367 | 2.45312 | 2.10954 |
| H | 3.35551 | 3.18720 | 1.53748 |
| C | 2.41817 | -2.66920 | 1.43347 |
| H | 1.59244 | -2.60575 | 2.14831 |
| H | 1.98724 | -2.92307 | 0.46072 |
| H | 3.06506 | -3.49309 | 1.73691 |
| C | 6.84263 | -0.32707 | 1.28448 |
| H | 7.19627 | -0.46858 | 0.25847 |
| H | 7.29483 | 0.59038 | 1.66409 |
| H | 7.21727 | -1.16561 | 1.87433 |
| C | -2.67225 | -1.38989 | 1.18872 |
| H | -1.70762 | -0.94109 | 1.42911 |
| H | -3.40086 | -0.57690 | 1.14512 |
| H | -2.94728 | -2.03938 | 2.02024 |
| C | -1.48330 | -2.21987 | -3.76873 |
| H | -1.82768 | -1.26445 | -4.16906 |
| H | -0.39620 | -2.17337 | -3.69557 |
| H | -1.73768 | -2.99637 | -4.48978 |
| C | -4.29400 | -5.41378 | -1.22300 |
| H | -4.35475 | -5.84097 | -0.22093 |
| H | -5.31677 | -5.21874 | -1.56046 |
| H | -3.86701 | -6.16091 | -1.89409 |

| | | | |
|----|----------|----------|----------|
| C | 6.19468 | -2.20720 | 1.53389 |
| H | 6.11262 | -1.60436 | 2.43995 |
| H | 5.23320 | -2.70341 | 1.38502 |
| H | 6.95475 | -2.97350 | 1.70893 |
| C | 7.92441 | -0.67216 | 0.58026 |
| H | 7.88217 | -0.02452 | 1.45826 |
| H | 8.70015 | -1.42241 | 0.75635 |
| H | 8.22843 | -0.06183 | -0.27390 |
| C | -2.36201 | 1.41229 | 0.28123 |
| C | -2.94943 | 0.83663 | 1.44726 |
| C | -3.17730 | 2.19635 | -0.57565 |
| C | -4.32963 | 0.72592 | 1.47543 |
| C | -4.55491 | 2.03838 | -0.47174 |
| C | -5.15481 | 1.22010 | 0.47256 |
| H | -4.78128 | 0.22587 | 2.32267 |
| H | -5.18096 | 2.58676 | -1.16185 |
| C | -2.20747 | 0.48091 | 2.75078 |
| C | -2.31088 | -1.00220 | 3.11131 |
| C | -2.88792 | 1.30119 | 3.86639 |
| H | -1.76642 | -1.62502 | 2.40229 |
| H | -1.88269 | -1.16741 | 4.10366 |
| H | -3.34835 | -1.34200 | 3.13188 |
| H | -2.86331 | 2.37032 | 3.64099 |
| H | -3.92693 | 1.01355 | 4.02790 |
| H | -2.35020 | 1.13824 | 4.80392 |
| C | -2.70366 | 3.35447 | -1.47609 |
| C | -3.35375 | 4.62256 | -0.88333 |
| C | -3.16609 | 3.21392 | -2.92862 |
| H | -3.05781 | 4.76290 | 0.15907 |
| H | -3.02362 | 5.49610 | -1.45219 |
| H | -4.44265 | 4.58728 | -0.92288 |
| H | -2.71846 | 2.34704 | -3.41334 |
| H | -4.25073 | 3.11764 | -3.00226 |
| H | -2.87641 | 4.10561 | -3.49126 |
| C | -6.64886 | 0.93042 | 0.49538 |
| C | -7.27133 | 1.53918 | 1.75777 |
| C | -6.85351 | -0.58979 | 0.50633 |
| H | -7.13830 | 2.62393 | 1.77965 |
| H | -8.34357 | 1.32687 | 1.78386 |
| H | -6.82920 | 1.12669 | 2.66688 |
| H | -6.40256 | -1.06190 | -0.36899 |
| H | -6.40925 | -1.05384 | 1.38871 |
| H | -7.92248 | -0.81971 | 0.51059 |
| Cl | 2.18325 | -1.44677 | 2.21666 |
| O | -0.93774 | -0.89041 | 0.14358 |
| Cl | -1.19537 | 0.39488 | -2.35896 |
| Au | -2.51832 | -2.20725 | -0.31500 |
| Cl | -4.16174 | -3.63697 | -0.79988 |
| C | -1.20239 | 3.61218 | -1.43773 |
| H | -0.83562 | 3.68963 | -0.41156 |
| H | -0.62382 | 2.85565 | -1.96369 |
| H | -0.99022 | 4.56523 | -1.92873 |
| C | -0.74576 | 0.91166 | 2.76257 |
| H | -0.10288 | 0.28840 | 2.14447 |
| H | -0.63572 | 1.95670 | 2.46115 |
| H | -0.35468 | 0.81788 | 3.77844 |
| C | -7.36548 | 1.50540 | -0.72347 |
| H | -7.31878 | 2.59743 | -0.75178 |
| H | -6.95033 | 1.11528 | -1.65597 |
| H | -8.42091 | 1.22599 | -0.68854 |
| Pb | 1.60702 | -1.33172 | -0.21863 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.72102 | 2.31195 | -0.18726 |
| C | 0.82149 | 0.92373 | -0.24172 |
| P | -0.87610 | 0.57350 | -0.33864 |
| C | 3.41059 | 1.55931 | -0.20361 |
| C | 4.17995 | 1.54676 | 0.98832 |
| C | 3.84945 | 0.81862 | -1.32388 |
| C | 5.19810 | 0.61023 | 1.09270 |
| C | 4.85333 | -0.13785 | -1.12464 |
| C | 5.50835 | -0.29708 | 0.08387 |
| H | 5.76268 | 0.55983 | 2.01193 |
| H | 5.15430 | -0.74594 | -1.96722 |
| C | 3.47079 | 1.09129 | -2.79847 |
| C | 3.96288 | 2.54743 | 2.13796 |
| C | 6.57867 | -1.35840 | 0.31605 |
| C | 2.63539 | 2.31601 | 2.86619 |
| H | 1.76971 | 2.55456 | 2.24289 |
| H | 2.53417 | 1.27784 | 3.18677 |
| H | 2.58172 | 2.96588 | 3.74452 |
| C | 4.01290 | 3.97629 | 1.58007 |
| H | 4.97089 | 4.16946 | 1.09087 |
| H | 3.21842 | 4.16997 | 0.85652 |
| H | 3.89524 | 4.69625 | 2.39460 |
| C | 5.06637 | 2.44579 | 3.19387 |
| H | 5.04383 | 1.49062 | 3.72351 |
| H | 6.06155 | 2.58685 | 2.76513 |
| H | 4.91256 | 3.23189 | 3.93639 |
| C | 2.81528 | -0.12290 | -3.46154 |
| H | 1.81582 | -0.30457 | -3.05796 |
| H | 2.69970 | 0.05393 | -4.53440 |
| H | 3.41157 | -1.02987 | -3.33996 |
| C | 2.57096 | 2.30457 | -3.02254 |
| H | 1.53881 | 2.12898 | -2.71831 |
| H | 2.94870 | 3.19449 | -2.51102 |
| H | 2.54634 | 2.53384 | -4.09156 |
| C | 4.78517 | 1.40683 | -3.53905 |
| H | 5.29278 | 2.26019 | -3.08295 |
| H | 5.47874 | 0.56585 | -3.54029 |
| H | 4.56600 | 1.65733 | -4.58020 |
| C | 6.74110 | -2.28798 | -0.88365 |
| H | 7.08136 | -1.75375 | -1.77464 |
| H | 7.49015 | -3.04941 | -0.65478 |
| H | 5.80919 | -2.80596 | -1.12532 |

Coordination through P(sp²) atom**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.70535 | 0.09431 | 0.86507 |
| C | 0.43930 | -0.22943 | -0.71387 |
| P | -1.07866 | -0.27753 | -1.56076 |
| O | -0.74098 | -0.09578 | -3.01909 |
| Pb | 1.62465 | -0.48751 | -2.83366 |
| Cl | 1.34742 | -2.95095 | -2.76806 |
| Au | -0.58472 | 0.57679 | 2.57750 |
| Cl | -1.89374 | 1.06734 | 4.34777 |
| Cl | -2.42307 | 1.06999 | -0.92886 |
| H | 2.10427 | 0.01539 | 1.04435 |
| H | -1.75391 | -1.48003 | -1.29849 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.80736 | 0.13245 | 0.80916 |
| C | 0.48623 | -0.15291 | -0.76470 |
| P | -1.08496 | -0.29468 | -1.51087 |
| O | -0.81073 | -0.28137 | -3.00084 |
| Pb | 1.54324 | -0.51275 | -2.91973 |
| Cl | 1.45050 | -2.98832 | -2.60824 |
| Cl | -1.97331 | -1.75075 | -0.98544 |
| H | -2.19009 | -1.69666 | 0.08223 |
| H | -2.90182 | -1.82255 | -1.55424 |
| H | -1.33709 | -2.61236 | -1.20209 |
| C | 2.58771 | 0.11689 | 1.13268 |
| H | 3.15702 | -0.07248 | 0.22371 |
| H | 2.87783 | 1.07487 | 1.57064 |
| H | 2.79907 | -0.66036 | 1.87130 |
| Au | -0.55994 | 0.47158 | 2.50762 |
| Cl | -1.95522 | 0.78663 | 4.25927 |
| Cl | -2.29996 | 1.24142 | -1.01853 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.76640 | 0.08766 | 0.91443 |
| C | 0.47641 | -0.16748 | -0.67354 |
| P | -1.06272 | -0.35743 | -1.48556 |
| O | -0.74057 | -0.17920 | -2.95809 |
| Pb | 1.60959 | 0.09829 | -2.80776 |
| Cl | 2.29386 | -2.29705 | -3.01871 |
| Au | -0.64819 | 0.29918 | 2.60713 |
| Cl | -2.07849 | 0.52479 | 4.35052 |
| C | 2.56849 | 0.19814 | 1.33309 |
| C | 2.86482 | -1.00563 | 2.23464 |
| C | 3.46183 | 0.16966 | 0.10460 |
| C | 2.77024 | 1.49546 | 2.11915 |
| H | 2.20979 | -1.02690 | 3.10901 |
| H | 2.75499 | -1.94986 | 1.69644 |
| H | 3.89694 | -0.93585 | 2.59131 |
| H | 3.29171 | 1.04247 | -0.53351 |
| H | 4.50890 | 0.20684 | 0.42000 |
| H | 3.32777 | -0.74548 | -0.47787 |
| H | 3.80728 | 1.54641 | 2.46388 |
| H | 2.57340 | 2.37772 | 1.50515 |
| H | 2.12175 | 1.54080 | 2.99722 |
| C | -1.96153 | -1.92636 | -1.18527 |
| C | -3.18591 | -1.92679 | -2.10358 |
| C | -1.01185 | -3.06060 | -1.57998 |
| C | -2.37952 | -2.06607 | 0.27311 |
| H | -3.90336 | -1.15301 | -1.82567 |
| H | -2.90481 | -1.78545 | -3.14841 |
| H | -3.68273 | -2.89651 | -2.01126 |
| H | -0.11219 | -3.07844 | -0.96246 |
| H | -1.53738 | -4.00937 | -1.44017 |
| H | -0.70161 | -2.99245 | -2.62317 |

| | | | |
|----|----------|----------|----------|
| H | -2.91861 | -3.01045 | 0.38949 |
| H | -1.51965 | -2.09572 | 0.94531 |
| H | -3.04095 | -1.26067 | 0.59559 |
| Cl | -2.34090 | 1.10896 | -0.90081 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.80165 | 0.28984 | 0.48061 |
| C | 0.64000 | -0.49824 | -0.94161 |
| P | -0.80753 | -0.84933 | -1.84301 |
| O | -0.31472 | -1.29134 | -3.20514 |
| Pb | 2.02437 | -1.20616 | -2.78365 |
| Cl | 2.21394 | -3.57493 | -1.99678 |
| Au | -0.71276 | 1.32594 | 1.71358 |
| Cl | -2.28806 | 2.35791 | 2.97077 |
| C | 2.50379 | 0.25942 | 1.03087 |
| C | 2.95179 | 1.28780 | 1.86099 |
| C | 3.37307 | -0.77460 | 0.67228 |
| C | 4.26811 | 1.30566 | 2.29163 |
| H | 2.26691 | 2.07357 | 2.16301 |
| C | 4.68352 | -0.75552 | 1.11688 |
| H | 3.01005 | -1.61496 | 0.08882 |
| C | 5.13353 | 0.28761 | 1.91726 |
| H | 4.61647 | 2.11174 | 2.92644 |
| H | 5.35217 | -1.56576 | 0.85046 |
| H | 6.16057 | 0.29730 | 2.26389 |
| C | -1.85083 | -2.07466 | -1.06906 |
| C | -2.75171 | -1.74558 | -0.05739 |
| C | -1.68615 | -3.40068 | -1.46540 |
| C | -3.48921 | -2.74551 | 0.55156 |
| H | -2.88392 | -0.71441 | 0.24988 |
| C | -2.43212 | -4.39363 | -0.85025 |
| H | -0.97700 | -3.64875 | -2.24571 |
| C | -3.33007 | -4.06723 | 0.15482 |
| H | -4.19185 | -2.49112 | 1.33610 |
| H | -2.30807 | -5.42510 | -1.15803 |
| H | -3.91159 | -4.84689 | 0.63358 |
| Cl | -1.96802 | 0.79818 | -2.01895 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.71475 | 0.51227 | 1.03246 |
| C | 0.41194 | -0.41769 | -0.27401 |
| P | -0.90420 | -0.69213 | -1.38184 |
| O | -0.20422 | -0.69308 | -2.72587 |
| Pb | 2.05594 | -0.88255 | -1.95456 |
| Cl | 1.99400 | -3.36822 | -1.65113 |
| Au | -0.57789 | 1.74075 | 2.34036 |
| Cl | -1.86898 | 3.00515 | 3.70605 |
| C | 2.49268 | 0.45430 | 1.34735 |
| C | 3.26072 | 1.60893 | 1.11831 |
| C | 3.08507 | -0.72010 | 1.84243 |
| C | 4.62666 | 1.55351 | 1.35781 |
| C | 4.45574 | -0.71723 | 2.07168 |
| C | 5.24421 | 0.40074 | 1.82943 |
| H | 5.22453 | 2.44183 | 1.17781 |
| H | 4.91848 | -1.61803 | 2.46301 |
| C | -1.87405 | -2.16770 | -1.05323 |
| C | -2.45239 | -2.35306 | 0.22028 |
| C | -2.06553 | -3.13609 | -2.06574 |
| C | -3.18468 | -3.50561 | 0.46451 |
| C | -2.80985 | -4.26715 | -1.75356 |
| C | -3.36866 | -4.48155 | -0.50272 |
| H | -3.63118 | -3.63578 | 1.44532 |
| H | -2.96179 | -5.00816 | -2.53184 |
| Cl | -2.23078 | 0.85310 | -1.38284 |
| C | 2.64122 | 2.88465 | 0.63014 |
| H | 2.08349 | 2.74114 | -0.29999 |

| | | | |
|---|----------|----------|----------|
| H | 1.93643 | 3.29040 | 1.36266 |
| H | 3.40529 | 3.64046 | 0.44710 |
| C | 2.28897 | -1.95450 | 2.14649 |
| H | 1.37750 | -1.71817 | 2.70311 |
| H | 1.98623 | -2.47679 | 1.23453 |
| H | 2.87768 | -2.64712 | 2.74860 |
| C | 6.72336 | 0.36138 | 2.05753 |
| H | 7.24562 | 0.05106 | 1.14703 |
| H | 7.10961 | 1.34301 | 2.33692 |
| H | 6.98625 | -0.34939 | 2.84250 |
| C | -2.31516 | -1.37725 | 1.34834 |
| H | -3.08404 | -1.56038 | 2.09916 |
| H | -1.34542 | -1.48387 | 1.84167 |
| H | -2.40905 | -0.33813 | 1.03216 |
| C | -1.53348 | -3.04660 | -3.46670 |
| H | -1.78430 | -2.10387 | -3.95102 |
| H | -0.44570 | -3.13366 | -3.47931 |
| H | -1.94657 | -3.86310 | -4.05956 |
| C | -4.13419 | -5.73176 | -0.20418 |
| H | -4.63464 | -6.11503 | -1.09496 |
| H | -3.45959 | -6.51552 | 0.15459 |
| H | -4.88399 | -5.56515 | 0.57088 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.90808 | 1.18045 | 0.07241 |
| C | -0.17986 | 0.24764 | 0.38936 |
| P | 1.39869 | -0.98582 | 0.49086 |
| Cl | -1.83137 | -2.66424 | -2.03183 |
| O | 1.16121 | -2.36998 | -0.07923 |
| C | 3.06830 | -0.43992 | 0.02203 |
| C | 3.59307 | -1.06324 | -1.14897 |
| C | 3.97011 | 0.12932 | 0.95893 |
| C | 4.93407 | -1.41342 | -1.13829 |
| C | 5.30467 | -0.25959 | 0.88401 |
| C | 5.79652 | -1.10598 | -0.09448 |
| H | 5.32421 | -1.94759 | -1.99486 |
| H | 5.98502 | 0.13141 | 1.62698 |
| C | -2.69441 | 0.80389 | 0.10930 |
| C | -3.42797 | 0.64720 | -1.09502 |
| C | -3.25405 | 0.37832 | 1.34065 |
| C | -4.57450 | -0.14091 | -1.04897 |
| C | -4.38253 | -0.43482 | 1.28847 |
| C | -5.03108 | -0.75669 | 0.10581 |
| H | -5.11402 | -0.31029 | -1.96558 |
| H | -4.78329 | -0.81466 | 2.21983 |
| C | -3.08477 | 1.35252 | -2.42070 |
| C | -2.81494 | 0.81969 | 2.75461 |
| C | -6.21572 | -1.71720 | 0.11739 |
| C | 3.68656 | 1.27792 | 1.94877 |
| C | 2.85690 | -1.26622 | -2.48887 |
| C | 7.23074 | -1.61989 | -0.10628 |
| C | -4.05969 | 1.37302 | 3.47450 |
| H | -3.77132 | 1.74005 | 4.46263 |
| H | -4.49459 | 2.20577 | 2.91688 |
| H | -4.83699 | 0.62291 | 3.61927 |
| C | -1.79195 | 1.95315 | 2.78985 |
| H | -0.78668 | 1.63563 | 2.51054 |
| H | -2.08669 | 2.79430 | 2.15736 |
| H | -1.71594 | 2.32873 | 3.81382 |
| C | -2.26543 | -0.36353 | 3.55638 |
| H | -2.97948 | -1.18932 | 3.59897 |
| H | -1.33200 | -0.73195 | 3.12499 |
| H | -2.05387 | -0.05432 | 4.58381 |
| C | -7.32324 | -1.16424 | 1.02170 |
| H | -8.17516 | -1.84951 | 1.03259 |
| H | -6.98549 | -1.03943 | 2.05260 |

| | | | |
|----|----------|----------|----------|
| H | -7.67291 | -0.19320 | 0.66280 |
| C | -6.79727 | -1.93693 | -1.27664 |
| H | -7.62338 | -2.64941 | -1.21690 |
| H | -7.19257 | -1.01202 | -1.70424 |
| H | -6.05458 | -2.34721 | -1.96499 |
| C | -5.74456 | -3.07285 | 0.65829 |
| H | -4.96707 | -3.49736 | 0.01781 |
| H | -5.34412 | -2.98760 | 1.67115 |
| H | -6.58009 | -3.77747 | 0.68884 |
| C | -4.09319 | 1.02096 | -3.52502 |
| H | -5.11252 | 1.30990 | -3.25869 |
| H | -3.82021 | 1.58422 | -4.41980 |
| H | -4.08164 | -0.03954 | -3.78784 |
| C | -3.16431 | 2.86757 | -2.18958 |
| H | -4.16610 | 3.15625 | -1.86135 |
| H | -2.45268 | 3.21197 | -1.43606 |
| H | -2.94155 | 3.40011 | -3.11782 |
| C | -1.71202 | 0.96572 | -2.97671 |
| H | -0.88167 | 1.32742 | -2.36715 |
| H | -1.61731 | -0.11622 | -3.07675 |
| H | -1.58164 | 1.42361 | -3.96122 |
| C | 2.26249 | 1.81413 | 1.91877 |
| H | 1.94944 | 2.03013 | 0.89467 |
| H | 1.53744 | 1.14942 | 2.38238 |
| H | 2.22421 | 2.76000 | 2.46389 |
| C | 4.57081 | 2.45364 | 1.48035 |
| H | 4.39416 | 3.31584 | 2.12846 |
| H | 5.63431 | 2.21630 | 1.51775 |
| H | 4.32206 | 2.74658 | 0.45789 |
| C | 4.07152 | 0.92676 | 3.38885 |
| H | 5.12285 | 0.64606 | 3.47525 |
| H | 3.91182 | 1.79858 | 4.02892 |
| H | 3.46956 | 0.10578 | 3.77792 |
| C | 1.50689 | -0.55882 | -2.57295 |
| H | 1.18410 | -0.53627 | -3.61645 |
| H | 0.71808 | -1.07156 | -2.02814 |
| H | 1.57668 | 0.47803 | -2.23174 |
| C | 2.68860 | -2.74977 | -2.82707 |
| H | 2.05956 | -3.24780 | -2.09099 |
| H | 2.22002 | -2.85220 | -3.80961 |
| H | 3.65396 | -3.26069 | -2.86292 |
| C | 3.72661 | -0.60643 | -3.57880 |
| H | 3.88922 | 0.45300 | -3.36587 |
| H | 4.70057 | -1.08177 | -3.69557 |
| H | 3.20829 | -0.68358 | -4.53778 |
| C | 8.01083 | -1.18811 | 1.13249 |
| H | 8.12236 | -0.10227 | 1.18774 |
| H | 7.53335 | -1.53356 | 2.05286 |
| H | 9.01479 | -1.61763 | 1.09828 |
| C | 7.95967 | -1.08817 | -1.34614 |
| H | 7.47939 | -1.41302 | -2.27113 |
| H | 7.98611 | 0.00418 | -1.34686 |
| H | 8.99010 | -1.45378 | -1.35984 |
| C | 7.20479 | -3.15255 | -0.15024 |
| H | 6.70012 | -3.56071 | 0.72871 |
| H | 6.68528 | -3.52321 | -1.03604 |
| H | 8.22529 | -3.54464 | -0.17097 |
| Au | -0.04250 | 3.18851 | -0.35134 |
| Cl | 0.85582 | 5.23378 | -0.75970 |
| Pb | -1.20566 | -2.45986 | 0.39070 |
| Cl | 1.56182 | -1.35197 | 2.51918 |

Coordination through $\pi(\text{C}=\text{P})$ bond**R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.74223 | -0.08108 | 0.95638 |
| C | 0.38133 | 0.10628 | -0.71677 |
| P | -1.15523 | -0.23261 | -1.48243 |
| O | -0.99795 | 0.12839 | -2.93782 |
| Pb | 1.41125 | 0.07018 | -2.95643 |
| Cl | 1.47272 | -2.41983 | -2.92198 |
| Au | 0.57405 | 2.11127 | 0.01859 |
| Cl | 0.71885 | 4.35007 | 0.15667 |
| Cl | -2.75907 | 0.66556 | -0.66780 |
| H | -1.47275 | -1.58588 | -1.28238 |
| H | 2.16828 | -0.10220 | 0.86011 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.76688 | 0.06467 | 0.86292 |
| C | 0.32686 | 0.23411 | -0.78865 |
| P | -1.22301 | -0.21131 | -1.48731 |
| O | -1.06379 | -0.01753 | -2.98080 |
| Pb | 1.30744 | 0.11867 | -3.03223 |
| Cl | 1.66132 | -2.35609 | -2.80575 |
| C | -1.66673 | -1.88812 | -1.05758 |
| H | -1.82796 | -1.97531 | 0.01746 |
| H | -2.57635 | -2.15704 | -1.59678 |
| H | -0.84427 | -2.53399 | -1.37560 |
| C | 2.59741 | -0.06510 | 0.84656 |
| H | 3.06103 | 0.36366 | -0.04128 |
| H | 3.00155 | 0.40958 | 1.74303 |
| H | 2.83792 | -1.13263 | 0.89439 |
| Au | 0.46773 | 2.25179 | -0.07581 |
| Cl | 0.56243 | 4.49334 | 0.12336 |
| Cl | -2.77786 | 0.89573 | -0.81465 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.71903 | -0.01283 | 0.70697 |
| C | 0.34737 | 0.28087 | -0.94766 |
| P | -1.10267 | -0.28886 | -1.79393 |
| O | -0.72379 | -0.27683 | -3.26173 |
| Pb | 1.50581 | 0.49880 | -3.10050 |
| Cl | 2.51948 | -1.79933 | -3.01646 |
| Au | 0.14814 | 2.20227 | 0.00019 |
| Cl | -0.07023 | 4.38759 | 0.51903 |
| C | 2.57039 | 0.10846 | 0.96315 |
| C | 3.00762 | -1.35503 | 1.11037 |
| C | 3.37650 | 0.78360 | -0.13116 |
| C | 2.75098 | 0.84089 | 2.29404 |
| H | 2.44085 | -1.87384 | 1.88888 |
| H | 2.89787 | -1.90319 | 0.17116 |
| H | 4.06377 | -1.38642 | 1.39673 |
| H | 3.01642 | 1.79378 | -0.34381 |
| H | 4.42162 | 0.86818 | 0.18483 |
| H | 3.38021 | 0.18454 | -1.04576 |
| H | 3.79837 | 0.77933 | 2.60504 |
| H | 2.48265 | 1.89699 | 2.21283 |
| H | 2.14218 | 0.39708 | 3.08693 |
| C | -1.79147 | -1.91680 | -1.30015 |
| C | -2.86753 | -2.27744 | -2.32711 |
| C | -0.64906 | -2.93405 | -1.36955 |
| C | -2.38257 | -1.86951 | 0.10532 |
| H | -3.70170 | -1.57384 | -2.30701 |
| H | -2.46135 | -2.30781 | -3.33895 |
| H | -3.25723 | -3.26947 | -2.08211 |
| H | 0.11767 | -2.74268 | -0.61696 |
| H | -1.06479 | -3.92715 | -1.17740 |
| H | -0.16611 | -2.94916 | -2.34758 |

| | | | |
|----|----------|----------|----------|
| H | -2.73956 | -2.87058 | 0.36366 |
| H | -1.64269 | -1.57865 | 0.85438 |
| H | -3.22827 | -1.18361 | 0.16884 |
| Cl | -2.63770 | 1.02066 | -1.51926 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.73086 | 0.29284 | 0.83340 |
| C | 0.20032 | 0.29381 | -0.79925 |
| P | -1.39627 | -0.12593 | -1.39179 |
| O | -1.35884 | 0.12832 | -2.88308 |
| Pb | 0.99600 | 0.42763 | -3.12616 |
| Cl | 1.49082 | -2.01610 | -3.43218 |
| Au | 0.40854 | 2.38842 | -0.29930 |
| Cl | 0.52931 | 4.63806 | -0.37258 |
| C | -1.82419 | -1.81759 | -1.00008 |
| C | -1.84406 | -2.75127 | -2.03163 |
| C | -2.10295 | -2.20611 | 0.30958 |
| C | -2.14814 | -4.07467 | -1.74914 |
| H | -1.61630 | -2.44110 | -3.04342 |
| C | -2.40210 | -3.52842 | 0.58216 |
| H | -2.09395 | -1.47650 | 1.11205 |
| C | -2.42510 | -4.46171 | -0.44769 |
| H | -2.16300 | -4.80374 | -2.55049 |
| H | -2.62136 | -3.83319 | 1.59864 |
| H | -2.66087 | -5.49732 | -0.23050 |
| C | 2.53744 | 0.14277 | 0.74019 |
| C | 3.18694 | -0.61450 | -0.23601 |
| C | 3.28559 | 0.73859 | 1.75799 |
| C | 4.56656 | -0.74279 | -0.20963 |
| H | 2.61327 | -1.13406 | -0.99691 |
| C | 4.66543 | 0.62334 | 1.76868 |
| H | 2.78459 | 1.30798 | 2.53477 |
| C | 5.30666 | -0.11630 | 0.78407 |
| H | 5.06336 | -1.34054 | -0.96529 |
| H | 5.24177 | 1.10630 | 2.54920 |
| H | 6.38607 | -0.21510 | 0.79877 |
| Cl | -2.87124 | 0.97364 | -0.53923 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.80797 | 0.34298 | 1.21908 |
| C | 0.15880 | 0.24399 | -0.37120 |
| P | -1.40336 | -0.12757 | -1.08958 |
| O | -1.27926 | 0.42861 | -2.49377 |
| Pb | 1.07969 | 0.69376 | -2.61364 |
| Cl | 1.52006 | -1.65926 | -3.39769 |
| Au | 0.16439 | 2.37056 | 0.10949 |
| Cl | 0.02146 | 4.62394 | 0.01550 |
| C | -1.84658 | -1.87106 | -1.02194 |
| C | -2.14902 | -2.57851 | -2.21084 |
| C | -1.91193 | -2.53038 | 0.22301 |
| C | -2.43562 | -3.93354 | -2.10845 |
| C | -2.20756 | -3.88673 | 0.25327 |
| C | -2.45253 | -4.61409 | -0.89955 |
| H | -2.66784 | -4.47484 | -3.02003 |
| H | -2.25968 | -4.38251 | 1.21785 |
| C | 2.61622 | 0.25522 | 0.96217 |
| C | 3.17281 | -0.94518 | 0.47692 |
| C | 3.45565 | 1.29241 | 1.40172 |
| C | 4.55161 | -1.03056 | 0.33966 |
| C | 4.82948 | 1.15667 | 1.23914 |
| C | 5.39714 | 0.01634 | 0.68856 |
| H | 4.97910 | -1.95715 | -0.03193 |
| H | 5.47465 | 1.96596 | 1.56845 |
| Cl | -2.97584 | 0.85079 | -0.22040 |
| C | 2.92696 | 2.53892 | 2.04633 |
| H | 2.62552 | 3.28808 | 1.30796 |

| | | | |
|---|----------|----------|----------|
| H | 2.05237 | 2.33911 | 2.67198 |
| H | 3.69168 | 2.99238 | 2.67898 |
| C | 2.34097 | -2.15824 | 0.17483 |
| H | 1.59505 | -2.33926 | 0.95453 |
| H | 1.80957 | -2.07778 | -0.77560 |
| H | 2.97707 | -3.04242 | 0.11857 |
| C | 6.87702 | -0.09241 | 0.48934 |
| H | 7.22729 | -1.11324 | 0.65358 |
| H | 7.14954 | 0.18330 | -0.53429 |
| H | 7.42042 | 0.57160 | 1.16343 |
| C | -1.69270 | -1.86437 | 1.54838 |
| H | -0.64874 | -1.94527 | 1.86504 |
| H | -1.95481 | -0.80819 | 1.55806 |
| H | -2.29582 | -2.35903 | 2.31150 |
| C | -2.73053 | -6.08314 | -0.84742 |
| H | -3.46876 | -6.37513 | -1.59661 |
| H | -1.81794 | -6.65165 | -1.05198 |
| H | -3.09479 | -6.38675 | 0.13511 |
| C | -2.21447 | -1.98164 | -3.58666 |
| H | -2.82776 | -1.08242 | -3.62123 |
| H | -1.22146 | -1.70977 | -3.94718 |
| H | -2.63463 | -2.71625 | -4.27423 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.65775 | 0.07201 | 1.16926 |
| C | 0.38139 | 0.08183 | -0.54173 |
| P | -1.03841 | -0.15397 | -1.62623 |
| O | -0.39666 | -0.06326 | -2.99702 |
| Pb | 1.82453 | 0.62517 | -2.49737 |
| Cl | 2.94796 | -1.45571 | -3.38137 |
| Au | 0.40554 | 2.18946 | 0.01289 |
| Cl | 0.32671 | 4.45742 | -0.09189 |
| C | 2.50843 | -0.02254 | 1.26483 |
| C | 3.18948 | -1.15843 | 0.74510 |
| C | 3.27766 | 1.09134 | 1.67877 |
| C | 4.49266 | -0.99151 | 0.30095 |
| C | 4.58662 | 1.18823 | 1.19870 |
| C | 5.18891 | 0.20641 | 0.43222 |
| H | 4.99524 | -1.84040 | -0.14334 |
| H | 5.15449 | 2.07093 | 1.45655 |
| C | 2.90620 | 2.12121 | 2.76709 |
| C | 2.70869 | -2.61385 | 0.90749 |
| C | 6.57664 | 0.36010 | -0.18003 |
| C | 3.86137 | 1.82682 | 3.94224 |
| H | 3.72452 | 0.80759 | 4.31271 |
| H | 4.90784 | 1.94289 | 3.65752 |
| H | 3.65466 | 2.51968 | 4.76252 |
| C | 3.12773 | 3.56588 | 2.31072 |
| H | 2.47954 | 3.83261 | 1.47527 |
| H | 2.90044 | 4.24615 | 3.13609 |
| H | 4.16141 | 3.75124 | 2.01434 |
| C | 1.49821 | 2.00674 | 3.34292 |
| H | 1.42452 | 2.65991 | 4.21663 |
| H | 0.72234 | 2.33406 | 2.64793 |
| H | 1.26870 | 0.99128 | 3.67491 |
| C | 3.04708 | -3.49291 | -0.29881 |
| H | 2.64359 | -3.08470 | -1.22423 |
| H | 4.12307 | -3.61509 | -0.43209 |
| H | 2.63148 | -4.49260 | -0.14609 |
| C | 3.48118 | -3.14929 | 2.12927 |
| H | 4.55957 | -3.09967 | 1.96905 |
| H | 3.24673 | -2.57242 | 3.02761 |
| H | 3.20874 | -4.19327 | 2.31082 |
| C | 1.22856 | -2.79031 | 1.22489 |
| H | 0.92295 | -2.22097 | 2.10985 |
| H | 0.58431 | -2.52410 | 0.38865 |

| | | | |
|----|----------|----------|----------|
| H | 1.03989 | -3.84238 | 1.45688 |
| C | 7.20550 | 1.71277 | 0.14272 |
| H | 6.59315 | 2.54243 | -0.21919 |
| H | 7.36394 | 1.84407 | 1.21639 |
| H | 8.18079 | 1.78604 | -0.34429 |
| C | 6.45511 | 0.23291 | -1.70347 |
| H | 7.44364 | 0.29466 | -2.16728 |
| H | 5.99795 | -0.71319 | -1.99936 |
| H | 5.84102 | 1.03903 | -2.11368 |
| C | 7.50752 | -0.73830 | 0.34715 |
| H | 7.59631 | -0.68806 | 1.43530 |
| H | 7.15362 | -1.73641 | 0.08266 |
| H | 8.50624 | -0.61863 | -0.08152 |
| C | -2.34088 | -1.45472 | -1.66349 |
| C | -2.31458 | -2.34407 | -2.78198 |
| C | -3.57781 | -1.26465 | -0.98908 |
| C | -3.52533 | -2.66038 | -3.37887 |
| C | -1.09127 | -3.11513 | -3.31442 |
| C | -4.74535 | -1.65180 | -1.63937 |
| C | -3.78337 | -0.81812 | 0.47065 |
| C | -4.75674 | -2.25673 | -2.88321 |
| H | -3.50065 | -3.27162 | -4.27110 |
| C | -0.61683 | -2.60595 | -4.67839 |
| C | -1.49911 | -4.59293 | -3.49232 |
| C | 0.04236 | -3.15217 | -2.29846 |
| H | -5.68514 | -1.46239 | -1.14080 |
| C | -2.50189 | -0.47352 | 1.20657 |
| C | -4.37546 | -2.04068 | 1.20099 |
| C | -4.76285 | 0.35176 | 0.60565 |
| C | -6.03560 | -2.56168 | -3.65203 |
| H | 0.20096 | -3.23456 | -5.03998 |
| H | -1.42950 | -2.65690 | -5.40813 |
| H | -0.26524 | -1.57975 | -4.62701 |
| H | -2.18632 | -4.75045 | -4.32415 |
| H | -0.60042 | -5.17693 | -3.70608 |
| H | -1.95843 | -4.99502 | -2.58611 |
| H | 0.46583 | -2.17691 | -2.07134 |
| H | -0.29731 | -3.61693 | -1.36950 |
| H | 0.86674 | -3.74755 | -2.69420 |
| H | -1.76207 | -1.27081 | 1.11087 |
| H | -2.06500 | 0.46648 | 0.87232 |
| H | -2.71177 | -0.35502 | 2.27221 |
| H | -4.51451 | -1.79729 | 2.25790 |
| H | -5.34214 | -2.33912 | 0.79404 |
| H | -3.70219 | -2.89888 | 1.13463 |
| H | -5.74178 | 0.12376 | 0.18094 |
| H | -4.91077 | 0.57872 | 1.66485 |
| H | -4.38228 | 1.24931 | 0.11850 |
| C | -7.27623 | -2.01499 | -2.95095 |
| C | -6.19548 | -4.07896 | -3.80602 |
| C | -5.94159 | -1.91700 | -5.04023 |
| H | -7.43724 | -2.48612 | -1.97791 |
| H | -7.21564 | -0.93361 | -2.80533 |
| H | -8.15895 | -2.21857 | -3.56161 |
| H | -5.35949 | -4.52274 | -4.35003 |
| H | -6.25890 | -4.56722 | -2.83042 |
| H | -7.11106 | -4.30458 | -4.35960 |
| H | -5.83681 | -0.83233 | -4.96164 |
| H | -5.08729 | -2.29517 | -5.60506 |
| H | -6.84612 | -2.13205 | -5.61563 |
| Cl | -2.24009 | 1.51804 | -1.55655 |

[R-P=C(Pb(II)Cl)-P(O)MeR](AuCl)**Coordination through Pb(II) atom****R = H**

| | | | |
|----|----------|----------|----------|
| P | 0.85769 | 0.09359 | 0.83241 |
| C | 0.44611 | -0.08511 | -0.75990 |
| P | -1.17105 | -0.18391 | -1.46739 |
| O | -0.92222 | 0.08841 | -2.94477 |
| Pb | 1.42477 | -0.06259 | -2.84848 |
| Cl | 1.47545 | -2.49625 | -3.08378 |
| C | -2.37059 | 0.92030 | -0.72982 |
| H | -3.32836 | 0.80688 | -1.24121 |
| H | -2.49021 | 0.67826 | 0.32887 |
| H | -2.02240 | 1.94876 | -0.83415 |
| Au | 2.77940 | 1.58768 | -4.31779 |
| Cl | 3.95172 | 3.08138 | -5.53379 |
| H | 2.27751 | 0.17652 | 0.68858 |
| H | -1.68596 | -1.47717 | -1.24145 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.84761 | 0.02686 | 0.84262 |
| C | 0.44498 | -0.10867 | -0.75169 |
| P | -1.17602 | -0.23325 | -1.45286 |
| O | -0.91479 | 0.04780 | -2.93504 |
| Pb | 1.40234 | -0.03306 | -2.83897 |
| Cl | 1.55310 | -2.47484 | -3.11098 |
| C | -2.33396 | 0.94289 | -0.74881 |
| H | -3.29901 | 0.84780 | -1.25070 |
| H | -2.45724 | 0.75686 | 0.32005 |
| H | -1.94929 | 1.95210 | -0.89910 |
| C | -1.85159 | -1.87381 | -1.19469 |
| H | -2.01560 | -2.05801 | -0.13134 |
| H | -2.79542 | -1.96539 | -1.73653 |
| H | -1.13769 | -2.59988 | -1.58798 |
| C | 2.67699 | 0.14378 | 0.88712 |
| H | 3.13062 | 0.24121 | -0.09944 |
| H | 2.96327 | 0.99560 | 1.50945 |
| H | 3.06605 | -0.75483 | 1.37546 |
| Au | 2.72067 | 1.60801 | -4.35130 |
| Cl | 3.87372 | 3.09986 | -5.59276 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.82827 | -0.23272 | 0.76305 |
| C | 0.50188 | -0.16410 | -0.85383 |
| P | -1.09120 | -0.35202 | -1.62202 |
| O | -0.77236 | -0.10574 | -3.10226 |
| Pb | 1.49883 | 0.30607 | -2.87544 |
| Cl | 2.33772 | -1.94962 | -3.39389 |
| C | -2.21840 | 0.90539 | -0.99703 |
| H | -3.17452 | 0.84913 | -1.51939 |
| H | -2.37210 | 0.79040 | 0.07662 |
| H | -1.76910 | 1.88067 | -1.18991 |
| Au | 2.38498 | 2.39208 | -4.13846 |
| Cl | 3.13874 | 4.27030 | -5.14437 |
| C | 2.65524 | 0.05975 | 1.05205 |
| C | 3.16486 | -1.22836 | 1.70688 |
| C | 3.47610 | 0.38347 | -0.18036 |
| C | 2.72503 | 1.21044 | 2.06017 |
| H | 2.57258 | -1.49942 | 2.58528 |
| H | 3.14644 | -2.06888 | 1.00901 |
| H | 4.19926 | -1.08526 | 2.03558 |
| H | 3.14175 | 1.30821 | -0.66089 |
| H | 4.52268 | 0.53959 | 0.10104 |
| H | 3.46451 | -0.43857 | -0.90260 |
| H | 3.76067 | 1.34930 | 2.38610 |
| H | 2.38186 | 2.15189 | 1.62382 |

| | | | |
|---|----------|----------|----------|
| H | 2.12084 | 1.00788 | 2.94877 |
| C | -1.86428 | -1.99951 | -1.38114 |
| C | -3.08667 | -2.06587 | -2.30120 |
| C | -0.85357 | -3.06900 | -1.79422 |
| C | -2.27732 | -2.19307 | 0.07559 |
| H | -3.86348 | -1.35454 | -2.01132 |
| H | -2.81410 | -1.87921 | -3.34133 |
| H | -3.52021 | -3.06794 | -2.23713 |
| H | 0.03040 | -3.06385 | -1.15450 |
| H | -1.32800 | -4.05091 | -1.71012 |
| H | -0.52184 | -2.93853 | -2.82521 |
| H | -2.67900 | -3.20304 | 0.19732 |
| H | -1.43142 | -2.09062 | 0.76014 |
| H | -3.05671 | -1.49175 | 0.38156 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.88868 | 0.16471 | 0.80502 |
| C | 0.45203 | -0.18061 | -0.75211 |
| P | -1.16127 | -0.33110 | -1.45832 |
| O | -0.88314 | -0.17885 | -2.95337 |
| Pb | 1.45867 | -0.15247 | -2.80339 |
| Cl | 1.76047 | -2.58134 | -3.09124 |
| C | -2.28570 | 0.93145 | -0.85307 |
| H | -3.24377 | 0.83143 | -1.36616 |
| H | -2.43643 | 0.82649 | 0.22288 |
| H | -1.85707 | 1.91215 | -1.06374 |
| Au | 2.69528 | 1.52027 | -4.35170 |
| Cl | 3.77110 | 3.02849 | -5.64489 |
| C | 2.69889 | 0.19951 | 0.77362 |
| C | 3.33719 | 1.11394 | 1.61357 |
| C | 3.47171 | -0.65473 | -0.01864 |
| C | 4.71934 | 1.21508 | 1.61690 |
| H | 2.74625 | 1.76073 | 2.25469 |
| C | 4.85347 | -0.56059 | -0.00099 |
| H | 2.99441 | -1.42617 | -0.61601 |
| C | 5.47714 | 0.38151 | 0.80703 |
| H | 5.20630 | 1.94346 | 2.25482 |
| H | 5.44564 | -1.23029 | -0.61383 |
| H | 6.55836 | 0.45631 | 0.81428 |
| C | -1.90006 | -1.92481 | -1.08970 |
| C | -2.05704 | -2.84168 | -2.12456 |
| C | -2.30181 | -2.25485 | 0.20390 |
| C | -2.62446 | -4.08044 | -1.86519 |
| H | -1.72866 | -2.58045 | -3.12328 |
| C | -2.86677 | -3.49266 | 0.45597 |
| H | -2.16383 | -1.55409 | 1.02124 |
| C | -3.02953 | -4.40441 | -0.57974 |
| H | -2.74437 | -4.79518 | -2.67077 |
| H | -3.17761 | -3.74990 | 1.46177 |
| H | -3.47026 | -5.37435 | -0.37958 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 1.03958 | -0.19707 | 1.30240 |
| C | 0.43492 | -0.31605 | -0.23267 |
| P | -1.15241 | -0.33163 | -1.03856 |
| O | -0.75640 | 0.14855 | -2.43555 |
| Pb | 1.57926 | 0.13591 | -2.13740 |
| Cl | 1.94637 | -2.17977 | -2.91675 |
| Au | 2.94056 | 2.08047 | -3.18201 |
| Cl | 4.14236 | 3.82808 | -3.97112 |
| C | 2.82088 | 0.04863 | 0.95857 |
| C | 3.34295 | 1.35276 | 0.93850 |
| C | 3.65639 | -1.05824 | 0.74642 |
| C | 4.69022 | 1.52785 | 0.65592 |
| C | 5.00032 | -0.83062 | 0.46958 |
| C | 5.53373 | 0.45016 | 0.40703 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| H | 5.09145 | 2.53635 | 0.62305 | C | -2.40181 | 1.06242 | 2.99767 |
| H | 5.64929 | -1.68461 | 0.30047 | C | -5.66252 | 1.17029 | -0.82924 |
| C | -1.95090 | -1.95549 | -1.02678 | C | 4.33728 | 1.36376 | 2.47964 |
| C | -2.19949 | -2.65583 | -2.22994 | C | 3.48411 | 0.50294 | -2.52912 |
| C | -2.33140 | -2.52830 | 0.20386 | C | 7.66481 | -1.13551 | -0.33415 |
| C | -2.79945 | -3.90765 | -2.14903 | C | -3.72843 | 0.97985 | 3.77017 |
| C | -2.91629 | -3.78696 | 0.21761 | H | -3.51209 | 0.83497 | 4.83126 |
| C | -3.15532 | -4.49945 | -0.94674 | H | -4.31506 | 1.89508 | 3.66373 |
| H | -2.99059 | -4.44146 | -3.07458 | H | -4.34462 | 0.13606 | 3.45671 |
| H | -3.19558 | -4.21888 | 1.17393 | C | -1.54901 | 2.09076 | 3.74314 |
| C | 2.47151 | 2.54875 | 1.18649 | H | -0.51844 | 2.14670 | 3.37441 |
| H | 1.78109 | 2.38428 | 2.01983 | H | -1.98129 | 3.09205 | 3.68055 |
| H | 3.07490 | 3.42732 | 1.41667 | H | -1.47876 | 1.81185 | 4.79787 |
| H | 1.86480 | 2.79186 | 0.30818 | C | -1.73464 | -0.31216 | 3.09627 |
| C | 3.13279 | -2.46256 | 0.80512 | H | -2.31467 | -1.07627 | 2.57219 |
| H | 2.44759 | -2.60378 | 1.64679 | H | -0.72569 | -0.29587 | 2.68343 |
| H | 2.58571 | -2.72183 | -0.10622 | H | -1.66148 | -0.61490 | 4.14492 |
| H | 3.95152 | -3.17465 | 0.91551 | C | -6.80945 | 1.43036 | 0.15445 |
| C | 6.97477 | 0.67437 | 0.06865 | H | -7.75293 | 1.07669 | -0.26999 |
| H | 7.07305 | 1.06950 | -0.94673 | H | -6.65964 | 0.91108 | 1.10307 |
| H | 7.43190 | 1.40183 | 0.74309 | H | -6.91055 | 2.49797 | 0.36603 |
| H | 7.54677 | -0.25263 | 0.12361 | C | -5.99585 | 1.86238 | -2.14824 |
| C | -2.18421 | -1.84302 | 1.53205 | H | -6.92869 | 1.45508 | -2.54503 |
| H | -1.30666 | -1.20079 | 1.60343 | H | -6.13549 | 2.93940 | -2.02208 |
| H | -3.06460 | -1.23172 | 1.75363 | H | -5.21845 | 1.69866 | -2.89847 |
| H | -2.10242 | -2.58372 | 2.32847 | C | -5.54801 | -0.33620 | -1.09271 |
| C | -1.86924 | -2.15857 | -3.60819 | H | -4.74686 | -0.54809 | -1.80505 |
| H | -2.26101 | -1.16057 | -3.79840 | H | -5.34131 | -0.89801 | -0.17946 |
| H | -0.79029 | -2.10886 | -3.76361 | H | -6.48341 | -0.71701 | -1.51164 |
| H | -2.28656 | -2.84413 | -4.34630 | C | -2.48671 | 4.90914 | -2.05617 |
| C | -3.75544 | -5.86975 | -0.90885 | H | -3.44532 | 5.23959 | -1.64950 |
| H | -2.96976 | -6.63168 | -0.90112 | H | -1.96365 | 5.79301 | -2.42812 |
| H | -4.36306 | -6.01565 | -0.01435 | H | -2.67511 | 4.25768 | -2.91256 |
| H | -4.37896 | -6.05516 | -1.78521 | C | -1.31967 | 5.28861 | 0.07758 |
| C | -2.27880 | 0.87997 | -0.32630 | H | -2.24290 | 5.61686 | 0.56141 |
| H | -3.19540 | 0.88677 | -0.91965 | H | -0.64616 | 4.91761 | 0.85322 |
| H | -2.51801 | 0.66952 | 0.71403 | H | -0.84458 | 6.16157 | -0.37869 |
| H | -1.79861 | 1.85710 | -0.40014 | C | -0.31017 | 3.83379 | -1.69857 |
| R = Mes* | | | | H | 0.46700 | 3.52238 | -0.99616 |
| P | -0.00912 | 2.38376 | 1.11188 | H | -0.47095 | 3.01307 | -2.39920 |
| C | 0.43179 | 0.88380 | 0.56155 | H | 0.08694 | 4.69322 | -2.24673 |
| P | 1.91384 | -0.10845 | 0.42728 | C | 2.98316 | 2.05385 | 2.56851 |
| Cl | -1.17175 | 0.26838 | -2.76657 | H | 2.77842 | 2.63941 | 1.67013 |
| O | 1.48045 | -1.08783 | -0.67288 | H | 2.14721 | 1.37658 | 2.73224 |
| C | 2.01653 | -1.12690 | 1.92109 | H | 2.98581 | 2.74716 | 3.41316 |
| H | 2.83921 | -1.83047 | 1.78188 | C | 5.36946 | 2.51005 | 2.43786 |
| H | 2.15182 | -0.58074 | 2.84883 | H | 5.23411 | 3.15185 | 3.31277 |
| H | 1.08432 | -1.69385 | 1.97194 | H | 6.39654 | 2.14499 | 2.44525 |
| C | 3.63999 | 0.42184 | 0.10830 | H | 5.23493 | 3.12157 | 1.54271 |
| C | 4.16508 | 0.15850 | -1.19053 | C | 4.59281 | 0.54502 | 3.74885 |
| C | 4.55650 | 0.55297 | 1.18523 | H | 5.60471 | 0.13672 | 3.76979 |
| C | 5.45904 | -0.33574 | -1.27427 | H | 4.47920 | 1.18468 | 4.62818 |
| C | 5.84668 | 0.05866 | 1.01458 | H | 3.90093 | -0.29151 | 3.85285 |
| C | 6.29544 | -0.48636 | -0.17669 | C | 2.30631 | 1.45626 | -2.35868 |
| H | 5.83307 | -0.60776 | -2.25264 | H | 1.95887 | 1.78079 | -3.34209 |
| H | 6.52744 | 0.11618 | 1.85252 | H | 1.44704 | 1.00192 | -1.87541 |
| C | -1.82159 | 2.34728 | 0.78136 | H | 2.60293 | 2.34630 | -1.79729 |
| C | -2.33193 | 3.03875 | -0.34038 | C | 3.06838 | -0.74646 | -3.31041 |
| C | -2.67399 | 1.50344 | 1.53998 | H | 2.31949 | -1.32025 | -2.76961 |
| C | -3.58132 | 2.65715 | -0.82424 | H | 2.65255 | -0.45306 | -4.27809 |
| C | -3.89746 | 1.15443 | 0.97733 | H | 3.93090 | -1.39125 | -3.49901 |
| C | -4.34842 | 1.66508 | -0.23387 | C | 4.50700 | 1.28010 | -3.38284 |
| H | -3.95945 | 3.13964 | -1.71093 | H | 4.89747 | 2.14826 | -2.84600 |
| H | -4.53834 | 0.47022 | 1.51631 | H | 5.35142 | 0.66906 | -3.70292 |
| C | -1.61172 | 4.23259 | -0.99770 | H | 4.00726 | 1.63698 | -4.28675 |
| | | | | C | 8.41971 | -1.22238 | 0.98960 |

| | | | |
|----|----------|----------|----------|
| H | 8.64618 | -0.23382 | 1.39735 |
| H | 7.85882 | -1.78548 | 1.73987 |
| H | 9.37122 | -1.73584 | 0.83324 |
| C | 8.51130 | -0.32241 | -1.32088 |
| H | 8.04741 | -0.27059 | -2.30769 |
| H | 8.65570 | 0.70006 | -0.96330 |
| H | 9.49549 | -0.78388 | -1.43918 |
| C | 7.47791 | -2.55722 | -0.87743 |
| H | 6.89006 | -3.16658 | -0.18673 |
| H | 6.96619 | -2.55781 | -1.84173 |
| H | 8.45028 | -3.03837 | -1.01320 |
| Au | -2.27276 | -2.77386 | 0.05353 |
| Cl | -3.53420 | -4.55227 | 0.67126 |
| Pb | -0.83261 | -0.68773 | -0.51729 |

Coordination through O atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.85986 | 0.08493 | 0.98463 |
| C | 0.59543 | -0.10644 | -0.63856 |
| P | -0.95630 | 0.02527 | -1.42480 |
| O | -0.55893 | 0.35200 | -2.88578 |
| Pb | 1.83898 | -0.35663 | -2.66779 |
| Cl | 1.21591 | -2.75110 | -2.80215 |
| C | -2.10282 | 1.21877 | -0.74733 |
| H | -3.03192 | 1.20537 | -1.32023 |
| H | -2.30605 | 0.96183 | 0.29555 |
| H | -1.65697 | 2.21308 | -0.79786 |
| Au | -1.99295 | 0.72093 | -4.36866 |
| Cl | -3.51824 | 1.14257 | -5.92985 |
| H | 2.28374 | -0.07360 | 1.00445 |
| H | -1.62301 | -1.21290 | -1.37057 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.82152 | -0.01704 | 0.97640 |
| C | 0.58239 | -0.13242 | -0.65372 |
| P | -0.99077 | -0.02081 | -1.40749 |
| O | -0.60494 | 0.29779 | -2.88443 |
| Pb | 1.79005 | -0.23646 | -2.71627 |
| Cl | 1.42762 | -2.69442 | -2.92014 |
| C | -2.05581 | 1.26316 | -0.75037 |
| H | -2.99817 | 1.28212 | -1.30156 |
| H | -2.24787 | 1.06821 | 0.30724 |
| H | -1.55712 | 2.22738 | -0.85419 |
| C | -1.87864 | -1.57239 | -1.31909 |
| H | -2.14260 | -1.78941 | -0.28215 |
| H | -2.78226 | -1.51036 | -1.92967 |
| H | -1.22715 | -2.35876 | -1.70545 |
| C | 2.63251 | -0.20315 | 1.22503 |
| H | 3.19907 | -0.19442 | 0.29346 |
| H | 2.98879 | 0.59431 | 1.88243 |
| H | 2.81281 | -1.14968 | 1.74386 |
| Au | -2.03975 | 0.66021 | -4.36165 |
| Cl | -3.57209 | 1.07126 | -5.92104 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.89950 | -0.50119 | 0.86098 |
| C | 0.49915 | -0.10952 | -0.69428 |
| P | -1.15859 | -0.06787 | -1.27044 |
| O | -0.98418 | 0.53563 | -2.69969 |
| Pb | 1.47550 | 0.79210 | -2.69236 |
| Cl | 2.09225 | -1.43093 | -3.65112 |
| C | -2.17780 | 1.02673 | -0.27113 |
| H | -3.18823 | 1.09653 | -0.67607 |
| H | -2.20584 | 0.66770 | 0.75906 |

| | | | |
|----|----------|----------|----------|
| H | -1.72285 | 2.01817 | -0.28936 |
| Au | -2.38235 | 1.65966 | -3.77094 |
| Cl | -3.84124 | 2.88800 | -4.91745 |
| C | 2.76104 | -0.39342 | 1.05627 |
| C | 3.21714 | -1.82499 | 1.35563 |
| C | 3.51024 | 0.15373 | -0.14289 |
| C | 2.99861 | 0.48786 | 2.28480 |
| H | 2.66947 | -2.25591 | 2.19840 |
| H | 3.08159 | -2.47836 | 0.49042 |
| H | 4.28056 | -1.82537 | 1.61684 |
| H | 3.19772 | 1.17756 | -0.37585 |
| H | 4.58413 | 0.19321 | 0.06876 |
| H | 3.38360 | -0.48795 | -1.02059 |
| H | 4.06252 | 0.48544 | 2.54289 |
| H | 2.69905 | 1.52362 | 2.10386 |
| H | 2.44451 | 0.12455 | 3.15455 |
| C | -1.97808 | -1.70842 | -1.37911 |
| C | -3.30639 | -1.54918 | -2.12262 |
| C | -1.06235 | -2.65356 | -2.15661 |
| C | -2.22398 | -2.24832 | 0.02891 |
| H | -4.00560 | -0.89529 | -1.59720 |
| H | -3.16588 | -1.16028 | -3.13246 |
| H | -3.77634 | -2.53358 | -2.20402 |
| H | -0.10820 | -2.80869 | -1.65104 |
| H | -1.56134 | -3.62223 | -2.25047 |
| H | -0.85118 | -2.28326 | -3.16072 |
| H | -2.64408 | -3.25464 | -0.05276 |
| H | -1.30199 | -2.32145 | 0.61099 |
| H | -2.93871 | -1.63907 | 0.58652 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78595 | 0.22950 | 0.92748 |
| C | 0.53483 | -0.23609 | -0.63963 |
| P | -0.96754 | -0.17812 | -1.52032 |
| O | -0.46664 | -0.10762 | -2.98932 |
| Pb | 1.97399 | -0.48629 | -2.51000 |
| Cl | 1.81416 | -2.97418 | -2.63851 |
| C | -1.99637 | 1.24151 | -1.13522 |
| H | -2.89535 | 1.22251 | -1.75370 |
| H | -2.27300 | 1.22612 | -0.07910 |
| H | -1.42799 | 2.14934 | -1.34243 |
| Au | -1.66563 | 0.36093 | -4.63665 |
| Cl | -2.91849 | 0.87902 | -6.40135 |
| C | 2.56580 | -0.05181 | 1.16858 |
| C | 3.25955 | -1.10760 | 0.56826 |
| C | 3.25529 | 0.81838 | 2.01406 |
| C | 4.62153 | -1.25844 | 0.77787 |
| H | 2.72080 | -1.84410 | -0.02203 |
| C | 4.61994 | 0.67288 | 2.21121 |
| H | 2.72044 | 1.62292 | 2.50961 |
| C | 5.30444 | -0.36228 | 1.59031 |
| H | 5.14768 | -2.08708 | 0.31759 |
| H | 5.14980 | 1.36532 | 2.85527 |
| H | 6.36941 | -0.48194 | 1.75294 |
| C | -1.95230 | -1.65348 | -1.26197 |
| C | -2.65030 | -1.83055 | -0.06762 |
| C | -1.99695 | -2.63423 | -2.24824 |
| C | -3.39764 | -2.97783 | 0.13100 |
| H | -2.60647 | -1.08042 | 0.71523 |
| C | -2.74885 | -3.78085 | -2.04246 |
| H | -1.44429 | -2.50184 | -3.16995 |
| C | -3.44834 | -3.95177 | -0.85822 |
| H | -3.94112 | -3.11398 | 1.05857 |
| H | -2.78482 | -4.54201 | -2.81259 |
| H | -4.03525 | -4.84952 | -0.70141 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.73022 | -0.16074 | 1.35667 |
| C | 0.38840 | -0.34502 | -0.24874 |
| P | -1.05194 | -0.22488 | -1.23499 |
| O | -0.41584 | 0.11953 | -2.61103 |
| Pb | 2.03072 | -0.15755 | -1.92783 |
| Cl | 2.16365 | -2.61016 | -2.41760 |
| Au | -1.17489 | 1.38707 | -4.08756 |
| Cl | -1.93250 | 2.75800 | -5.66954 |
| C | 2.56828 | -0.20114 | 1.33176 |
| C | 3.25024 | -1.42949 | 1.35996 |
| C | 3.28470 | 1.00691 | 1.34681 |
| C | 4.64022 | -1.42017 | 1.35787 |
| C | 4.67408 | 0.96474 | 1.34328 |
| C | 5.37071 | -0.23777 | 1.34047 |
| H | 5.16731 | -2.36948 | 1.38020 |
| H | 5.22697 | 1.89957 | 1.35402 |
| C | -2.02221 | -1.75238 | -1.27841 |
| C | -2.69911 | -2.14450 | -0.10419 |
| C | -2.10520 | -2.56273 | -2.43501 |
| C | -3.43567 | -3.32103 | -0.10340 |
| C | -2.86717 | -3.72386 | -2.36974 |
| C | -3.53999 | -4.12556 | -1.22628 |
| H | -3.94094 | -3.61477 | 0.81162 |
| H | -2.92509 | -4.34374 | -3.25869 |
| C | 2.57956 | 2.33221 | 1.36483 |
| H | 2.10069 | 2.55278 | 0.40554 |
| H | 1.79060 | 2.35831 | 2.12283 |
| H | 3.27843 | 3.14163 | 1.57864 |
| C | 2.51290 | -2.73446 | 1.39496 |
| H | 1.68084 | -2.70723 | 2.10514 |
| H | 2.09541 | -2.97892 | 0.41380 |
| H | 3.17979 | -3.54668 | 1.68668 |
| C | 6.86804 | -0.26191 | 1.31068 |
| H | 7.23293 | -0.39845 | 0.28794 |
| H | 7.28976 | 0.67080 | 1.68835 |
| H | 7.26409 | -1.08541 | 1.90789 |
| C | -2.70417 | -1.35481 | 1.17375 |
| H | -1.76144 | -0.84756 | 1.38154 |
| H | -3.49791 | -0.60196 | 1.16619 |
| H | -2.90149 | -2.01713 | 2.01741 |
| C | -1.43114 | -2.28230 | -3.74613 |
| H | -1.75220 | -1.33430 | -4.18159 |
| H | -0.34631 | -2.24585 | -3.64391 |
| H | -1.67549 | -3.07522 | -4.45298 |
| C | -4.36280 | -5.37529 | -1.21470 |
| H | -4.51101 | -5.74661 | -0.19962 |
| H | -5.35106 | -5.18836 | -1.64617 |
| H | -3.89468 | -6.16386 | -1.80681 |
| C | -2.11589 | 1.15713 | -0.78244 |
| H | -2.98843 | 1.17555 | -1.43802 |
| H | -2.43121 | 1.10155 | 0.25739 |
| H | -1.53963 | 2.07127 | -0.93702 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.71145 | 2.29999 | -0.39784 |
| C | 0.79787 | 0.92201 | -0.35122 |
| P | -0.91606 | 0.56987 | -0.48255 |
| C | 3.40643 | 1.55273 | -0.33699 |
| C | 4.14538 | 1.60142 | 0.87372 |
| C | 3.88086 | 0.76410 | -1.40794 |
| C | 5.16053 | 0.67292 | 1.05191 |
| C | 4.87850 | -0.17979 | -1.13576 |
| C | 5.49760 | -0.28213 | 0.09733 |
| H | 5.70169 | 0.67002 | 1.98653 |
| H | 5.19920 | -0.83195 | -1.93647 |

| | | | |
|---|----------|----------|----------|
| C | 3.51492 | 0.94860 | -2.89916 |
| C | 3.90689 | 2.66530 | 1.96150 |
| C | 6.55868 | -1.33209 | 0.41058 |
| C | 2.56771 | 2.47657 | 2.68010 |
| H | 1.71282 | 2.67775 | 2.03046 |
| H | 2.46116 | 1.45861 | 3.05859 |
| H | 2.50162 | 3.17549 | 3.51914 |
| C | 3.96732 | 4.06024 | 1.32429 |
| H | 4.93375 | 4.22591 | 0.84149 |
| H | 3.18532 | 4.21157 | 0.57741 |
| H | 3.83602 | 4.82511 | 2.09470 |
| C | 4.99242 | 2.62541 | 3.04012 |
| H | 4.95912 | 1.70314 | 3.62469 |
| H | 5.99505 | 2.74014 | 2.62094 |
| H | 4.82691 | 3.45388 | 3.73240 |
| C | 2.73148 | -0.24575 | -3.44850 |
| H | 1.73767 | -0.30282 | -2.99805 |
| H | 2.59621 | -0.14587 | -4.52922 |
| H | 3.25033 | -1.18953 | -3.26473 |
| C | 2.73875 | 2.22883 | -3.20461 |
| H | 1.70340 | 2.19320 | -2.86224 |
| H | 3.21848 | 3.10809 | -2.76727 |
| H | 2.70469 | 2.37569 | -4.28771 |
| C | 4.83080 | 1.07177 | -3.69127 |
| H | 5.44372 | 1.88919 | -3.30446 |
| H | 5.42893 | 0.16110 | -3.66438 |
| H | 4.60438 | 1.28236 | -4.73960 |
| C | 6.75547 | -2.31658 | -0.73908 |
| H | 7.12312 | -1.82419 | -1.64323 |
| H | 7.49596 | -3.06697 | -0.45273 |
| H | 5.83020 | -2.84466 | -0.98434 |
| C | 6.13663 | -2.12307 | 1.65438 |
| H | 6.02382 | -1.47782 | 2.52727 |
| H | 5.18112 | -2.62856 | 1.49826 |
| H | 6.89127 | -2.87837 | 1.89059 |
| C | 7.89757 | -0.63581 | 0.68315 |
| H | 7.83061 | 0.05160 | 1.52876 |
| H | 8.66621 | -1.37774 | 0.91664 |
| H | 8.22807 | -0.06561 | -0.18874 |
| C | -2.37677 | 1.43020 | 0.20634 |
| C | -2.95029 | 0.88412 | 1.39032 |
| C | -3.21320 | 2.19173 | -0.65087 |
| C | -4.33108 | 0.76683 | 1.44091 |
| C | -4.58984 | 2.03440 | -0.52845 |
| C | -5.17425 | 1.23461 | 0.44157 |
| H | -4.76695 | 0.28061 | 2.30439 |
| H | -5.22714 | 2.56816 | -1.22027 |
| C | -2.18835 | 0.55736 | 2.68841 |
| C | -2.24444 | -0.92551 | 3.06086 |
| C | -2.87576 | 1.36213 | 3.81077 |
| H | -1.68514 | -1.53643 | 2.35409 |
| H | -1.80663 | -1.07007 | 4.05222 |
| H | -3.27233 | -1.29373 | 3.08975 |
| H | -2.90052 | 2.42887 | 3.57440 |
| H | -3.89759 | 1.03378 | 4.00264 |
| H | -2.30915 | 1.23160 | 4.73628 |
| C | -2.74926 | 3.32936 | -1.58321 |
| C | -3.43292 | 4.60892 | -1.05754 |
| C | -3.18309 | 3.13067 | -3.03837 |
| H | -3.17308 | 4.78750 | -0.01167 |
| H | -3.09492 | 5.46726 | -1.64481 |
| H | -4.51932 | 4.55945 | -1.13126 |
| H | -2.72083 | 2.25663 | -3.49707 |
| H | -4.26488 | 3.01068 | -3.12049 |
| H | -2.90313 | 4.00688 | -3.62953 |
| C | -6.66698 | 0.93973 | 0.49275 |

| | | | |
|----|----------|----------|----------|
| C | -7.27346 | 1.56800 | 1.75320 |
| C | -6.86600 | -0.58063 | 0.53340 |
| H | -7.14510 | 2.65353 | 1.75337 |
| H | -8.34420 | 1.35142 | 1.80034 |
| H | -6.81471 | 1.17445 | 2.66242 |
| H | -6.42710 | -1.06604 | -0.34094 |
| H | -6.40543 | -1.02672 | 1.41669 |
| H | -7.93370 | -0.81526 | 0.55877 |
| Cl | 2.10615 | -1.32336 | 2.31658 |
| O | -0.94864 | -0.88372 | 0.10137 |
| Au | -2.49941 | -2.21219 | -0.36766 |
| Cl | -4.12927 | -3.64637 | -0.88708 |
| C | -1.25494 | 3.62207 | -1.51089 |
| H | -0.92946 | 3.77314 | -0.47951 |
| H | -0.62573 | 2.85072 | -1.95005 |
| H | -1.04005 | 4.54190 | -2.06041 |
| C | -0.74303 | 1.03635 | 2.67059 |
| H | -0.10122 | 0.45201 | 2.01602 |
| H | -0.67934 | 2.08995 | 2.38635 |
| H | -0.31704 | 0.93268 | 3.67117 |
| C | -7.40473 | 1.49059 | -0.72471 |
| H | -7.36076 | 2.58202 | -0.77365 |
| H | -7.00391 | 1.08447 | -1.65677 |
| H | -8.45890 | 1.20983 | -0.66801 |
| Pb | 1.54587 | -1.33492 | -0.12610 |
| C | -1.25513 | 0.33087 | -2.24759 |
| H | -2.30621 | 0.07068 | -2.37970 |
| H | -0.99511 | 1.18265 | -2.86914 |
| H | -0.65167 | -0.52688 | -2.55225 |

Coordination through P(sp²) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.76399 | 0.09517 | 0.85531 |
| C | 0.47319 | -0.19967 | -0.72261 |
| P | -1.06986 | -0.19935 | -1.56142 |
| O | -0.69607 | -0.06128 | -3.03118 |
| Pb | 1.61655 | -0.53787 | -2.85142 |
| Cl | 1.24869 | -2.99296 | -2.70670 |
| C | -2.24150 | 1.04339 | -1.02687 |
| H | -3.14550 | 0.96394 | -1.63396 |
| H | -2.49238 | 0.89062 | 0.02571 |
| H | -1.80313 | 2.03374 | -1.15697 |
| Au | -0.55091 | 0.57656 | 2.56026 |
| Cl | -1.93823 | 1.08835 | 4.26914 |
| H | 2.16257 | 0.01745 | 1.03793 |
| H | -1.69829 | -1.43073 | -1.28545 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.81955 | 0.11719 | 0.81681 |
| C | 0.47446 | -0.15413 | -0.75173 |
| P | -1.12108 | -0.25044 | -1.49222 |
| O | -0.81850 | -0.23797 | -2.99267 |
| Pb | 1.49943 | -0.51829 | -2.92136 |
| Cl | 1.40107 | -3.00131 | -2.62107 |
| C | -2.20126 | 1.11105 | -1.04429 |
| H | -3.13985 | 1.01751 | -1.59473 |
| H | -2.40333 | 1.10074 | 0.02902 |
| H | -1.72121 | 2.05260 | -1.31321 |
| C | -1.93413 | -1.76738 | -0.99133 |
| H | -2.14219 | -1.75191 | 0.08039 |
| H | -2.86750 | -1.87541 | -1.54813 |
| H | -1.27134 | -2.60154 | -1.22918 |
| C | 2.60176 | 0.09902 | 1.13825 |
| H | 3.16354 | -0.08661 | 0.22357 |

| | | | |
|----|----------|----------|---------|
| H | 2.89730 | 1.05422 | 1.57815 |
| H | 2.81713 | -0.68358 | 1.86975 |
| Au | -0.55985 | 0.48205 | 2.51030 |
| Cl | -2.01493 | 0.85764 | 4.20550 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.76293 | 0.08924 | 0.91570 |
| C | 0.45849 | -0.15373 | -0.66906 |
| P | -1.10288 | -0.29345 | -1.48277 |
| O | -0.74198 | -0.12700 | -2.96429 |
| Pb | 1.58299 | 0.10481 | -2.81009 |
| Cl | 2.29063 | -2.28738 | -3.04513 |
| C | -2.22056 | 1.02046 | -0.96604 |
| H | -3.14729 | 0.97010 | -1.53940 |
| H | -2.43838 | 0.95481 | 0.10128 |
| H | -1.73217 | 1.97457 | -1.16937 |
| Au | -0.67199 | 0.32837 | 2.59753 |
| Cl | -2.16827 | 0.61143 | 4.28053 |
| C | 2.56444 | 0.18956 | 1.34490 |
| C | 2.84992 | -1.00926 | 2.25569 |
| C | 3.45828 | 0.14434 | 0.11727 |
| C | 2.77526 | 1.49048 | 2.12159 |
| H | 2.19198 | -1.01960 | 3.12818 |
| H | 2.73361 | -1.95629 | 1.72383 |
| H | 3.88156 | -0.94579 | 2.61510 |
| H | 3.29873 | 1.01543 | -0.52550 |
| H | 4.50565 | 0.16913 | 0.43323 |
| H | 3.31140 | -0.77009 | -0.46293 |
| H | 3.81066 | 1.53483 | 2.47235 |
| H | 2.59063 | 2.36937 | 1.49896 |
| H | 2.12219 | 1.54971 | 2.99563 |
| C | -1.93814 | -1.90771 | -1.20648 |
| C | -3.13687 | -1.95450 | -2.15926 |
| C | -0.95923 | -3.02564 | -1.56220 |
| C | -2.40180 | -2.05470 | 0.23887 |
| H | -3.90348 | -1.22189 | -1.89685 |
| H | -2.83307 | -1.78845 | -3.19429 |
| H | -3.59559 | -2.94518 | -2.09366 |
| H | -0.08312 | -3.02426 | -0.91157 |
| H | -1.46814 | -3.98672 | -1.44420 |
| H | -0.60812 | -2.95015 | -2.59191 |
| H | -2.88543 | -3.02894 | 0.35517 |
| H | -1.56855 | -2.01871 | 0.94388 |
| H | -3.12788 | -1.29282 | 0.52944 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77892 | 0.33462 | 0.64238 |
| C | 0.55538 | -0.38892 | -0.80227 |
| P | -0.93457 | -0.65562 | -1.69505 |
| O | -0.44758 | -1.01925 | -3.09842 |
| Pb | 1.87258 | -1.04007 | -2.71429 |
| Cl | 2.04406 | -3.44837 | -2.04332 |
| C | -1.99973 | 0.78948 | -1.73608 |
| H | -2.86831 | 0.57077 | -2.35997 |
| H | -2.32923 | 1.06295 | -0.73191 |
| H | -1.44146 | 1.62224 | -2.16635 |
| Au | -0.70214 | 1.34600 | 1.94745 |
| Cl | -2.27881 | 2.36093 | 3.22185 |
| C | 2.49746 | 0.27502 | 1.14377 |
| C | 2.98164 | 1.26956 | 1.99368 |
| C | 3.34389 | -0.75381 | 0.72296 |
| C | 4.31059 | 1.25959 | 2.38448 |
| H | 2.31502 | 2.05139 | 2.34329 |
| C | 4.66793 | -0.76248 | 1.12661 |
| H | 2.95396 | -1.56802 | 0.11998 |
| C | 5.15349 | 0.24711 | 1.94862 |

| | | | |
|---|----------|----------|----------|
| H | 4.68674 | 2.03970 | 3.03578 |
| H | 5.31954 | -1.56881 | 0.81058 |
| H | 6.19071 | 0.23487 | 2.26343 |
| C | -1.87855 | -1.99912 | -0.96893 |
| C | -2.61756 | -1.81836 | 0.19990 |
| C | -1.84541 | -3.24577 | -1.58744 |
| C | -3.32464 | -2.87896 | 0.73942 |
| H | -2.63950 | -0.85600 | 0.70109 |
| C | -2.55615 | -4.30368 | -1.04119 |
| H | -1.25997 | -3.38042 | -2.48873 |
| C | -3.29457 | -4.12086 | 0.11798 |
| H | -3.89823 | -2.73586 | 1.64761 |
| H | -2.52779 | -5.27438 | -1.52213 |
| H | -3.84813 | -4.95017 | 0.54354 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.73454 | 0.52191 | 1.00353 |
| C | 0.42080 | -0.43399 | -0.28025 |
| P | -0.93507 | -0.66269 | -1.38092 |
| O | -0.20244 | -0.69256 | -2.72487 |
| Pb | 2.01994 | -0.97667 | -1.97715 |
| Cl | 1.87074 | -3.45923 | -1.63770 |
| Au | -0.59326 | 1.79992 | 2.23854 |
| Cl | -1.96481 | 3.11891 | 3.47332 |
| C | 2.50772 | 0.47140 | 1.34738 |
| C | 3.28106 | 1.62247 | 1.12014 |
| C | 3.09226 | -0.69805 | 1.86312 |
| C | 4.64234 | 1.57055 | 1.38546 |
| C | 4.45879 | -0.69298 | 2.11640 |
| C | 5.25157 | 0.42269 | 1.87877 |
| H | 5.24330 | 2.45718 | 1.20715 |
| H | 4.91459 | -1.59047 | 2.52328 |
| C | -1.86716 | -2.17932 | -1.04366 |
| C | -2.39200 | -2.41148 | 0.24355 |
| C | -2.11652 | -3.11195 | -2.07594 |
| C | -3.13581 | -3.56047 | 0.47837 |
| C | -2.86728 | -4.24291 | -1.77693 |
| C | -3.37954 | -4.49602 | -0.51375 |
| H | -3.53829 | -3.72177 | 1.47376 |
| H | -3.06012 | -4.95318 | -2.57490 |
| C | 2.67340 | 2.89173 | 0.60139 |
| H | 2.15934 | 2.73755 | -0.35194 |
| H | 1.93357 | 3.29526 | 1.29969 |
| H | 3.43906 | 3.65256 | 0.44791 |
| C | 2.29348 | -1.93155 | 2.16482 |
| H | 1.37976 | -1.69246 | 2.71657 |
| H | 1.99288 | -2.45553 | 1.25318 |
| H | 2.87869 | -2.62342 | 2.77126 |
| C | 6.72652 | 0.38555 | 2.13352 |
| H | 7.26512 | 0.06794 | 1.23513 |
| H | 7.10767 | 1.36953 | 2.41184 |
| H | 6.97546 | -0.31867 | 2.92893 |
| C | -2.17454 | -1.50046 | 1.41456 |
| H | -2.93636 | -1.67558 | 2.17479 |
| H | -1.20091 | -1.68675 | 1.87535 |
| H | -2.20713 | -0.44008 | 1.16562 |
| C | -1.63046 | -2.98850 | -3.49233 |
| H | -1.85321 | -2.01899 | -3.93572 |
| H | -0.54826 | -3.11862 | -3.54472 |
| H | -2.09680 | -3.76400 | -4.10101 |
| C | -4.15368 | -5.74501 | -0.23011 |
| H | -4.72857 | -6.06386 | -1.10143 |
| H | -3.47637 | -6.56410 | 0.03117 |
| H | -4.84058 | -5.60776 | 0.60657 |
| C | -2.11043 | 0.70168 | -1.40755 |
| H | -2.67046 | 0.78860 | -0.47691 |

| | | | |
|---|----------|---------|----------|
| H | -1.56362 | 1.62827 | -1.58907 |
| H | -2.80797 | 0.52754 | -2.22966 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.91516 | 1.17362 | -0.03155 |
| C | 0.10410 | -0.18526 | -0.42968 |
| P | -1.49825 | -0.86533 | -0.72290 |
| Cl | 1.56825 | -2.93693 | 1.81614 |
| O | -1.27334 | -2.34166 | -0.36130 |
| C | -3.14919 | -0.40253 | -0.06571 |
| C | -3.66485 | -1.22137 | 0.97897 |
| C | -4.07300 | 0.31560 | -0.86991 |
| C | -5.00466 | -1.57771 | 0.92048 |
| C | -5.40450 | -0.09168 | -0.86227 |
| C | -5.88112 | -1.10328 | -0.04580 |
| H | -5.38048 | -2.25723 | 1.67468 |
| H | -6.09481 | 0.42198 | -1.51686 |
| C | 2.68240 | 0.69969 | -0.05903 |
| C | 3.36484 | 0.39527 | 1.14778 |
| C | 3.27153 | 0.37212 | -1.30646 |
| C | 4.48283 | -0.42984 | 1.06342 |
| C | 4.37213 | -0.48087 | -1.29598 |
| C | 4.96521 | -0.94116 | -0.13113 |
| H | 4.97916 | -0.71152 | 1.97670 |
| H | 4.79265 | -0.78639 | -2.24561 |
| C | 3.00546 | 0.98643 | 2.52522 |
| C | 2.89070 | 0.93994 | -2.69324 |
| C | 6.12150 | -1.93378 | -0.19862 |
| C | -3.79690 | 1.63267 | -1.62319 |
| C | -2.91086 | -1.64438 | 2.25349 |
| C | -7.31189 | -1.62352 | -0.11116 |
| C | 4.17338 | 1.49209 | -3.34402 |
| H | 3.92364 | 1.94488 | -4.30681 |
| H | 4.62768 | 2.26136 | -2.71542 |
| H | 4.92367 | 0.72412 | -3.53043 |
| C | 1.91485 | 2.11473 | -2.67380 |
| H | 0.89101 | 1.82070 | -2.44056 |
| H | 2.22214 | 2.89506 | -1.97364 |
| H | 1.88489 | 2.56480 | -3.66979 |
| C | 2.31456 | -0.15763 | -3.59230 |
| H | 2.99510 | -1.00710 | -3.68311 |
| H | 1.36225 | -0.52036 | -3.19839 |
| H | 2.13228 | 0.23453 | -4.59686 |
| C | 7.27964 | -1.32558 | -0.99795 |
| H | 8.11164 | -2.03312 | -1.05025 |
| H | 6.98646 | -1.08237 | -2.02136 |
| H | 7.64194 | -0.40919 | -0.52576 |
| C | 6.63983 | -2.31435 | 1.18567 |
| H | 7.44731 | -3.04316 | 1.08303 |
| H | 7.04336 | -1.45139 | 1.72137 |
| H | 5.85878 | -2.76881 | 1.79983 |
| C | 5.63660 | -3.21100 | -0.89557 |
| H | 4.82149 | -3.67470 | -0.33409 |
| H | 5.28102 | -3.00951 | -1.90865 |
| H | 6.45320 | -3.93466 | -0.96695 |
| C | 3.93297 | 0.47124 | 3.63029 |
| H | 4.98059 | 0.71957 | 3.44544 |
| H | 3.64862 | 0.95137 | 4.56889 |
| H | 3.84265 | -0.60854 | 3.77149 |
| C | 3.20110 | 2.50704 | 2.45365 |
| H | 4.23444 | 2.75289 | 2.19582 |
| H | 2.54975 | 2.97480 | 1.71203 |
| H | 2.97334 | 2.95927 | 3.42252 |
| C | 1.58366 | 0.65339 | 2.98466 |
| H | 0.81099 | 1.15411 | 2.39814 |
| H | 1.39924 | -0.42106 | 2.95238 |

| | | | |
|----|----------|----------|----------|
| H | 1.44976 | 1.00151 | 4.01269 |
| C | -2.39777 | 2.18995 | -1.39895 |
| H | -2.18616 | 2.27176 | -0.33088 |
| H | -1.59761 | 1.61218 | -1.85646 |
| H | -2.33361 | 3.19769 | -1.81506 |
| C | -4.73969 | 2.68650 | -1.00363 |
| H | -4.53441 | 3.66168 | -1.45263 |
| H | -5.79183 | 2.45512 | -1.17065 |
| H | -4.57588 | 2.77070 | 0.07273 |
| C | -4.11364 | 1.54735 | -3.11937 |
| H | -5.15048 | 1.25186 | -3.29223 |
| H | -3.97000 | 2.52793 | -3.58094 |
| H | -3.47785 | 0.83449 | -3.64456 |
| C | -1.57857 | -0.92620 | 2.43582 |
| H | -1.20708 | -1.11373 | 3.44591 |
| H | -0.80489 | -1.28524 | 1.76307 |
| H | -1.68976 | 0.15510 | 2.31821 |
| C | -2.70838 | -3.16006 | 2.32475 |
| H | -2.08550 | -3.50792 | 1.50288 |
| H | -2.21926 | -3.42286 | 3.26657 |
| H | -3.66485 | -3.68787 | 2.28563 |
| C | -3.77495 | -1.20848 | 3.45424 |
| H | -3.97507 | -0.13441 | 3.42819 |
| H | -4.73092 | -1.73028 | 3.50568 |
| H | -3.23254 | -1.42982 | 4.37686 |
| C | -8.10657 | -0.99019 | -1.25007 |
| H | -8.22609 | 0.08781 | -1.11523 |
| H | -7.63494 | -1.16649 | -2.22019 |
| H | -9.10724 | -1.42750 | -1.28351 |
| C | -8.03239 | -1.31929 | 1.20773 |
| H | -7.53990 | -1.79423 | 2.05837 |
| H | -8.06511 | -0.24354 | 1.39658 |
| H | -9.06048 | -1.68983 | 1.16807 |
| C | -7.27761 | -3.14044 | -0.33247 |
| H | -6.78158 | -3.38727 | -1.27436 |
| H | -6.74478 | -3.65410 | 0.47006 |
| H | -8.29544 | -3.53852 | -0.36856 |
| Au | 0.23461 | 3.24123 | 0.44907 |
| Cl | -0.45446 | 5.36232 | 0.89156 |
| C | -1.68494 | -0.88189 | -2.52868 |
| H | -2.62909 | -1.37614 | -2.76303 |
| H | -1.64074 | 0.08557 | -3.01746 |
| H | -0.87067 | -1.50513 | -2.90503 |
| Pb | 1.07975 | -2.41537 | -0.59441 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.86528 | -0.13003 | 0.91378 |
| C | 0.44558 | 0.14599 | -0.73017 |
| P | -1.14434 | -0.11045 | -1.46380 |
| O | -0.93478 | 0.14511 | -2.94915 |
| Pb | 1.43415 | 0.02133 | -2.97404 |
| Cl | 1.44704 | -2.47139 | -2.80976 |
| C | -2.50964 | 0.84047 | -0.79800 |
| H | -3.42273 | 0.57129 | -1.33316 |
| H | -2.63078 | 0.62160 | 0.26524 |
| H | -2.31365 | 1.90555 | -0.93125 |
| Au | 0.69731 | 2.11447 | 0.09103 |
| Cl | 0.79977 | 4.36066 | 0.23917 |
| H | -1.48547 | -1.45315 | -1.19966 |
| H | 2.28896 | -0.15552 | 0.77977 |

R = Me

| | | | |
|---|---------|----------|---------|
| P | 0.87335 | -0.03786 | 0.84513 |
|---|---------|----------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.37261 | 0.25739 | -0.76780 |
| P | -1.21595 | -0.14519 | -1.45380 |
| O | -0.99870 | -0.05747 | -2.96493 |
| Pb | 1.33815 | 0.09725 | -3.00537 |
| Cl | 1.74178 | -2.36228 | -2.64492 |
| C | -2.56079 | 0.93198 | -0.94473 |
| H | -3.47610 | 0.61605 | -1.45052 |
| H | -2.70431 | 0.88135 | 0.13616 |
| H | -2.33353 | 1.96004 | -1.22967 |
| C | -1.66064 | -1.81053 | -0.95383 |
| H | -1.81842 | -1.85930 | 0.12541 |
| H | -2.57156 | -2.11082 | -1.47573 |
| H | -0.84520 | -2.47838 | -1.23925 |
| C | 2.70537 | -0.13021 | 0.76508 |
| H | 3.13336 | 0.41042 | -0.07884 |
| H | 3.13102 | 0.24273 | 1.69880 |
| H | 2.96208 | -1.19116 | 0.67443 |
| Au | 0.50631 | 2.21825 | 0.09289 |
| Cl | 0.48473 | 4.45794 | 0.37666 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.75871 | -0.03767 | 0.78657 |
| C | 0.32754 | 0.29319 | -0.84059 |
| P | -1.18865 | -0.19432 | -1.65349 |
| O | -0.83400 | -0.12269 | -3.14274 |
| Pb | 1.38794 | 0.58732 | -3.03699 |
| Cl | 2.43305 | -1.70427 | -3.09916 |
| C | -2.54391 | 0.94428 | -1.30812 |
| H | -3.42666 | 0.63504 | -1.87112 |
| H | -2.77842 | 0.98342 | -0.24436 |
| H | -2.25132 | 1.94051 | -1.64350 |
| Au | 0.18196 | 2.20742 | 0.14709 |
| Cl | -0.09141 | 4.40936 | 0.57766 |
| C | 2.61998 | 0.06400 | 0.98595 |
| C | 3.05115 | -1.40491 | 1.08565 |
| C | 3.39172 | 0.75605 | -0.12234 |
| C | 2.85341 | 0.76559 | 2.32463 |
| H | 2.50455 | -1.93838 | 1.86878 |
| H | 2.90747 | -1.92976 | 0.13773 |
| H | 4.11555 | -1.45112 | 1.33770 |
| H | 3.03842 | 1.77628 | -0.29488 |
| H | 4.44999 | 0.81773 | 0.15301 |
| H | 3.34734 | 0.18306 | -1.05214 |
| H | 3.91100 | 0.69354 | 2.59676 |
| H | 2.58814 | 1.82470 | 2.27637 |
| H | 2.27088 | 0.30755 | 3.12915 |
| C | -1.76864 | -1.88603 | -1.21527 |
| C | -2.83193 | -2.27306 | -2.24787 |
| C | -0.59813 | -2.86348 | -1.31039 |
| C | -2.36301 | -1.90600 | 0.19165 |
| H | -3.71396 | -1.63043 | -2.19813 |
| H | -2.43347 | -2.23650 | -3.26267 |
| H | -3.16082 | -3.29614 | -2.04379 |
| H | 0.15714 | -2.67277 | -0.54619 |
| H | -0.97703 | -3.87830 | -1.15760 |
| H | -0.10654 | -2.82532 | -2.28356 |
| H | -2.64478 | -2.93337 | 0.44031 |
| H | -1.64724 | -1.57063 | 0.94648 |
| H | -3.26285 | -1.29216 | 0.26852 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.77688 | 0.24336 | 0.81323 |
| C | 0.25704 | 0.28535 | -0.81959 |
| P | -1.36723 | -0.08598 | -1.42769 |
| O | -1.25424 | 0.10747 | -2.93840 |
| Pb | 1.07828 | 0.35924 | -3.13600 |

| | | | |
|----|----------|----------|----------|
| Cl | 1.55422 | -2.10243 | -3.36020 |
| C | -2.68666 | 0.93313 | -0.75395 |
| H | -3.63221 | 0.62115 | -1.20195 |
| H | -2.74454 | 0.82197 | 0.33022 |
| H | -2.49367 | 1.97885 | -0.99862 |
| Au | 0.45748 | 2.37172 | -0.26391 |
| Cl | 0.48846 | 4.62802 | -0.35661 |
| C | -1.77990 | -1.78765 | -1.01825 |
| C | -1.86855 | -2.72230 | -2.04477 |
| C | -2.01542 | -2.17608 | 0.30008 |
| C | -2.19847 | -4.03754 | -1.75259 |
| H | -1.66902 | -2.41573 | -3.06402 |
| C | -2.34400 | -3.48993 | 0.58563 |
| H | -1.93255 | -1.45872 | 1.11039 |
| C | -2.43681 | -4.42028 | -0.44197 |
| H | -2.26166 | -4.76529 | -2.55300 |
| H | -2.52516 | -3.79063 | 1.61097 |
| H | -2.69163 | -5.44952 | -0.21618 |
| C | 2.58819 | 0.11480 | 0.74407 |
| C | 3.25345 | -0.63775 | -0.22457 |
| C | 3.32123 | 0.71862 | 1.76769 |
| C | 4.63421 | -0.75306 | -0.18530 |
| H | 2.69166 | -1.16354 | -0.99020 |
| C | 4.70205 | 0.61624 | 1.79157 |
| H | 2.80782 | 1.28418 | 2.53924 |
| C | 5.35947 | -0.11863 | 0.81404 |
| H | 5.14320 | -1.34706 | -0.93583 |
| H | 5.26659 | 1.10572 | 2.57675 |
| H | 6.43962 | -0.20719 | 0.83878 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.81420 | 0.15097 | 1.21337 |
| C | 0.09886 | 0.31466 | -0.34194 |
| P | -1.49650 | -0.04587 | -1.06220 |
| O | -1.32091 | 0.46802 | -2.49165 |
| Pb | 0.96230 | 1.01237 | -2.53175 |
| Cl | 1.77457 | -1.18187 | -3.48098 |
| Au | 0.03298 | 2.31345 | 0.50698 |
| Cl | -0.36783 | 4.53353 | 0.70157 |
| C | -1.85726 | -1.82246 | -0.97096 |
| C | -1.94037 | -2.61705 | -2.13797 |
| C | -2.06802 | -2.41971 | 0.28942 |
| C | -2.16778 | -3.98166 | -1.99168 |
| C | -2.27989 | -3.78948 | 0.36906 |
| C | -2.31868 | -4.59499 | -0.75800 |
| H | -2.22838 | -4.58659 | -2.89092 |
| H | -2.42958 | -4.23471 | 1.34817 |
| C | 2.61601 | 0.15166 | 0.89650 |
| C | 3.15956 | -1.01610 | 0.32716 |
| C | 3.46483 | 1.17061 | 1.35644 |
| C | 4.53245 | -1.08788 | 0.13478 |
| C | 4.83227 | 1.05150 | 1.13617 |
| C | 5.38492 | -0.05605 | 0.50771 |
| H | 4.94800 | -1.98882 | -0.30679 |
| H | 5.48610 | 1.84657 | 1.48287 |
| C | 2.95666 | 2.37678 | 2.08859 |
| H | 2.58717 | 3.14841 | 1.40610 |
| H | 2.13540 | 2.12902 | 2.76695 |
| H | 3.75421 | 2.82492 | 2.68344 |
| C | 2.31077 | -2.20210 | -0.02675 |
| H | 1.56499 | -2.41480 | 0.74616 |
| H | 1.77768 | -2.05520 | -0.96867 |
| H | 2.93385 | -3.09052 | -0.13786 |
| C | 6.85709 | -0.14350 | 0.24831 |
| H | 7.21926 | -1.16841 | 0.34952 |
| H | 7.08920 | 0.18331 | -0.77019 |

| | | | |
|---|----------|----------|----------|
| H | 7.42172 | 0.49099 | 0.93345 |
| C | -2.15359 | -1.65928 | 1.58249 |
| H | -1.85852 | -2.29850 | 2.41557 |
| H | -1.52182 | -0.77344 | 1.62309 |
| H | -3.18499 | -1.34330 | 1.76853 |
| C | -2.50771 | -6.07546 | -0.64814 |
| H | -3.04449 | -6.47322 | -1.51114 |
| H | -1.53904 | -6.58318 | -0.60450 |
| H | -3.05846 | -6.34231 | 0.25540 |
| C | -1.82495 | -2.10736 | -3.54585 |
| H | -2.46841 | -1.24865 | -3.73024 |
| H | -0.80464 | -1.79652 | -3.77589 |
| H | -2.09860 | -2.90455 | -4.23799 |
| C | -2.90625 | 0.84357 | -0.36844 |
| H | -3.04270 | 0.67278 | 0.69679 |
| H | -2.75098 | 1.90898 | -0.54846 |
| H | -3.79961 | 0.51980 | -0.90778 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.67231 | -0.01869 | 1.17244 |
| C | 0.38926 | 0.06609 | -0.53312 |
| P | -1.05176 | -0.11111 | -1.63549 |
| O | -0.35319 | -0.09476 | -3.00104 |
| Pb | 1.83023 | 0.58859 | -2.48907 |
| Cl | 2.96456 | -1.49313 | -3.36593 |
| Au | 0.36961 | 2.14547 | 0.11359 |
| Cl | 0.12809 | 4.40173 | -0.06756 |
| C | 2.52807 | -0.07193 | 1.27023 |
| C | 3.23180 | -1.19339 | 0.75121 |
| C | 3.27549 | 1.05933 | 1.67646 |
| C | 4.52962 | -0.99936 | 0.30125 |
| C | 4.57867 | 1.18557 | 1.18785 |
| C | 5.19931 | 0.21416 | 0.42247 |
| H | 5.04787 | -1.83872 | -0.14342 |
| H | 5.12802 | 2.08196 | 1.43946 |
| C | 2.88822 | 2.08102 | 2.76775 |
| C | 2.78043 | -2.65888 | 0.90777 |
| C | 6.57927 | 0.39660 | -0.19944 |
| C | -2.09594 | 1.37164 | -1.67128 |
| H | -2.59266 | 1.60811 | -0.73566 |
| H | -1.47206 | 2.21607 | -1.96899 |
| H | -2.84317 | 1.19607 | -2.44831 |
| C | 3.87465 | 1.82975 | 3.92706 |
| H | 3.78436 | 0.80732 | 4.30273 |
| H | 4.91073 | 1.98566 | 3.62451 |
| H | 3.65504 | 2.51699 | 4.74877 |
| C | 3.04794 | 3.53050 | 2.30137 |
| H | 2.36939 | 3.77335 | 1.48236 |
| H | 2.82084 | 4.20755 | 3.12949 |
| H | 4.06602 | 3.74764 | 1.97408 |
| C | 1.49739 | 1.91435 | 3.37238 |
| H | 1.41770 | 2.56041 | 4.25085 |
| H | 0.69456 | 2.21580 | 2.69580 |
| H | 1.31094 | 0.88910 | 3.70104 |
| C | 3.10692 | -3.51916 | -0.31484 |
| H | 2.66425 | -3.11614 | -1.22433 |
| H | 4.18128 | -3.60854 | -0.48276 |
| H | 2.72472 | -4.53142 | -0.15709 |
| C | 3.58529 | -3.19557 | 2.10761 |
| H | 4.65944 | -3.13241 | 1.92515 |
| H | 3.36361 | -2.62924 | 3.01589 |
| H | 3.32887 | -4.24421 | 2.28570 |
| C | 1.30985 | -2.86024 | 1.25313 |
| H | 1.01884 | -2.31641 | 2.15790 |
| H | 0.64460 | -2.58089 | 0.43705 |
| H | 1.13677 | -3.92034 | 1.45965 |

| | | | |
|---|----------|----------|----------|
| C | 7.17933 | 1.76453 | 0.11377 |
| H | 6.54599 | 2.57844 | -0.24785 |
| H | 7.34128 | 1.90405 | 1.18593 |
| H | 8.14968 | 1.85786 | -0.37969 |
| C | 6.45090 | 0.26039 | -1.72153 |
| H | 7.43475 | 0.34281 | -2.19215 |
| H | 6.01320 | -0.69692 | -2.01059 |
| H | 5.81532 | 1.05007 | -2.13090 |
| C | 7.53838 | -0.67798 | 0.32605 |
| H | 7.63349 | -0.62079 | 1.41335 |
| H | 7.20498 | -1.68492 | 0.06859 |
| H | 8.53120 | -0.53806 | -0.11024 |
| C | -2.34321 | -1.44109 | -1.65342 |
| C | -2.32234 | -2.34702 | -2.75554 |
| C | -3.58990 | -1.22324 | -1.00455 |
| C | -3.52965 | -2.65501 | -3.36758 |
| C | -1.10255 | -3.14033 | -3.26095 |
| C | -4.75705 | -1.59800 | -1.66507 |
| C | -3.80535 | -0.76867 | 0.45299 |
| C | -4.76183 | -2.22432 | -2.89885 |
| H | -3.50005 | -3.27932 | -4.25089 |
| C | -0.61703 | -2.66749 | -4.63395 |
| C | -1.52291 | -4.61838 | -3.40211 |
| C | 0.02615 | -3.15779 | -2.23943 |
| H | -5.70084 | -1.38983 | -1.18096 |
| C | -2.52622 | -0.44557 | 1.20436 |
| C | -4.41956 | -1.98112 | 1.18230 |
| C | -4.77999 | 0.40685 | 0.58035 |
| C | -6.03496 | -2.52488 | -3.67986 |
| H | 0.20287 | -3.30579 | -4.97330 |
| H | -1.42381 | -2.73601 | -5.36907 |
| H | -0.26377 | -1.64086 | -4.60210 |
| H | -2.21421 | -4.79062 | -4.22775 |
| H | -0.62981 | -5.21543 | -3.60314 |
| H | -1.98338 | -4.99400 | -2.48500 |
| H | 0.45465 | -2.17856 | -2.04347 |
| H | -0.32327 | -3.59026 | -1.29849 |
| H | 0.84516 | -3.77486 | -2.61270 |
| H | -1.80396 | -1.25947 | 1.12256 |
| H | -2.04865 | 0.47720 | 0.87695 |
| H | -2.74750 | -0.31410 | 2.26612 |
| H | -4.56724 | -1.73474 | 2.23747 |
| H | -5.38466 | -2.26926 | 0.76437 |
| H | -3.75508 | -2.84641 | 1.12378 |
| H | -5.76189 | 0.17459 | 0.16509 |
| H | -4.92125 | 0.64978 | 1.63679 |
| H | -4.41591 | 1.30534 | 0.08011 |
| C | -7.27739 | -1.95191 | -3.00331 |
| C | -6.21322 | -4.04202 | -3.81260 |
| C | -5.91656 | -1.90404 | -5.07689 |
| H | -7.45622 | -2.40553 | -2.02506 |
| H | -7.20525 | -0.86910 | -2.87352 |
| H | -8.15518 | -2.15393 | -3.62163 |
| H | -5.37601 | -4.50474 | -4.33859 |
| H | -6.29472 | -4.51390 | -2.83033 |
| H | -7.12458 | -4.26513 | -4.37423 |
| H | -5.80368 | -0.81894 | -5.01463 |
| H | -5.05758 | -2.29854 | -5.62310 |
| H | -6.81468 | -2.12008 | -5.66200 |

[R-P=C(Pb(II)Cl)-P(S)ClR](AuCl)

Coordination through Pb(II) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.85812 | 0.50629 | 0.64378 |
| C | 0.40446 | -0.01987 | -0.86145 |
| P | -1.23757 | -0.32377 | -1.38076 |
| Pb | 1.36022 | -0.05595 | -2.95982 |
| Cl | 1.26032 | -2.49436 | -3.19750 |
| Au | 2.99073 | 1.51417 | -4.23192 |
| Cl | 4.42334 | 2.90982 | -5.26705 |
| Cl | -2.64504 | 0.40798 | -0.14131 |
| H | 2.25804 | 0.64239 | 0.38661 |
| H | -1.49865 | -1.70043 | -1.27550 |
| S | -1.36300 | 0.34842 | -3.24003 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.85491 | 0.24846 | 0.73057 |
| C | 0.36468 | -0.11953 | -0.80731 |
| P | -1.30102 | -0.28861 | -1.31766 |
| Pb | 1.30844 | -0.05470 | -2.90540 |
| Cl | 1.24558 | -2.48774 | -3.31164 |
| C | -1.83956 | -1.99551 | -1.19862 |
| H | -1.82217 | -2.31259 | -0.15486 |
| H | -2.84810 | -2.07825 | -1.60585 |
| H | -1.14541 | -2.59601 | -1.79184 |
| C | 2.68192 | 0.34242 | 0.64230 |
| H | 3.10036 | 0.09940 | -0.33440 |
| H | 2.99112 | 1.35122 | 0.93157 |
| H | 3.09252 | -0.34102 | 1.39135 |
| Au | 3.03475 | 1.48858 | -4.08163 |
| Cl | 4.57344 | 2.85670 | -5.00134 |
| Cl | -2.59720 | 0.69327 | -0.10996 |
| S | -1.35417 | 0.41416 | -3.18617 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.72458 | -0.02975 | 0.61390 |
| C | 0.47614 | -0.13425 | -1.02295 |
| P | -1.14086 | -0.39920 | -1.68462 |
| Pb | 1.60422 | 0.30153 | -2.98327 |
| Cl | 2.37482 | -1.99285 | -3.46219 |
| Au | 2.88512 | 2.34060 | -3.96348 |
| Cl | 4.00735 | 4.15141 | -4.71323 |
| C | 2.54338 | 0.19272 | 0.97536 |
| C | 2.91404 | -1.04305 | 1.80481 |
| C | 3.46682 | 0.31884 | -0.21996 |
| C | 2.62838 | 1.44376 | 1.85564 |
| H | 2.24702 | -1.17617 | 2.66116 |
| H | 2.88814 | -1.95522 | 1.20378 |
| H | 3.93078 | -0.92366 | 2.19235 |
| H | 3.26262 | 1.22439 | -0.79874 |
| H | 4.50371 | 0.40006 | 0.12235 |
| H | 3.41748 | -0.55910 | -0.87091 |
| H | 3.64986 | 1.55294 | 2.23315 |
| H | 2.37904 | 2.34929 | 1.29725 |
| H | 1.95954 | 1.38044 | 2.71828 |
| C | -1.82514 | -2.09898 | -1.40797 |
| C | -3.16432 | -2.19341 | -2.13715 |
| C | -0.82557 | -3.08785 | -2.00807 |
| C | -2.00538 | -2.36410 | 0.08301 |
| H | -3.90586 | -1.50859 | -1.72254 |
| H | -3.05787 | -1.99225 | -3.20465 |
| H | -3.54457 | -3.21216 | -2.02297 |
| H | 0.14757 | -3.04176 | -1.51706 |
| H | -1.22595 | -4.09686 | -1.87598 |
| H | -0.67234 | -2.91967 | -3.07467 |

| | | | |
|----|----------|----------|----------|
| H | -2.38050 | -3.38413 | 0.20407 |
| H | -1.06372 | -2.29130 | 0.63071 |
| H | -2.72532 | -1.68357 | 0.53898 |
| Cl | -2.48283 | 0.81869 | -0.75396 |
| S | -1.02122 | 0.06946 | -3.62405 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78939 | 0.38577 | 0.70801 |
| C | 0.34226 | -0.11496 | -0.81010 |
| P | -1.28980 | -0.28215 | -1.41691 |
| Pb | 1.48037 | -0.14154 | -2.79155 |
| Cl | 1.59531 | -2.58655 | -3.11295 |
| Au | 3.18676 | 1.41451 | -3.98331 |
| Cl | 4.70005 | 2.78322 | -4.95012 |
| C | 2.59582 | 0.31260 | 0.66255 |
| C | 3.29098 | 1.29620 | 1.36953 |
| C | 3.31359 | -0.68031 | -0.01307 |
| C | 4.67620 | 1.32274 | 1.35157 |
| H | 2.74262 | 2.05433 | 1.91990 |
| C | 4.69837 | -0.65847 | -0.01444 |
| H | 2.78934 | -1.49522 | -0.50396 |
| C | 5.37925 | 0.34908 | 0.65677 |
| H | 5.20838 | 2.10376 | 1.88178 |
| H | 5.24771 | -1.43235 | -0.53770 |
| H | 6.46276 | 0.36834 | 0.64594 |
| C | -1.94700 | -1.92505 | -1.09532 |
| C | -2.10301 | -2.82258 | -2.14525 |
| C | -2.24313 | -2.30874 | 0.21267 |
| C | -2.56609 | -4.10395 | -1.88575 |
| H | -1.85678 | -2.51979 | -3.15545 |
| C | -2.70320 | -3.58840 | 0.46117 |
| H | -2.12096 | -1.60953 | 1.03235 |
| C | -2.86550 | -4.48554 | -0.58814 |
| H | -2.68748 | -4.80441 | -2.70324 |
| H | -2.93728 | -3.88821 | 1.47579 |
| H | -3.22604 | -5.48816 | -0.38885 |
| Cl | -2.56136 | 0.94363 | -0.41326 |
| S | -1.19376 | 0.17858 | -3.35128 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.85888 | 0.20176 | 1.23168 |
| C | 0.32162 | -0.20772 | -0.28574 |
| P | -1.28470 | -0.22698 | -1.00709 |
| Pb | 1.61916 | 0.01627 | -2.14056 |
| Cl | 1.51561 | -2.32766 | -2.93346 |
| Au | 3.61557 | 1.50313 | -2.89810 |
| Cl | 5.42403 | 2.77270 | -3.39924 |
| C | 2.66187 | 0.24999 | 0.94768 |
| C | 3.28700 | 1.50778 | 0.89232 |
| C | 3.40827 | -0.92725 | 0.77887 |
| C | 4.64170 | 1.56752 | 0.60264 |
| C | 4.76610 | -0.81297 | 0.49638 |
| C | 5.39704 | 0.41940 | 0.38374 |
| H | 5.11922 | 2.53929 | 0.52426 |
| H | 5.34753 | -1.71978 | 0.35980 |
| C | -1.99639 | -1.89325 | -1.05608 |
| C | -2.30933 | -2.55793 | -2.26644 |
| C | -2.18335 | -2.56280 | 0.17823 |
| C | -2.73676 | -3.87863 | -2.19657 |
| C | -2.60264 | -3.88557 | 0.16823 |
| C | -2.87197 | -4.57117 | -1.00467 |
| H | -2.97229 | -4.38422 | -3.12721 |
| H | -2.73287 | -4.38955 | 1.12066 |
| Cl | -2.61939 | 0.88794 | 0.06427 |
| C | 2.50743 | 2.77539 | 1.08449 |
| H | 1.81833 | 2.70654 | 1.93218 |

| | | | |
|---|----------|----------|----------|
| H | 3.17614 | 3.61811 | 1.26192 |
| H | 1.90752 | 3.01488 | 0.20063 |
| C | 2.78977 | -2.29004 | 0.90394 |
| H | 2.08806 | -2.33912 | 1.74137 |
| H | 2.23671 | -2.57435 | 0.00380 |
| H | 3.56130 | -3.04350 | 1.06705 |
| C | 6.84351 | 0.52572 | 0.01798 |
| H | 6.94891 | 0.99533 | -0.96474 |
| H | 7.38710 | 1.14758 | 0.73351 |
| H | 7.32070 | -0.45419 | -0.01800 |
| C | -2.02802 | -1.93342 | 1.52993 |
| H | -1.15860 | -1.28394 | 1.62077 |
| H | -2.90345 | -1.32722 | 1.77473 |
| H | -1.93737 | -2.71015 | 2.28961 |
| C | -2.24079 | -1.97029 | -3.64532 |
| H | -2.79429 | -1.03585 | -3.72934 |
| H | -1.21187 | -1.77122 | -3.94741 |
| H | -2.66684 | -2.68081 | -4.35396 |
| C | -3.28458 | -6.00840 | -0.98752 |
| H | -2.40824 | -6.65641 | -1.08787 |
| H | -3.78157 | -6.27076 | -0.05232 |
| H | -3.95677 | -6.23971 | -1.81544 |
| S | -0.95733 | 0.75304 | -2.71993 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.13246 | 2.21629 | 1.01999 |
| C | 0.46114 | 0.70095 | 0.41208 |
| P | 1.97783 | -0.19212 | 0.24493 |
| Cl | -1.28020 | 0.47491 | -2.81078 |
| C | 3.71792 | 0.37948 | 0.14180 |
| C | 4.30788 | 0.36927 | -1.15879 |
| C | 4.57667 | 0.31459 | 1.27246 |
| C | 5.59772 | -0.12553 | -1.26824 |
| C | 5.86311 | -0.17737 | 1.07227 |
| C | 6.36394 | -0.51085 | -0.17522 |
| H | 6.02987 | -0.19384 | -2.25870 |
| H | 6.49977 | -0.28880 | 1.93876 |
| C | -1.69630 | 2.28192 | 0.85341 |
| C | -2.26825 | 3.07956 | -0.16637 |
| C | -2.52590 | 1.43807 | 1.63643 |
| C | -3.57689 | 2.80037 | -0.54935 |
| C | -3.81502 | 1.19537 | 1.17379 |
| C | -4.34581 | 1.81328 | 0.04889 |
| H | -4.00782 | 3.36587 | -1.35945 |
| H | -4.44160 | 0.51006 | 1.72856 |
| C | -1.55093 | 4.28805 | -0.79751 |
| C | -2.15990 | 0.88925 | 3.03438 |
| C | -5.74434 | 1.44769 | -0.43726 |
| C | 4.32253 | 0.93259 | 2.66417 |
| C | 3.74881 | 1.05828 | -2.42153 |
| C | 7.72205 | -1.16862 | -0.37888 |
| C | -3.39613 | 0.96894 | 3.94699 |
| H | -3.09774 | 0.73186 | 4.97104 |
| H | -3.83538 | 1.96913 | 3.94197 |
| H | -4.16974 | 0.25219 | 3.67007 |
| C | -1.08861 | 1.73555 | 3.72114 |
| H | -0.10279 | 1.65122 | 3.24998 |
| H | -1.36399 | 2.79257 | 3.74798 |
| H | -0.95484 | 1.39102 | 4.75001 |
| C | -1.70706 | -0.57189 | 2.99602 |
| H | -2.45211 | -1.20673 | 2.50999 |
| H | -0.75729 | -0.68790 | 2.47265 |
| H | -1.56766 | -0.94556 | 4.01464 |
| C | -6.76567 | 1.73075 | 0.67106 |
| H | -7.77058 | 1.47121 | 0.32735 |
| H | -6.56340 | 1.14608 | 1.57057 |

| | | | |
|----|----------|----------|----------|
| H | -6.76285 | 2.78836 | 0.94733 |
| C | -6.15049 | 2.24010 | -1.67714 |
| H | -7.14366 | 1.92040 | -2.00089 |
| H | -6.20014 | 3.31439 | -1.48000 |
| H | -5.46182 | 2.07115 | -2.50860 |
| C | -5.77516 | -0.04425 | -0.78879 |
| H | -5.06652 | -0.27256 | -1.58855 |
| H | -5.52711 | -0.67589 | 0.06639 |
| H | -6.77395 | -0.32868 | -1.13070 |
| C | -2.46440 | 5.05846 | -1.75386 |
| H | -3.37522 | 5.40892 | -1.26312 |
| H | -1.92719 | 5.93763 | -2.11672 |
| H | -2.74281 | 4.46238 | -2.62590 |
| C | -1.15389 | 5.26014 | 0.32297 |
| H | -2.03187 | 5.58138 | 0.88863 |
| H | -0.44481 | 4.81577 | 1.02493 |
| H | -0.68022 | 6.14793 | -0.10533 |
| C | -0.31046 | 3.89532 | -1.60064 |
| H | 0.49092 | 3.51050 | -0.96371 |
| H | -0.53903 | 3.13081 | -2.34421 |
| H | 0.09297 | 4.77671 | -2.10796 |
| C | 2.97546 | 1.62513 | 2.81949 |
| H | 2.79711 | 2.33434 | 2.00860 |
| H | 2.13984 | 0.93124 | 2.87501 |
| H | 2.97384 | 2.19538 | 3.75186 |
| C | 5.37383 | 2.05628 | 2.79833 |
| H | 5.22126 | 2.57825 | 3.74681 |
| H | 6.39494 | 1.67471 | 2.78525 |
| H | 5.27407 | 2.78409 | 1.98953 |
| C | 4.53254 | -0.05481 | 3.81497 |
| H | 5.52573 | -0.50670 | 3.78957 |
| H | 4.43816 | 0.47382 | 4.76724 |
| H | 3.79637 | -0.85733 | 3.80021 |
| C | 2.41569 | 1.76666 | -2.22009 |
| H | 2.22099 | 2.40606 | -3.08443 |
| H | 1.56789 | 1.08900 | -2.14492 |
| H | 2.44379 | 2.41102 | -1.33807 |
| C | 3.65861 | 0.12542 | -3.63081 |
| H | 2.91921 | -0.65866 | -3.47355 |
| H | 3.36060 | 0.70130 | -4.51078 |
| H | 4.61734 | -0.34654 | -3.85548 |
| C | 4.76292 | 2.17690 | -2.74680 |
| H | 4.86959 | 2.86685 | -1.90595 |
| H | 5.75162 | 1.78754 | -2.99136 |
| H | 4.40260 | 2.74439 | -3.60878 |
| C | 8.39428 | -1.52793 | 0.94342 |
| H | 8.62606 | -0.64136 | 1.53926 |
| H | 7.77327 | -2.19637 | 1.54491 |
| H | 9.33751 | -2.04165 | 0.74418 |
| C | 8.64704 | -0.21973 | -1.15055 |
| H | 8.24698 | 0.02755 | -2.13577 |
| H | 8.79659 | 0.71415 | -0.60314 |
| H | 9.62398 | -0.68812 | -1.29721 |
| C | 7.52567 | -2.45679 | -1.18772 |
| H | 6.87810 | -3.15817 | -0.65641 |
| H | 7.07458 | -2.25788 | -2.16181 |
| H | 8.48990 | -2.94347 | -1.35706 |
| Au | -2.70598 | -2.58387 | -0.15540 |
| Cl | -4.27195 | -4.12669 | 0.39302 |
| Pb | -0.93951 | -0.74667 | -0.68171 |
| Cl | 1.99537 | -1.39739 | 1.91620 |
| S | 1.61714 | -1.48550 | -1.24142 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.89866 | 0.11767 | 1.05349 |
| C | 0.60297 | -0.15506 | -0.55454 |
| P | -0.89646 | 0.16422 | -1.35234 |
| Pb | 1.92303 | -0.53152 | -2.53831 |
| Cl | 0.69129 | -2.62896 | -3.03933 |
| Au | -1.96850 | 0.77745 | -4.53975 |
| Cl | -3.56313 | 0.41534 | -6.08544 |
| Cl | -2.35203 | 1.06322 | -0.29241 |
| H | 2.27610 | -0.27562 | 1.07470 |
| H | -1.49938 | -1.04877 | -1.71195 |
| S | -0.34773 | 1.20752 | -3.00574 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.90809 | 0.13432 | 1.05823 |
| C | 0.59150 | -0.11794 | -0.54762 |
| P | -0.96160 | 0.15765 | -1.25899 |
| Pb | 1.92088 | -0.32733 | -2.55009 |
| Cl | 1.14746 | -2.63851 | -3.08058 |
| C | -1.86839 | -1.36655 | -1.50334 |
| H | -2.07648 | -1.80108 | -0.52364 |
| H | -2.79620 | -1.14862 | -2.03392 |
| H | -1.24152 | -2.03980 | -2.09346 |
| C | 2.67234 | -0.32531 | 1.27370 |
| H | 3.15297 | -0.69006 | 0.36569 |
| H | 3.21702 | 0.54132 | 1.65999 |
| H | 2.72920 | -1.10091 | 2.04339 |
| Au | -2.09761 | 0.54633 | -4.53164 |
| Cl | -3.68092 | 0.04988 | -6.05478 |
| Cl | -2.23015 | 1.29897 | -0.16304 |
| S | -0.50068 | 1.10249 | -3.01108 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.98540 | 0.11770 | 0.74989 |
| C | 0.75370 | -0.10741 | -0.87928 |
| P | -0.84438 | 0.14707 | -1.53834 |
| Pb | 2.15016 | -0.21936 | -2.83763 |
| Cl | 2.11455 | -2.70815 | -3.09639 |
| C | -1.97298 | -1.32898 | -1.41637 |
| C | 2.74123 | -0.34494 | 1.20201 |
| Au | -2.05810 | 0.32090 | -4.95008 |
| Cl | -3.59924 | -0.12081 | -6.53605 |
| Cl | -1.86056 | 1.60640 | -0.54140 |
| S | -0.44927 | 0.82333 | -3.42536 |
| C | 3.69125 | -0.61249 | 0.05146 |
| H | 3.35191 | -1.44688 | -0.56989 |
| H | 3.83642 | 0.28222 | -0.56355 |
| H | 4.67902 | -0.88708 | 0.43691 |
| C | 3.25926 | 0.80610 | 2.06849 |
| H | 2.57981 | 1.02589 | 2.89626 |
| H | 4.23046 | 0.53765 | 2.49614 |
| H | 3.38956 | 1.72322 | 1.48805 |
| C | 2.58903 | -1.60462 | 2.06334 |
| H | 3.55708 | -1.86155 | 2.50588 |
| H | 1.88134 | -1.45419 | 2.88354 |
| H | 2.25117 | -2.45826 | 1.47098 |
| C | -1.98607 | -1.78092 | 0.04378 |
| H | -2.69722 | -2.60713 | 0.12751 |
| H | -1.01083 | -2.14479 | 0.36857 |
| H | -2.31254 | -0.99023 | 0.72209 |
| C | -3.38459 | -0.94931 | -1.85597 |
| H | -3.84503 | -0.22474 | -1.18438 |
| H | -3.41127 | -0.55488 | -2.87465 |
| H | -3.99107 | -1.85882 | -1.84437 |

| | | | |
|---|----------|----------|----------|
| C | -1.41359 | -2.43390 | -2.30834 |
| H | -1.43631 | -2.15529 | -3.36320 |
| H | -0.39159 | -2.71086 | -2.04617 |
| H | -2.04651 | -3.31698 | -2.18413 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.85993 | 0.54383 | 0.85395 |
| C | 0.55410 | -0.07172 | -0.65641 |
| P | -0.95175 | 0.03249 | -1.49942 |
| Pb | 2.13505 | -0.56272 | -2.37340 |
| Cl | 1.73159 | -3.02537 | -2.50231 |
| Au | -2.03098 | 0.02904 | -4.86595 |
| Cl | -3.63556 | -0.40207 | -6.39010 |
| C | 2.58411 | 0.05021 | 1.14301 |
| C | 3.12291 | -1.16230 | 0.69691 |
| C | 3.39211 | 0.92225 | 1.87522 |
| C | 4.45216 | -1.47020 | 0.94404 |
| H | 2.48646 | -1.89023 | 0.20104 |
| C | 4.72386 | 0.61684 | 2.10895 |
| H | 2.97646 | 1.85154 | 2.25255 |
| C | 5.25541 | -0.57666 | 1.64045 |
| H | 4.85638 | -2.41658 | 0.60333 |
| H | 5.34738 | 1.30880 | 2.66326 |
| H | 6.29416 | -0.81923 | 1.83277 |
| C | -1.90033 | -1.48613 | -1.35685 |
| C | -2.66849 | -1.70248 | -0.21239 |
| C | -1.80666 | -2.46724 | -2.33854 |
| C | -3.34954 | -2.89665 | -0.06380 |
| H | -2.74458 | -0.93929 | 0.55278 |
| C | -2.49548 | -3.65925 | -2.17967 |
| H | -1.20145 | -2.30835 | -3.22106 |
| C | -3.26565 | -3.87318 | -1.04827 |
| H | -3.95426 | -3.06245 | 0.81986 |
| H | -2.42888 | -4.41801 | -2.94964 |
| H | -3.80718 | -4.80482 | -0.93132 |
| Cl | -2.19204 | 1.46701 | -0.76897 |
| S | -0.37344 | 0.51287 | -3.38546 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.71571 | 0.24598 | 1.25883 |
| C | 0.38582 | -0.18340 | -0.30738 |
| P | -1.06333 | -0.05692 | -1.25537 |
| Pb | 2.21152 | -0.35906 | -1.81145 |
| Cl | 1.93055 | -2.80362 | -2.28194 |
| Au | -1.83996 | 1.49155 | -4.39522 |
| Cl | -3.36242 | 2.23507 | -5.88403 |
| C | 2.52759 | -0.05626 | 1.31607 |
| C | 3.03894 | -1.35898 | 1.45599 |
| C | 3.39855 | 1.04772 | 1.28068 |
| C | 4.41894 | -1.52917 | 1.50600 |
| C | 4.76808 | 0.82498 | 1.33404 |
| C | 5.29915 | -0.45637 | 1.43717 |
| H | 4.81535 | -2.53406 | 1.61621 |
| H | 5.43951 | 1.67810 | 1.30320 |
| C | -1.94944 | -1.63783 | -1.33403 |
| C | -2.53423 | -2.10152 | -0.13079 |
| C | -2.02023 | -2.43459 | -2.50241 |
| C | -3.16530 | -3.33831 | -0.12618 |
| C | -2.67817 | -3.65542 | -2.42220 |
| C | -3.25851 | -4.13066 | -1.25726 |
| H | -3.60151 | -3.68686 | 0.80463 |
| H | -2.72780 | -4.26241 | -3.32007 |
| Cl | -2.42953 | 1.29497 | -0.57035 |
| C | 2.87060 | 2.44863 | 1.17520 |
| H | 2.42502 | 2.64383 | 0.19459 |
| H | 2.09006 | 2.64112 | 1.91778 |

| | | | |
|---|----------|----------|----------|
| H | 3.66712 | 3.17750 | 1.32803 |
| C | 2.13963 | -2.55425 | 1.57062 |
| H | 1.30224 | -2.36219 | 2.24745 |
| H | 1.71563 | -2.83403 | 0.60181 |
| H | 2.69271 | -3.41350 | 1.95155 |
| C | 6.78054 | -0.67369 | 1.46574 |
| H | 7.17487 | -0.78262 | 0.45059 |
| H | 7.29791 | 0.16890 | 1.92768 |
| H | 7.03934 | -1.58044 | 2.01466 |
| C | -2.56572 | -1.35020 | 1.16785 |
| H | -1.65734 | -0.78716 | 1.37847 |
| H | -3.39419 | -0.63857 | 1.18515 |
| H | -2.71338 | -2.05196 | 1.98946 |
| C | -1.44592 | -2.08892 | -3.84203 |
| H | -1.90244 | -1.19230 | -4.26517 |
| H | -0.36975 | -1.92511 | -3.79598 |
| H | -1.62721 | -2.91180 | -4.53291 |
| C | -3.97383 | -5.44384 | -1.23278 |
| H | -4.07905 | -5.82296 | -0.21544 |
| H | -4.97839 | -5.33997 | -1.65423 |
| H | -3.44835 | -6.19198 | -1.82939 |
| S | -0.25854 | 0.79151 | -2.91487 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | 1.78778 | 2.14533 | 0.10305 |
| C | 0.92176 | 0.75060 | -0.15515 |
| P | -0.80082 | 0.50801 | -0.22643 |
| C | 3.51607 | 1.50978 | -0.03967 |
| C | 4.30222 | 1.37185 | 1.13423 |
| C | 4.00421 | 1.00331 | -1.26595 |
| C | 5.38866 | 0.51083 | 1.08781 |
| C | 5.08222 | 0.11482 | -1.22315 |
| C | 5.75440 | -0.19451 | -0.05355 |
| H | 5.96799 | 0.35984 | 1.98647 |
| H | 5.42329 | -0.32241 | -2.15052 |
| C | 3.54355 | 1.46569 | -2.66705 |
| C | 4.04721 | 2.18006 | 2.41977 |
| C | 6.89890 | -1.20044 | 0.00575 |
| C | 2.73559 | 1.79306 | 3.10513 |
| H | 1.86062 | 2.08190 | 2.51756 |
| H | 2.67730 | 0.71738 | 3.27776 |
| H | 2.65489 | 2.31366 | 4.06402 |
| C | 4.03293 | 3.67549 | 2.07308 |
| H | 4.97815 | 3.97783 | 1.61539 |
| H | 3.22579 | 3.93516 | 1.38490 |
| H | 3.89060 | 4.26565 | 2.98262 |
| C | 5.15860 | 1.97434 | 3.45184 |
| H | 5.18655 | 0.94890 | 3.82745 |
| H | 6.14377 | 2.23109 | 3.05508 |
| H | 4.96678 | 2.62815 | 4.30553 |
| C | 2.64039 | 0.43752 | -3.35224 |
| H | 1.68069 | 0.34255 | -2.84192 |
| H | 2.43540 | 0.74376 | -4.38224 |
| H | 3.11889 | -0.54488 | -3.38972 |
| C | 2.83953 | 2.82115 | -2.63672 |
| H | 1.86076 | 2.78925 | -2.15003 |
| H | 3.44734 | 3.57705 | -2.13387 |
| H | 2.65583 | 3.15947 | -3.66008 |
| C | 4.78358 | 1.67072 | -3.55624 |
| H | 5.51382 | 2.32560 | -3.07557 |
| H | 5.28167 | 0.73509 | -3.81223 |
| H | 4.47575 | 2.13536 | -4.49619 |
| C | 7.12327 | -1.90101 | -1.33164 |
| H | 7.42182 | -1.20128 | -2.11666 |
| H | 7.92501 | -2.63571 | -1.22752 |
| H | 6.22924 | -2.43426 | -1.66538 |

| | | | |
|----|----------|----------|----------|
| C | 6.57730 | -2.26642 | 1.06003 |
| H | 6.45233 | -1.83095 | 2.05290 |
| H | 5.65308 | -2.79612 | 0.81881 |
| H | 7.38952 | -2.99664 | 1.11308 |
| C | 8.19426 | -0.47748 | 0.39428 |
| H | 8.10981 | 0.00767 | 1.36871 |
| H | 9.02110 | -1.19111 | 0.44786 |
| H | 8.45225 | 0.28813 | -0.34179 |
| C | -2.25398 | 1.49572 | 0.27097 |
| C | -2.89724 | 1.10686 | 1.47939 |
| C | -3.01560 | 2.19963 | -0.70841 |
| C | -4.28621 | 1.04102 | 1.47131 |
| C | -4.39383 | 2.09673 | -0.63374 |
| C | -5.05615 | 1.41570 | 0.38284 |
| H | -4.77943 | 0.67556 | 2.36103 |
| H | -4.98327 | 2.58175 | -1.40178 |
| C | -2.22844 | 0.95178 | 2.86015 |
| C | -2.55536 | -0.37277 | 3.55314 |
| C | -2.81920 | 2.09983 | 3.70810 |
| H | -2.11507 | -1.21929 | 3.02792 |
| H | -2.15103 | -0.35737 | 4.56870 |
| H | -3.63057 | -0.54300 | 3.62906 |
| H | -2.61623 | 3.07111 | 3.25001 |
| H | -3.89773 | 2.00584 | 3.83749 |
| H | -2.35721 | 2.08657 | 4.69889 |
| C | -2.47420 | 3.24269 | -1.70864 |
| C | -3.07949 | 4.58680 | -1.25072 |
| C | -2.91988 | 2.98491 | -3.15022 |
| H | -2.79394 | 4.81337 | -0.22068 |
| H | -2.70493 | 5.38875 | -1.89287 |
| H | -4.16828 | 4.59026 | -1.30692 |
| H | -2.50332 | 2.05868 | -3.54427 |
| H | -4.00612 | 2.92841 | -3.23768 |
| H | -2.58239 | 3.80698 | -3.78721 |
| C | -6.56098 | 1.20183 | 0.31498 |
| C | -7.27262 | 2.55989 | 0.34693 |
| C | -7.07203 | 0.35213 | 1.47546 |
| H | -6.98079 | 3.19167 | -0.49492 |
| H | -8.35470 | 2.41335 | 0.29275 |
| H | -7.04878 | 3.10156 | 1.26963 |
| H | -6.58017 | -0.62304 | 1.50331 |
| H | -6.93220 | 0.84620 | 2.44081 |
| H | -8.14356 | 0.17922 | 1.35216 |
| Cl | 2.50134 | -1.80468 | 1.99850 |
| Cl | -1.12595 | 0.17506 | -2.22866 |
| Au | -2.94552 | -2.24617 | -0.18194 |
| Cl | -4.93650 | -3.11681 | -0.82060 |
| C | -0.96434 | 3.44321 | -1.66946 |
| H | -0.60867 | 3.61562 | -0.65108 |
| H | -0.41218 | 2.61149 | -2.10169 |
| H | -0.70934 | 4.32972 | -2.25577 |
| C | -0.72086 | 1.17155 | 2.86952 |
| H | -0.15504 | 0.34807 | 2.43577 |
| H | -0.45398 | 2.09994 | 2.35776 |
| H | -0.38543 | 1.26249 | 3.90554 |
| C | -6.89630 | 0.47563 | -0.99419 |
| H | -6.59051 | 1.05466 | -1.86842 |
| H | -6.40402 | -0.49859 | -1.04156 |
| H | -7.97621 | 0.31800 | -1.06117 |
| Pb | 1.73725 | -1.50115 | -0.37462 |
| S | -0.97291 | -1.37952 | 0.55991 |

Coordination through P(sp²) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.68557 | 0.07500 | 0.87784 |
| C | 0.41465 | -0.33302 | -0.68271 |
| P | -1.08390 | -0.32739 | -1.55340 |
| Pb | 1.82468 | -0.56723 | -2.64739 |
| Cl | 1.17171 | -2.96149 | -2.89655 |
| Au | -0.57097 | 0.73981 | 2.55412 |
| Cl | -1.82910 | 1.42606 | 4.29609 |
| Cl | -2.64384 | 0.56170 | -0.63561 |
| H | 2.08176 | -0.04902 | 1.05383 |
| H | -1.53746 | -1.65514 | -1.60741 |
| S | -0.69892 | 0.43004 | -3.34178 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.76845 | 0.17666 | 0.86028 |
| C | 0.40447 | -0.22646 | -0.68127 |
| P | -1.16812 | -0.28630 | -1.41817 |
| Pb | 1.69182 | -0.53123 | -2.70752 |
| Cl | 1.35004 | -3.01781 | -2.68955 |
| C | -1.88950 | -1.91115 | -1.17902 |
| H | -2.05991 | -2.08022 | -0.11458 |
| H | -2.83133 | -1.96015 | -1.72718 |
| H | -1.18228 | -2.64348 | -1.57666 |
| C | 2.55081 | 0.05124 | 1.15378 |
| H | 3.08453 | -0.31454 | 0.27730 |
| H | 2.93205 | 1.03237 | 1.44691 |
| H | 2.71324 | -0.62867 | 1.99362 |
| Au | -0.50574 | 0.79197 | 2.55196 |
| Cl | -1.77784 | 1.40012 | 4.31926 |
| Cl | -2.53036 | 0.95662 | -0.57114 |
| S | -0.90059 | 0.17229 | -3.33890 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.72545 | 0.19242 | 0.83753 |
| C | 0.45432 | -0.11506 | -0.75085 |
| P | -1.12620 | -0.28354 | -1.48170 |
| Pb | 1.77076 | 0.12960 | -2.77886 |
| Cl | 2.37858 | -2.29605 | -3.01118 |
| Au | -0.71581 | 0.55653 | 2.48229 |
| Cl | -2.15772 | 0.91892 | 4.19256 |
| C | 2.51248 | 0.18494 | 1.33111 |
| C | 2.66473 | -1.00492 | 2.28677 |
| C | 3.46696 | 0.03945 | 0.15877 |
| C | 2.77806 | 1.48960 | 2.08543 |
| H | 1.96623 | -0.94485 | 3.12490 |
| H | 2.51112 | -1.95708 | 1.77384 |
| H | 3.67960 | -0.99953 | 2.69585 |
| H | 3.42347 | 0.90895 | -0.50383 |
| H | 4.49229 | -0.01629 | 0.53695 |
| H | 3.28199 | -0.87242 | -0.41469 |
| H | 3.79850 | 1.47096 | 2.47944 |
| H | 2.68214 | 2.36218 | 1.43474 |
| H | 2.09467 | 1.61632 | 2.92829 |
| C | -1.90348 | -1.94372 | -1.19348 |
| C | -3.23579 | -1.97199 | -1.94086 |
| C | -0.95722 | -2.99809 | -1.76584 |
| C | -2.11983 | -2.17906 | 0.29709 |
| H | -3.95197 | -1.25919 | -1.52974 |
| H | -3.10663 | -1.76834 | -3.00547 |
| H | -3.66024 | -2.97445 | -1.83899 |
| H | 0.01629 | -2.99422 | -1.27376 |
| H | -1.41269 | -3.98052 | -1.61256 |
| H | -0.79163 | -2.86259 | -2.83515 |
| H | -2.59353 | -3.15694 | 0.42143 |

| | | | |
|----|----------|----------|----------|
| H | -1.17894 | -2.19943 | 0.84960 |
| H | -2.77302 | -1.43146 | 0.74919 |
| Cl | -2.46568 | 1.02597 | -0.67480 |
| S | -0.91145 | 0.11813 | -3.42592 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.74203 | 0.43860 | 0.43091 |
| C | 0.55167 | -0.43352 | -0.94204 |
| P | -0.90744 | -0.73189 | -1.83395 |
| Pb | 2.15713 | -1.17237 | -2.57073 |
| Cl | 2.13127 | -3.58195 | -1.85200 |
| Au | -0.68162 | 1.69207 | 1.56491 |
| Cl | -2.14122 | 2.95341 | 2.74854 |
| C | 2.42545 | 0.29301 | 1.02165 |
| C | 2.97155 | 1.35735 | 1.74059 |
| C | 3.18298 | -0.86170 | 0.80363 |
| C | 4.27674 | 1.28541 | 2.19817 |
| H | 2.37188 | 2.24040 | 1.93595 |
| C | 4.48354 | -0.92889 | 1.27388 |
| H | 2.74194 | -1.72249 | 0.31007 |
| C | 5.03287 | 0.14578 | 1.96179 |
| H | 4.70182 | 2.11776 | 2.74645 |
| H | 5.06424 | -1.82996 | 1.11467 |
| H | 6.05097 | 0.08764 | 2.32935 |
| C | -1.82840 | -2.08449 | -1.08483 |
| C | -2.60987 | -1.86113 | 0.04860 |
| C | -1.69077 | -3.36746 | -1.60494 |
| C | -3.25856 | -2.92447 | 0.65025 |
| H | -2.72036 | -0.86260 | 0.45573 |
| C | -2.34461 | -4.42602 | -0.99325 |
| H | -1.07141 | -3.53503 | -2.47737 |
| C | -3.12673 | -4.20575 | 0.12949 |
| H | -3.87134 | -2.75110 | 1.52692 |
| H | -2.23755 | -5.42547 | -1.39758 |
| H | -3.63796 | -5.03564 | 0.60389 |
| Cl | -2.19632 | 0.83853 | -1.75203 |
| S | -0.36852 | -1.08458 | -3.71658 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.67340 | 0.61820 | 0.95879 |
| C | 0.35685 | -0.35241 | -0.31999 |
| P | -0.99954 | -0.54774 | -1.39060 |
| Pb | 2.14868 | -0.97271 | -1.79051 |
| Cl | 1.70473 | -3.44325 | -1.63972 |
| Au | -0.60153 | 1.97095 | 2.15792 |
| Cl | -1.87262 | 3.35691 | 3.42008 |
| C | 2.43634 | 0.47729 | 1.33155 |
| C | 3.27630 | 1.56895 | 1.05268 |
| C | 2.94652 | -0.69346 | 1.91852 |
| C | 4.62943 | 1.45349 | 1.33973 |
| C | 4.30808 | -0.75339 | 2.18911 |
| C | 5.16614 | 0.30130 | 1.90231 |
| H | 5.28244 | 2.29328 | 1.12244 |
| H | 4.70735 | -1.65198 | 2.64931 |
| C | -1.86837 | -2.11232 | -1.09789 |
| C | -2.29754 | -2.38617 | 0.22149 |
| C | -2.12469 | -3.04971 | -2.12549 |
| C | -2.92282 | -3.59647 | 0.48762 |
| C | -2.75400 | -4.24072 | -1.78518 |
| C | -3.14768 | -4.54781 | -0.49285 |
| H | -3.25207 | -3.79066 | 1.50358 |
| H | -2.94902 | -4.95572 | -2.57780 |
| Cl | -2.44873 | 0.88047 | -1.15752 |
| C | 2.74512 | 2.84023 | 0.46062 |
| H | 2.20691 | 2.66302 | -0.47532 |
| H | 2.04366 | 3.33316 | 1.14096 |

| | | | |
|---|----------|----------|----------|
| H | 3.55589 | 3.53864 | 0.25225 |
| C | 2.07080 | -1.85824 | 2.27449 |
| H | 1.18542 | -1.53536 | 2.83024 |
| H | 1.72083 | -2.39317 | 1.38693 |
| H | 2.61544 | -2.56748 | 2.89816 |
| C | 6.63360 | 0.19381 | 2.17871 |
| H | 7.15996 | -0.21658 | 1.31121 |
| H | 7.07088 | 1.17000 | 2.39443 |
| H | 6.83211 | -0.46781 | 3.02334 |
| C | -2.13108 | -1.45965 | 1.38851 |
| H | -2.85821 | -1.70982 | 2.16145 |
| H | -1.13674 | -1.56230 | 1.82942 |
| H | -2.27374 | -0.40969 | 1.13796 |
| C | -1.78949 | -2.88133 | -3.57801 |
| H | -2.16124 | -1.94391 | -3.99037 |
| H | -0.71134 | -2.90490 | -3.74300 |
| H | -2.23589 | -3.70026 | -4.14275 |
| C | -3.78685 | -5.86092 | -0.17022 |
| H | -4.38399 | -6.22958 | -1.00602 |
| H | -3.02179 | -6.61438 | 0.04185 |
| H | -4.42835 | -5.78765 | 0.70932 |
| S | -0.14613 | -0.22407 | -3.16834 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.85435 | 1.09617 | 0.13034 |
| C | -0.25346 | -0.42114 | 0.29683 |
| P | 1.34047 | -1.13304 | 0.30009 |
| Cl | -2.44120 | -2.37799 | -2.20365 |
| C | 3.01605 | -0.43359 | 0.05643 |
| C | 3.61940 | -0.68525 | -1.21380 |
| C | 3.85915 | -0.13760 | 1.16267 |
| C | 4.96192 | -1.02913 | -1.22342 |
| C | 5.19793 | -0.50640 | 1.06098 |
| C | 5.75450 | -1.05042 | -0.08352 |
| H | 5.41394 | -1.27377 | -2.17615 |
| H | 5.83122 | -0.33978 | 1.92060 |
| C | -2.66874 | 0.92863 | 0.19602 |
| C | -3.44349 | 0.96562 | -0.99213 |
| C | -3.25622 | 0.49123 | 1.41177 |
| C | -4.68589 | 0.33897 | -0.96654 |
| C | -4.48559 | -0.15381 | 1.33578 |
| C | -5.19598 | -0.29654 | 0.15342 |
| H | -5.26313 | 0.31437 | -1.87527 |
| H | -4.91577 | -0.54593 | 2.24788 |
| C | -3.04195 | 1.72231 | -2.27237 |
| C | -2.71502 | 0.75298 | 2.83469 |
| C | -6.49766 | -1.09042 | 0.13203 |
| C | 3.52711 | 0.73745 | 2.39232 |
| C | 3.00313 | -0.41254 | -2.60351 |
| C | 7.18891 | -1.55776 | -0.15191 |
| C | -3.87645 | 1.24593 | 3.71785 |
| H | -3.48350 | 1.53258 | 4.69626 |
| H | -4.36348 | 2.11934 | 3.27831 |
| H | -4.63688 | 0.48424 | 3.89007 |
| C | -1.66287 | 1.85821 | 2.90142 |
| H | -0.69522 | 1.56007 | 2.49506 |
| H | -1.99141 | 2.76642 | 2.39067 |
| H | -1.47729 | 2.11436 | 3.94790 |
| C | -2.14596 | -0.52592 | 3.45500 |
| H | -2.88637 | -1.32989 | 3.45337 |
| H | -1.26066 | -0.86883 | 2.91650 |
| H | -1.85433 | -0.34308 | 4.49325 |
| C | -7.50363 | -0.46555 | 1.10544 |
| H | -8.43783 | -1.03362 | 1.09462 |
| H | -7.13072 | -0.46046 | 2.13175 |
| H | -7.73015 | 0.56609 | 0.82524 |

| | | | |
|----|----------|----------|----------|
| C | -7.13025 | -1.12815 | -1.25652 |
| H | -8.04237 | -1.72872 | -1.22336 |
| H | -7.40761 | -0.13025 | -1.60570 |
| H | -6.46166 | -1.57998 | -1.99306 |
| C | -6.19918 | -2.53243 | 0.56118 |
| H | -5.49096 | -3.00235 | -0.12590 |
| H | -5.77770 | -2.57561 | 1.56812 |
| H | -7.11901 | -3.12367 | 0.55933 |
| C | -4.10308 | 1.59878 | -3.37004 |
| H | -5.07326 | 1.99256 | -3.05857 |
| H | -3.77676 | 2.18624 | -4.23082 |
| H | -4.22892 | 0.56620 | -3.70426 |
| C | -2.93037 | 3.21378 | -1.92790 |
| H | -3.88175 | 3.59563 | -1.54890 |
| H | -2.16591 | 3.40958 | -1.17265 |
| H | -2.66332 | 3.78535 | -2.82064 |
| C | -1.73654 | 1.21940 | -2.89157 |
| H | -0.85955 | 1.44627 | -2.28317 |
| H | -1.76768 | 0.14261 | -3.06343 |
| H | -1.57435 | 1.72491 | -3.84775 |
| C | 2.10373 | 1.27544 | 2.45276 |
| H | 1.81902 | 1.73739 | 1.50435 |
| H | 1.36549 | 0.52506 | 2.72279 |
| H | 2.05630 | 2.06039 | 3.21137 |
| C | 4.42026 | 1.98917 | 2.24035 |
| H | 4.22560 | 2.66992 | 3.07323 |
| H | 5.48290 | 1.74551 | 2.24531 |
| H | 4.19463 | 2.52059 | 1.31301 |
| C | 3.87109 | 0.05783 | 3.72095 |
| H | 4.92204 | -0.23131 | 3.77635 |
| H | 3.68159 | 0.75493 | 4.54148 |
| H | 3.26646 | -0.83328 | 3.88791 |
| C | 1.57785 | 0.12427 | -2.58942 |
| H | 1.33207 | 0.48799 | -3.59005 |
| H | 0.83402 | -0.62923 | -2.33793 |
| H | 1.48313 | 0.97432 | -1.90789 |
| C | 3.07538 | -1.62572 | -3.53382 |
| H | 2.45878 | -2.44496 | -3.16451 |
| H | 2.70904 | -1.34396 | -4.52450 |
| H | 4.09676 | -1.99228 | -3.65393 |
| C | 3.85978 | 0.72236 | -3.20612 |
| H | 3.83130 | 1.61292 | -2.57377 |
| H | 4.90280 | 0.43365 | -3.33946 |
| H | 3.45723 | 0.99067 | -4.18639 |
| C | 7.88222 | -1.51710 | 1.20722 |
| H | 7.98862 | -0.49597 | 1.58212 |
| H | 7.34335 | -2.10513 | 1.95436 |
| H | 8.88676 | -1.93670 | 1.11591 |
| C | 7.99511 | -0.69774 | -1.13265 |
| H | 7.58035 | -0.73398 | -2.14186 |
| H | 8.01406 | 0.34728 | -0.81410 |
| H | 9.02657 | -1.05692 | -1.18415 |
| C | 7.17375 | -3.01040 | -0.64322 |
| H | 6.61404 | -3.65006 | 0.04332 |
| H | 6.71589 | -3.09876 | -1.63039 |
| H | 8.19545 | -3.39381 | -0.71127 |
| Au | 0.26999 | 3.00142 | -0.16467 |
| Cl | 1.46591 | 4.91220 | -0.44327 |
| Pb | -1.47817 | -2.52928 | 0.12185 |
| Cl | 1.43782 | -1.89617 | 2.22690 |
| S | 1.13025 | -2.79236 | -0.79429 |

Coordination through $\pi(\text{C}=\text{P})$ bond

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.68291 | -0.00181 | 1.00197 |
| C | 0.38199 | 0.08014 | -0.69485 |
| P | -1.15377 | -0.21235 | -1.47027 |
| Pb | 1.62312 | -0.01380 | -2.81056 |
| Cl | 1.31045 | -2.49667 | -2.91934 |
| Au | 0.58793 | 2.12408 | -0.07253 |
| Cl | 0.77210 | 4.36437 | -0.04834 |
| Cl | -2.80326 | 0.32238 | -0.42245 |
| H | -1.31787 | -1.60651 | -1.50512 |
| H | 2.10928 | -0.07681 | 0.94500 |
| S | -1.07734 | 0.60017 | -3.27187 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.72839 | 0.17031 | 0.91650 |
| C | 0.31221 | 0.19277 | -0.75316 |
| P | -1.27341 | -0.17989 | -1.39377 |
| Pb | 1.46080 | 0.07964 | -2.91359 |
| Cl | 1.58162 | -2.43801 | -2.86772 |
| C | -1.60582 | -1.92838 | -1.16042 |
| H | -1.65916 | -2.15044 | -0.09340 |
| H | -2.55388 | -2.16745 | -1.64361 |
| H | -0.79273 | -2.48708 | -1.63126 |
| C | 2.55034 | -0.04895 | 0.93321 |
| H | 3.04123 | 0.24725 | 0.00642 |
| H | 2.97204 | 0.51136 | 1.77019 |
| H | 2.74033 | -1.11248 | 1.11273 |
| Au | 0.52099 | 2.26660 | -0.22162 |
| Cl | 0.69933 | 4.51084 | -0.22673 |
| Cl | -2.81241 | 0.70280 | -0.38923 |
| S | -1.26790 | 0.36371 | -3.30755 |

R = *t*-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.59335 | 0.26567 | 0.76539 |
| C | 0.32975 | 0.25049 | -0.93696 |
| P | -1.21763 | -0.18855 | -1.65747 |
| Pb | 1.58159 | 0.59207 | -3.03604 |
| Cl | 2.48283 | -1.74360 | -3.33601 |
| Au | 0.34963 | 2.35272 | -0.38402 |
| Cl | 0.41590 | 4.60479 | -0.33370 |
| C | 2.43077 | 0.15202 | 1.10638 |
| C | 2.61619 | -1.30253 | 1.55793 |
| C | 3.36456 | 0.45915 | -0.04914 |
| C | 2.69407 | 1.09519 | 2.28105 |
| H | 1.94804 | -1.56403 | 2.38352 |
| H | 2.44678 | -2.00432 | 0.73728 |
| H | 3.64360 | -1.44097 | 1.90917 |
| H | 3.21958 | 1.47501 | -0.42808 |
| H | 4.40315 | 0.38737 | 0.29079 |
| H | 3.24993 | -0.26285 | -0.86225 |
| H | 3.71241 | 0.94262 | 2.65152 |
| H | 2.59485 | 2.14257 | 1.98596 |
| H | 2.00654 | 0.91127 | 3.11148 |
| C | -1.68245 | -1.96525 | -1.37382 |
| C | -2.96503 | -2.23883 | -2.15916 |
| C | -0.55102 | -2.84081 | -1.90715 |
| C | -1.90539 | -2.23360 | 0.11121 |
| H | -3.80586 | -1.64884 | -1.79123 |
| H | -2.83558 | -2.04008 | -3.22420 |
| H | -3.21608 | -3.29644 | -2.04034 |
| H | 0.38747 | -2.68022 | -1.37530 |
| H | -0.84056 | -3.88745 | -1.77622 |
| H | -0.36384 | -2.67094 | -2.96771 |
| H | -2.17108 | -3.28804 | 0.22854 |

| | | | |
|----|----------|----------|----------|
| H | -1.00739 | -2.05292 | 0.70511 |
| H | -2.71699 | -1.63312 | 0.52305 |
| Cl | -2.77910 | 0.82415 | -0.79802 |
| S | -1.11855 | 0.27661 | -3.59372 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.67974 | 0.42885 | 0.85725 |
| C | 0.16174 | 0.32061 | -0.78075 |
| P | -1.45829 | -0.05346 | -1.32302 |
| Pb | 1.20718 | 0.31255 | -2.99948 |
| Cl | 1.42857 | -2.18769 | -3.24568 |
| Au | 0.41411 | 2.44123 | -0.41553 |
| Cl | 0.59061 | 4.67882 | -0.61870 |
| C | -1.80584 | -1.79452 | -1.02598 |
| C | -1.94148 | -2.66983 | -2.09634 |
| C | -1.91138 | -2.26077 | 0.28444 |
| C | -2.18823 | -4.01316 | -1.85474 |
| H | -1.84530 | -2.30091 | -3.10965 |
| C | -2.15492 | -3.60191 | 0.51597 |
| H | -1.81328 | -1.57756 | 1.12103 |
| C | -2.29405 | -4.47792 | -0.55421 |
| H | -2.29068 | -4.69635 | -2.68928 |
| H | -2.23938 | -3.96563 | 1.53323 |
| H | -2.48481 | -5.52884 | -0.36902 |
| C | 2.47812 | 0.19085 | 0.77641 |
| C | 3.07506 | -0.72906 | -0.08774 |
| C | 3.26990 | 0.88851 | 1.69107 |
| C | 4.44813 | -0.91907 | -0.05708 |
| H | 2.46740 | -1.32321 | -0.76331 |
| C | 4.64251 | 0.70722 | 1.70529 |
| H | 2.81012 | 1.58817 | 2.38204 |
| C | 5.23252 | -0.19532 | 0.83020 |
| H | 4.90315 | -1.64019 | -0.72640 |
| H | 5.25358 | 1.26762 | 2.40327 |
| H | 6.30625 | -0.34302 | 0.84845 |
| Cl | -2.89889 | 0.89313 | -0.22723 |
| S | -1.56959 | 0.47596 | -3.23452 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.73478 | 0.44223 | 1.27528 |
| C | 0.10278 | 0.27250 | -0.32355 |
| P | -1.46203 | -0.03796 | -1.04649 |
| Pb | 1.38638 | 0.52021 | -2.40369 |
| Cl | 1.41419 | -1.88380 | -3.18538 |
| Au | 0.16511 | 2.41453 | 0.05321 |
| Cl | 0.11038 | 4.67403 | -0.06334 |
| C | -1.84608 | -1.81272 | -1.06012 |
| C | -2.13623 | -2.52645 | -2.24906 |
| C | -1.85078 | -2.49359 | 0.17833 |
| C | -2.34017 | -3.89674 | -2.15782 |
| C | -2.06551 | -3.86638 | 0.19335 |
| C | -2.28911 | -4.59480 | -0.96088 |
| H | -2.55901 | -4.43803 | -3.07247 |
| H | -2.06934 | -4.37392 | 1.15325 |
| C | 2.53974 | 0.27092 | 1.00953 |
| C | 3.05043 | -0.97361 | 0.58365 |
| C | 3.42110 | 1.30666 | 1.36286 |
| C | 4.42106 | -1.10402 | 0.40411 |
| C | 4.78529 | 1.12152 | 1.16611 |
| C | 5.30476 | -0.06217 | 0.66255 |
| H | 4.81137 | -2.06215 | 0.07435 |
| H | 5.46181 | 1.92959 | 1.42854 |
| Cl | -3.07093 | 0.79632 | -0.06032 |
| C | 2.95177 | 2.60256 | 1.95356 |
| H | 2.65160 | 3.32149 | 1.18531 |
| H | 2.09061 | 2.46674 | 2.61308 |

| | | | |
|---|----------|----------|----------|
| H | 3.75066 | 3.06172 | 2.53803 |
| C | 2.18273 | -2.18702 | 0.40876 |
| H | 1.57453 | -2.36281 | 1.30153 |
| H | 1.50650 | -2.11463 | -0.44456 |
| H | 2.80189 | -3.07105 | 0.25493 |
| C | 6.77335 | -0.22252 | 0.42005 |
| H | 7.10487 | -1.23916 | 0.63984 |
| H | 7.01496 | -0.02228 | -0.62855 |
| H | 7.35635 | 0.47002 | 1.02910 |
| C | -1.65544 | -1.85777 | 1.52364 |
| H | -0.61807 | -1.95363 | 1.85601 |
| H | -1.91712 | -0.80427 | 1.56479 |
| H | -2.27367 | -2.37515 | 2.25937 |
| C | -2.47710 | -6.07817 | -0.92489 |
| H | -3.25123 | -6.39762 | -1.62534 |
| H | -1.55134 | -6.58678 | -1.21112 |
| H | -2.74958 | -6.42305 | 0.07350 |
| C | -2.27362 | -1.93611 | -3.62108 |
| H | -2.96875 | -1.09755 | -3.64649 |
| H | -1.31485 | -1.58209 | -4.00113 |
| H | -2.64291 | -2.70394 | -4.30157 |
| S | -1.33097 | 0.95629 | -2.77610 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.64543 | 0.20898 | 1.14854 |
| C | 0.38950 | 0.06861 | -0.56152 |
| P | -1.08713 | -0.09066 | -1.56075 |
| Pb | 2.10879 | 0.52683 | -2.32226 |
| Cl | 3.01678 | -1.58429 | -3.42441 |
| Au | 0.49275 | 2.23234 | -0.17299 |
| Cl | 0.52481 | 4.48832 | -0.42055 |
| C | 2.49029 | 0.06022 | 1.26052 |
| C | 3.14547 | -1.10295 | 0.76509 |
| C | 3.28369 | 1.16775 | 1.64493 |
| C | 4.45146 | -0.97577 | 0.31411 |
| C | 4.59748 | 1.21888 | 1.16932 |
| C | 5.17774 | 0.20713 | 0.42579 |
| H | 4.93337 | -1.84525 | -0.11282 |
| H | 5.18473 | 2.09481 | 1.40512 |
| C | 2.92770 | 2.25125 | 2.68506 |
| C | 2.63549 | -2.54246 | 0.97173 |
| C | 6.57074 | 0.31390 | -0.18435 |
| C | 3.86145 | 1.98218 | 3.88291 |
| H | 3.69064 | 0.98515 | 4.29718 |
| H | 4.91396 | 2.05511 | 3.60606 |
| H | 3.66654 | 2.71696 | 4.66880 |
| C | 3.19178 | 3.66850 | 2.16809 |
| H | 2.56153 | 3.91233 | 1.31194 |
| H | 2.96976 | 4.38952 | 2.95954 |
| H | 4.23339 | 3.81694 | 1.87897 |
| C | 1.50971 | 2.20383 | 3.24561 |
| H | 1.44574 | 2.89867 | 4.08735 |
| H | 0.75427 | 2.52064 | 2.52424 |
| H | 1.24491 | 1.21244 | 3.62101 |
| C | 2.96769 | -3.46760 | -0.20154 |
| H | 2.59026 | -3.07927 | -1.14668 |
| H | 4.04159 | -3.62415 | -0.31351 |
| H | 2.52192 | -4.45005 | -0.02471 |
| C | 3.38954 | -3.04797 | 2.21778 |
| H | 4.46989 | -3.01910 | 2.06580 |
| H | 3.15544 | -2.43881 | 3.09466 |
| H | 3.10020 | -4.08137 | 2.43050 |
| C | 1.15029 | -2.68162 | 1.28118 |
| H | 0.84128 | -2.06198 | 2.13122 |
| H | 0.52189 | -2.44707 | 0.42427 |
| H | 0.94442 | -3.71719 | 1.56611 |

| | | | |
|----|----------|----------|----------|
| C | 7.23356 | 1.65515 | 0.11742 |
| H | 6.64555 | 2.49405 | -0.26302 |
| H | 7.39046 | 1.80169 | 1.18937 |
| H | 8.21270 | 1.69348 | -0.36572 |
| C | 6.45053 | 0.16336 | -1.70581 |
| H | 7.44185 | 0.19170 | -2.16673 |
| H | 5.97081 | -0.77572 | -1.98855 |
| H | 5.85990 | 0.97880 | -2.13203 |
| C | 7.47059 | -0.79923 | 0.36544 |
| H | 7.55654 | -0.73305 | 1.45298 |
| H | 7.09270 | -1.79228 | 0.11556 |
| H | 8.47362 | -0.71210 | -0.06084 |
| C | -2.32677 | -1.47324 | -1.65299 |
| C | -2.30182 | -2.30477 | -2.81448 |
| C | -3.55965 | -1.35816 | -0.95273 |
| C | -3.50896 | -2.55935 | -3.44595 |
| C | -1.10676 | -3.14636 | -3.30165 |
| C | -4.72790 | -1.68009 | -1.63691 |
| C | -3.73969 | -1.11224 | 0.55771 |
| C | -4.73843 | -2.16866 | -2.93264 |
| H | -3.48197 | -3.12249 | -4.37056 |
| C | -0.65923 | -2.83335 | -4.73059 |
| C | -1.58266 | -4.61554 | -3.27294 |
| C | 0.06770 | -3.09300 | -2.34017 |
| H | -5.66737 | -1.53893 | -1.12152 |
| C | -2.45442 | -0.80483 | 1.30693 |
| C | -4.24676 | -2.45892 | 1.11605 |
| C | -4.77584 | -0.03405 | 0.88586 |
| C | -6.01471 | -2.37910 | -3.73557 |
| H | 0.06418 | -3.58518 | -5.05605 |
| H | -1.50288 | -2.85684 | -5.42466 |
| H | -0.18328 | -1.85822 | -4.80076 |
| H | -2.34004 | -4.82837 | -4.02806 |
| H | -0.72594 | -5.26483 | -3.47209 |
| H | -1.99214 | -4.88135 | -2.29534 |
| H | 0.50875 | -2.10311 | -2.25316 |
| H | -0.23528 | -3.43970 | -1.34955 |
| H | 0.86481 | -3.74512 | -2.70052 |
| H | -1.67266 | -1.53065 | 1.07281 |
| H | -2.08299 | 0.19856 | 1.11024 |
| H | -2.63843 | -0.86247 | 2.38257 |
| H | -4.37167 | -2.37652 | 2.19932 |
| H | -5.20582 | -2.74787 | 0.68455 |
| H | -3.53100 | -3.25984 | 0.91493 |
| H | -5.75746 | -0.25891 | 0.46593 |
| H | -4.89431 | 0.03219 | 1.97065 |
| H | -4.46582 | 0.94455 | 0.52049 |
| C | -7.25102 | -1.87062 | -2.99900 |
| C | -6.20471 | -3.87245 | -4.02752 |
| C | -5.89069 | -1.61450 | -5.05915 |
| H | -7.43430 | -2.42585 | -2.07546 |
| H | -7.16730 | -0.80917 | -2.75309 |
| H | -8.13082 | -1.99603 | -3.63442 |
| H | -5.37574 | -4.28255 | -4.60752 |
| H | -6.28401 | -4.44635 | -3.10095 |
| H | -7.12152 | -4.02700 | -4.60296 |
| H | -5.76560 | -0.54367 | -4.88241 |
| H | -5.03607 | -1.95817 | -5.64521 |
| H | -6.79174 | -1.75866 | -5.66153 |
| Cl | -2.40696 | 1.45609 | -1.14480 |
| S | -0.43732 | 0.35482 | -3.39961 |

[R-P=C(Pb(II)Cl)-P(S)MeR](AuCl)

Coordination through Pb(II) atom

R = H

| | | | |
|----|----------|----------|----------|
| P | 0.85630 | 0.64014 | 0.55373 |
| C | 0.41450 | 0.12878 | -0.96024 |
| P | -1.25216 | -0.11359 | -1.49080 |
| Pb | 1.41507 | -0.00147 | -3.02438 |
| Cl | 1.22481 | -2.44876 | -3.17166 |
| C | -2.51333 | 0.65878 | -0.46736 |
| H | -3.49858 | 0.41644 | -0.86924 |
| H | -2.43284 | 0.28585 | 0.55623 |
| H | -2.36974 | 1.73957 | -0.48133 |
| Au | 3.18987 | 1.39802 | -4.29998 |
| Cl | 4.74142 | 2.66690 | -5.33465 |
| H | 2.26486 | 0.75223 | 0.33830 |
| H | -1.51415 | -1.49433 | -1.38813 |
| S | -1.25679 | 0.50006 | -3.39456 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.82398 | 0.29423 | 0.65593 |
| C | 0.37355 | -0.05441 | -0.89769 |
| P | -1.30842 | -0.20109 | -1.42025 |
| Pb | 1.37009 | -0.06773 | -2.96373 |
| Cl | 1.32766 | -2.52303 | -3.25852 |
| C | -2.46132 | 0.78291 | -0.44498 |
| H | -3.47117 | 0.64698 | -0.83637 |
| H | -2.42692 | 0.46592 | 0.59960 |
| H | -2.18284 | 1.83394 | -0.51915 |
| C | -1.83390 | -1.91595 | -1.26354 |
| H | -1.85136 | -2.20288 | -0.20993 |
| H | -2.82744 | -2.02962 | -1.70120 |
| H | -1.12203 | -2.54049 | -1.80643 |
| C | 2.65332 | 0.39187 | 0.63281 |
| H | 3.09165 | 0.25387 | -0.35590 |
| H | 2.95857 | 1.36189 | 1.03469 |
| H | 3.04470 | -0.37228 | 1.31084 |
| Au | 3.15936 | 1.39051 | -4.15192 |
| Cl | 4.74431 | 2.70589 | -5.07883 |
| S | -1.26494 | 0.39221 | -3.34572 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.75755 | -0.07018 | 0.61755 |
| C | 0.47016 | -0.12045 | -1.01401 |
| P | -1.18969 | -0.32041 | -1.63050 |
| Pb | 1.55925 | 0.32601 | -2.99226 |
| Cl | 2.32487 | -1.96300 | -3.52234 |
| C | -2.31647 | 0.81973 | -0.79378 |
| H | -3.32312 | 0.72068 | -1.20142 |
| H | -2.32406 | 0.62592 | 0.27981 |
| H | -1.95766 | 1.83273 | -0.97664 |
| Au | 2.85480 | 2.38157 | -3.91731 |
| Cl | 3.97177 | 4.22151 | -4.61149 |
| C | 2.58356 | 0.13647 | 0.96060 |
| C | 2.96474 | -1.11185 | 1.76495 |
| C | 3.48401 | 0.27499 | -0.25089 |
| C | 2.69163 | 1.37429 | 1.85603 |
| H | 2.31407 | -1.25325 | 2.63247 |
| H | 2.92036 | -2.01528 | 1.15193 |
| H | 3.99009 | -1.00462 | 2.13300 |
| H | 3.27446 | 1.19008 | -0.81210 |
| H | 4.52810 | 0.34274 | 0.07212 |
| H | 3.41350 | -0.59118 | -0.91527 |
| H | 3.71973 | 1.47261 | 2.21842 |

| | | | |
|---|----------|----------|----------|
| H | 2.43922 | 2.28875 | 1.31372 |
| H | 2.03671 | 1.30324 | 2.72886 |
| C | -1.85373 | -2.03683 | -1.39139 |
| C | -3.17194 | -2.14387 | -2.15866 |
| C | -0.84280 | -3.03034 | -1.95705 |
| C | -2.08482 | -2.30304 | 0.09421 |
| H | -3.93932 | -1.47265 | -1.76629 |
| H | -3.03679 | -1.93752 | -3.22182 |
| H | -3.54892 | -3.16558 | -2.05882 |
| H | 0.10842 | -2.99574 | -1.42398 |
| H | -1.25273 | -4.03946 | -1.85805 |
| H | -0.63991 | -2.84765 | -3.01327 |
| H | -2.41197 | -3.33978 | 0.21365 |
| H | -1.17428 | -2.17516 | 0.68382 |
| H | -2.86312 | -1.66331 | 0.51518 |
| S | -1.05935 | 0.14664 | -3.59158 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.78295 | 0.37194 | 0.66198 |
| C | 0.36338 | -0.10789 | -0.86942 |
| P | -1.29088 | -0.25723 | -1.46729 |
| Pb | 1.50582 | -0.18791 | -2.84371 |
| Cl | 1.63196 | -2.64640 | -3.07044 |
| C | -2.43283 | 0.87465 | -0.64746 |
| H | -3.42673 | 0.74789 | -1.07930 |
| H | -2.47080 | 0.66203 | 0.42256 |
| H | -2.08808 | 1.89637 | -0.80785 |
| Au | 3.24565 | 1.31116 | -4.05768 |
| Cl | 4.77889 | 2.64940 | -5.04265 |
| C | 2.59166 | 0.32850 | 0.66344 |
| C | 3.25891 | 1.31300 | 1.39479 |
| C | 3.33511 | -0.65001 | -0.00383 |
| C | 4.64382 | 1.35417 | 1.41048 |
| H | 2.68960 | 2.06038 | 1.93862 |
| C | 4.71936 | -0.61286 | 0.02674 |
| H | 2.83122 | -1.46460 | -0.51609 |
| C | 5.37363 | 0.39481 | 0.72334 |
| H | 5.15491 | 2.13565 | 1.96054 |
| H | 5.28889 | -1.37502 | -0.49211 |
| H | 6.45685 | 0.42574 | 0.73796 |
| C | -1.91443 | -1.92026 | -1.13730 |
| C | -2.22989 | -2.77976 | -2.18220 |
| C | -2.07166 | -2.33840 | 0.18393 |
| C | -2.71579 | -4.04933 | -1.90603 |
| H | -2.08366 | -2.45482 | -3.20552 |
| C | -2.55736 | -3.60573 | 0.45270 |
| H | -1.80044 | -1.68452 | 1.00673 |
| C | -2.88157 | -4.46069 | -0.59328 |
| H | -2.95703 | -4.71984 | -2.72227 |
| H | -2.67699 | -3.93061 | 1.47961 |
| H | -3.25730 | -5.45494 | -0.38057 |
| S | -1.14224 | 0.14004 | -3.43133 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.89492 | 0.16027 | 1.20728 |
| C | 0.35937 | -0.22148 | -0.31837 |
| P | -1.28093 | -0.22234 | -1.00744 |
| Pb | 1.64663 | 0.00471 | -2.17315 |
| Cl | 1.57089 | -2.35466 | -2.94182 |
| Au | 3.66022 | 1.46351 | -2.93399 |
| Cl | 5.48054 | 2.72452 | -3.42904 |
| C | 2.69819 | 0.24810 | 0.93277 |
| C | 3.30356 | 1.51503 | 0.87467 |
| C | 3.46432 | -0.91682 | 0.77021 |
| C | 4.65825 | 1.59596 | 0.59092 |
| C | 4.82130 | -0.78196 | 0.49227 |

| | | | |
|---|----------|----------|----------|
| C | 5.43295 | 0.45963 | 0.37829 |
| H | 5.12024 | 2.57502 | 0.51003 |
| H | 5.41694 | -1.67990 | 0.35816 |
| C | -1.97714 | -1.91097 | -1.07005 |
| C | -2.28620 | -2.58776 | -2.27474 |
| C | -2.19499 | -2.56765 | 0.16271 |
| C | -2.76770 | -3.88932 | -2.19678 |
| C | -2.66687 | -3.87438 | 0.16643 |
| C | -2.95356 | -4.56146 | -0.99946 |
| H | -3.00096 | -4.39913 | -3.12590 |
| H | -2.81670 | -4.36406 | 1.12385 |
| C | 2.50386 | 2.77140 | 1.05798 |
| H | 1.81698 | 2.69744 | 1.90698 |
| H | 3.15917 | 3.62613 | 1.22807 |
| H | 1.90028 | 2.99346 | 0.17197 |
| C | 2.86614 | -2.28891 | 0.89072 |
| H | 2.15904 | -2.34895 | 1.72301 |
| H | 2.32375 | -2.57995 | -0.01383 |
| H | 3.64785 | -3.03081 | 1.05868 |
| C | 6.87799 | 0.58818 | 0.01395 |
| H | 6.97563 | 1.04326 | -0.97649 |
| H | 7.40806 | 1.23222 | 0.71992 |
| H | 7.37404 | -0.38287 | -0.00525 |
| C | -2.00228 | -1.95185 | 1.51953 |
| H | -1.20611 | -1.21208 | 1.57090 |
| H | -2.92632 | -1.47487 | 1.86102 |
| H | -1.76088 | -2.72904 | 2.24575 |
| C | -2.15105 | -2.03015 | -3.66172 |
| H | -2.68604 | -1.08992 | -3.79041 |
| H | -1.10751 | -1.84927 | -3.92088 |
| H | -2.55469 | -2.74981 | -4.37445 |
| C | -3.42694 | -5.98026 | -0.97448 |
| H | -2.59281 | -6.66456 | -1.15760 |
| H | -3.86158 | -6.24026 | -0.00824 |
| H | -4.17255 | -6.16381 | -1.75043 |
| C | -2.45438 | 0.82093 | -0.10600 |
| H | -3.38942 | 0.83936 | -0.66911 |
| H | -2.64359 | 0.45981 | 0.90225 |
| H | -2.03732 | 1.82763 | -0.06941 |
| S | -0.91536 | 0.73058 | -2.75153 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.12632 | 2.18114 | 1.03975 |
| C | 0.48116 | 0.67365 | 0.43478 |
| P | 2.00861 | -0.24587 | 0.34537 |
| Cl | -1.21391 | 0.41206 | -2.85851 |
| C | 3.74489 | 0.35811 | 0.20227 |
| C | 4.34999 | 0.34275 | -1.08844 |
| C | 4.59838 | 0.29962 | 1.33757 |
| C | 5.64597 | -0.14284 | -1.18518 |
| C | 5.88964 | -0.18818 | 1.15625 |
| C | 6.40612 | -0.51960 | -0.08592 |
| H | 6.08504 | -0.21507 | -2.17240 |
| H | 6.51890 | -0.29258 | 2.02939 |
| C | -1.70272 | 2.24537 | 0.84193 |
| C | -2.25917 | 3.02678 | -0.19793 |
| C | -2.54865 | 1.42772 | 1.63727 |
| C | -3.56682 | 2.75068 | -0.58879 |
| C | -3.83830 | 1.19437 | 1.17272 |
| C | -4.35187 | 1.78873 | 0.02706 |
| H | -3.98385 | 3.30080 | -1.41656 |
| H | -4.47958 | 0.53273 | 1.73813 |
| C | -1.53250 | 4.22538 | -0.83918 |
| C | -2.19067 | 0.89903 | 3.04643 |
| C | -5.74963 | 1.42468 | -0.46253 |
| C | 4.32164 | 0.92233 | 2.72379 |

| | | | |
|---|----------|----------|----------|
| C | 3.79270 | 1.00913 | -2.36239 |
| C | 7.77276 | -1.16463 | -0.27594 |
| C | -3.45481 | 0.83613 | 3.91885 |
| H | -3.16176 | 0.62815 | 4.95069 |
| H | -4.00379 | 1.78033 | 3.90432 |
| H | -4.13281 | 0.03653 | 3.61728 |
| C | -1.23531 | 1.84996 | 3.77033 |
| H | -0.23774 | 1.88960 | 3.31819 |
| H | -1.62889 | 2.86871 | 3.79730 |
| H | -1.08947 | 1.51012 | 4.79922 |
| C | -1.58965 | -0.50845 | 3.02530 |
| H | -2.25212 | -1.21455 | 2.51810 |
| H | -0.62233 | -0.52056 | 2.52415 |
| H | -1.44411 | -0.86581 | 4.04911 |
| C | -6.77835 | 1.74218 | 0.62941 |
| H | -7.78254 | 1.48336 | 0.28287 |
| H | -6.58916 | 1.17708 | 1.54417 |
| H | -6.76854 | 2.80595 | 0.88085 |
| C | -6.13782 | 2.19166 | -1.72395 |
| H | -7.13134 | 1.87401 | -2.04886 |
| H | -6.17839 | 3.27067 | -1.55216 |
| H | -5.44378 | 1.99705 | -2.54525 |
| C | -5.79073 | -0.07476 | -0.77982 |
| H | -5.07648 | -0.32752 | -1.56714 |
| H | -5.55524 | -0.68813 | 0.09201 |
| H | -6.78888 | -0.35837 | -1.12454 |
| C | -2.43249 | 4.97980 | -1.82093 |
| H | -3.35042 | 5.33826 | -1.34957 |
| H | -1.88994 | 5.85295 | -2.19039 |
| H | -2.69803 | 4.36925 | -2.68702 |
| C | -1.15507 | 5.21524 | 0.27267 |
| H | -2.04238 | 5.54317 | 0.81973 |
| H | -0.45651 | 4.78190 | 0.99191 |
| H | -0.67620 | 6.09747 | -0.16156 |
| C | -0.27825 | 3.82635 | -1.61729 |
| H | 0.51624 | 3.45853 | -0.96318 |
| H | -0.49140 | 3.04775 | -2.35075 |
| H | 0.12526 | 4.70168 | -2.13504 |
| C | 2.99441 | 1.66409 | 2.82852 |
| H | 2.88712 | 2.39490 | 2.02481 |
| H | 2.11484 | 1.02446 | 2.81846 |
| H | 2.96421 | 2.21222 | 3.77347 |
| C | 5.39609 | 2.01700 | 2.90480 |
| H | 5.21787 | 2.54455 | 3.84576 |
| H | 6.40605 | 1.60841 | 2.93625 |
| H | 5.35079 | 2.74546 | 2.09210 |
| C | 4.47457 | -0.07267 | 3.87818 |
| H | 5.46451 | -0.53256 | 3.88252 |
| H | 4.35196 | 0.44946 | 4.83077 |
| H | 3.74041 | -0.87735 | 3.84279 |
| C | 2.44831 | 1.69768 | -2.17444 |
| H | 2.24091 | 2.31727 | -3.05009 |
| H | 1.61603 | 1.00290 | -2.08581 |
| H | 2.46422 | 2.35632 | -1.30303 |
| C | 3.72361 | 0.06025 | -3.56089 |
| H | 2.99931 | -0.73576 | -3.39454 |
| H | 3.41632 | 0.62005 | -4.44807 |
| H | 4.69238 | -0.39470 | -3.77835 |
| C | 4.79290 | 2.13764 | -2.69452 |
| H | 4.88392 | 2.83963 | -1.86172 |
| H | 5.78891 | 1.75963 | -2.92792 |
| H | 4.43039 | 2.68926 | -3.56587 |
| C | 8.43810 | -1.51139 | 1.05323 |
| H | 8.65442 | -0.61999 | 1.64773 |
| H | 7.82012 | -2.18504 | 1.65222 |
| H | 9.38892 | -2.01485 | 0.86410 |

| | | | |
|----|----------|----------|----------|
| C | 8.69447 | -0.20933 | -1.04347 |
| H | 8.29947 | 0.03036 | -2.03254 |
| H | 8.82958 | 0.72808 | -0.49836 |
| H | 9.67750 | -0.66782 | -1.18078 |
| C | 7.59795 | -2.45799 | -1.08120 |
| H | 6.95549 | -3.16564 | -0.55178 |
| H | 7.15069 | -2.26807 | -2.05879 |
| H | 8.56898 | -2.93389 | -1.24246 |
| Au | -2.65514 | -2.57591 | -0.08806 |
| Cl | -4.20452 | -4.09478 | 0.57387 |
| Pb | -0.88005 | -0.77692 | -0.71190 |
| S | 1.65340 | -1.54425 | -1.18190 |
| C | 2.01090 | -1.36410 | 1.78058 |
| H | 2.02722 | -0.86378 | 2.74331 |
| H | 1.10282 | -1.96255 | 1.70004 |
| H | 2.87008 | -2.02869 | 1.68299 |

Coordination through S atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.91170 | 0.24836 | 0.96279 |
| C | 0.65282 | -0.10507 | -0.63681 |
| P | -0.85325 | 0.23811 | -1.45726 |
| Pb | 1.98097 | -0.71173 | -2.53358 |
| Cl | 0.64164 | -2.78671 | -2.84352 |
| C | -2.10843 | 1.21380 | -0.61881 |
| H | -2.96774 | 1.32480 | -1.28305 |
| H | -2.41236 | 0.70041 | 0.29633 |
| H | -1.70252 | 2.19601 | -0.37545 |
| Au | -1.94121 | 0.75312 | -4.61362 |
| Cl | -3.70216 | 0.48076 | -5.99315 |
| H | 2.28146 | -0.15982 | 1.06164 |
| H | -1.45647 | -0.99607 | -1.75074 |
| S | -0.19418 | 1.09684 | -3.19094 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.86716 | 0.15174 | 0.96534 |
| C | 0.62387 | -0.11567 | -0.65054 |
| P | -0.94154 | 0.17343 | -1.38162 |
| Pb | 1.99349 | -0.48318 | -2.58417 |
| Cl | 1.20891 | -2.83302 | -2.91958 |
| C | -2.03369 | 1.32392 | -0.52738 |
| H | -2.94151 | 1.45393 | -1.12007 |
| H | -2.28989 | 0.92633 | 0.45710 |
| H | -1.53101 | 2.28430 | -0.41482 |
| C | -1.84323 | -1.37072 | -1.54927 |
| H | -2.08328 | -1.74165 | -0.54979 |
| H | -2.75617 | -1.19688 | -2.12182 |
| H | -1.21070 | -2.09319 | -2.06815 |
| C | 2.62534 | -0.27763 | 1.27765 |
| H | 3.17295 | -0.55983 | 0.37778 |
| H | 3.11944 | 0.57054 | 1.75964 |
| H | 2.65518 | -1.10911 | 1.98815 |
| Au | -2.12659 | 0.49286 | -4.61927 |
| Cl | -3.87534 | 0.10516 | -5.99009 |
| S | -0.39783 | 0.94817 | -3.20640 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.86972 | -0.04154 | 0.81879 |
| C | 0.65893 | -0.14041 | -0.82515 |
| P | -0.97013 | 0.10983 | -1.45422 |
| Pb | 2.07449 | -0.05617 | -2.76175 |
| Cl | 2.14454 | -2.52169 | -3.20152 |
| C | -1.91796 | 1.33441 | -0.52176 |
| H | -2.82109 | 1.59405 | -1.07493 |
| H | -2.18099 | 0.94806 | 0.46448 |

| | | | |
|----|----------|----------|----------|
| H | -1.29588 | 2.22191 | -0.40724 |
| Au | -2.29520 | 0.72144 | -4.74108 |
| Cl | -4.02518 | 0.59389 | -6.18587 |
| S | -0.54683 | 0.91833 | -3.29868 |
| C | -1.99106 | -1.44771 | -1.50063 |
| C | -3.44778 | -1.08387 | -1.78889 |
| C | -1.45989 | -2.38923 | -2.57499 |
| C | -1.89036 | -2.11403 | -0.12739 |
| H | -3.90536 | -0.52090 | -0.97327 |
| H | -3.56123 | -0.51998 | -2.71875 |
| H | -4.01158 | -2.01320 | -1.90571 |
| H | -0.40961 | -2.64422 | -2.42582 |
| H | -2.04142 | -3.31476 | -2.53710 |
| H | -1.57309 | -1.96535 | -3.57417 |
| H | -2.57038 | -2.97039 | -0.11889 |
| H | -0.88355 | -2.48044 | 0.07306 |
| H | -2.18761 | -1.45269 | 0.69049 |
| C | 2.68581 | -0.33573 | 1.19623 |
| C | 3.11860 | -1.70937 | 0.69424 |
| C | 3.54811 | 0.77046 | 0.59740 |
| C | 2.79330 | -0.28572 | 2.72176 |
| H | 2.52169 | -2.50641 | 1.14539 |
| H | 3.02635 | -1.81295 | -0.38890 |
| H | 4.16509 | -1.88768 | 0.96447 |
| H | 3.21960 | 1.76366 | 0.91466 |
| H | 4.58734 | 0.64414 | 0.91924 |
| H | 3.54709 | 0.75494 | -0.49579 |
| H | 3.82889 | -0.46176 | 3.02805 |
| H | 2.48602 | 0.68597 | 3.11779 |
| H | 2.17060 | -1.05014 | 3.19372 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.83316 | 0.50304 | 0.82893 |
| C | 0.57693 | -0.11329 | -0.68961 |
| P | -0.94574 | 0.01085 | -1.54160 |
| Cl | 2.17143 | -0.71269 | -2.34372 |
| Cl | 1.67507 | -3.16357 | -2.34260 |
| C | -2.05531 | 1.31661 | -0.97891 |
| H | -2.94032 | 1.32048 | -1.61773 |
| H | -2.35075 | 1.14664 | 0.05769 |
| H | -1.53753 | 2.27259 | -1.05976 |
| Au | -2.09011 | 0.22911 | -4.83966 |
| Cl | -3.85671 | 0.11325 | -6.24000 |
| C | 2.56049 | 0.04566 | 1.16810 |
| C | 3.11445 | -1.17388 | 0.76337 |
| C | 3.35133 | 0.94378 | 1.88603 |
| C | 4.44333 | -1.46377 | 1.03532 |
| H | 2.48955 | -1.92051 | 0.28024 |
| C | 4.68232 | 0.65577 | 2.14579 |
| H | 2.92404 | 1.88020 | 2.23136 |
| C | 5.23032 | -0.54527 | 1.71711 |
| H | 4.85937 | -2.41576 | 0.72572 |
| H | 5.29290 | 1.36818 | 2.68865 |
| H | 6.26853 | -0.77336 | 1.92912 |
| C | -1.84825 | -1.54154 | -1.38244 |
| C | -2.44203 | -1.82974 | -0.15277 |
| C | -1.93108 | -2.45463 | -2.42620 |
| C | -3.13027 | -3.01735 | 0.01895 |
| H | -2.36067 | -1.13741 | 0.67851 |
| C | -2.62325 | -3.64245 | -2.24697 |
| H | -1.45688 | -2.24132 | -3.37558 |
| C | -3.22401 | -3.92232 | -1.03051 |
| H | -3.59339 | -3.23780 | 0.97353 |
| H | -2.68968 | -4.34899 | -3.06532 |
| H | -3.76528 | -4.85160 | -0.89504 |
| S | -0.30221 | 0.41206 | -3.43624 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.73072 | 0.16466 | 1.24070 |
| C | 0.42645 | -0.22597 | -0.34213 |
| P | -1.06808 | -0.07328 | -1.25701 |
| Pb | 2.25585 | -0.36755 | -1.82292 |
| Cl | 2.02248 | -2.82504 | -2.27702 |
| Au | -1.90540 | 1.49639 | -4.31531 |
| Cl | -3.54567 | 2.31207 | -5.63607 |
| C | 2.55200 | -0.07853 | 1.31280 |
| C | 3.09711 | -1.36678 | 1.45760 |
| C | 3.39480 | 1.04713 | 1.28214 |
| C | 4.48081 | -1.50122 | 1.51734 |
| C | 4.76923 | 0.86071 | 1.34654 |
| C | 5.33310 | -0.40614 | 1.45447 |
| H | 4.90240 | -2.49562 | 1.62951 |
| H | 5.41837 | 1.73111 | 1.31944 |
| C | -1.94960 | -1.67122 | -1.33959 |
| C | -2.56844 | -2.11693 | -0.14902 |
| C | -2.02198 | -2.47964 | -2.49979 |
| C | -3.25170 | -3.32678 | -0.14838 |
| C | -2.73110 | -3.67277 | -2.42953 |
| C | -3.35879 | -4.11840 | -1.27754 |
| H | -3.71159 | -3.65625 | 0.77831 |
| H | -2.78160 | -4.28374 | -3.32481 |
| C | 2.83283 | 2.43432 | 1.17121 |
| H | 2.38777 | 2.61521 | 0.18763 |
| H | 2.04423 | 2.60829 | 1.90974 |
| H | 3.61046 | 3.18298 | 1.32606 |
| C | 2.22891 | -2.58547 | 1.56343 |
| H | 1.38102 | -2.41607 | 2.23331 |
| H | 1.82069 | -2.87370 | 0.59027 |
| H | 2.80118 | -3.43064 | 1.94765 |
| C | 6.81955 | -0.58428 | 1.49308 |
| H | 7.22480 | -0.67241 | 0.48020 |
| H | 7.31063 | 0.26717 | 1.96751 |
| H | 7.09811 | -1.48918 | 2.03535 |
| C | -2.56900 | -1.38055 | 1.16152 |
| H | -1.66565 | -0.80122 | 1.34835 |
| H | -3.42668 | -0.70553 | 1.23326 |
| H | -2.66093 | -2.09635 | 1.97934 |
| C | -1.39172 | -2.17619 | -3.82561 |
| H | -1.80540 | -1.27563 | -4.28184 |
| H | -0.31366 | -2.04304 | -3.74287 |
| H | -1.57279 | -3.00802 | -4.50618 |
| C | -4.12606 | -5.40247 | -1.26381 |
| H | -4.30901 | -5.74808 | -0.24552 |
| H | -5.09701 | -5.27493 | -1.75194 |
| H | -3.59322 | -6.18717 | -1.80476 |
| S | -0.24741 | 0.70956 | -2.95963 |
| C | -2.22797 | 1.18979 | -0.67489 |
| H | -1.71538 | 2.14931 | -0.74723 |
| H | -3.09186 | 1.19745 | -1.34239 |
| H | -2.54959 | 1.01928 | 0.34913 |

R = Mes*

| | | | |
|---|----------|----------|----------|
| P | -1.76371 | 2.14815 | 0.27786 |
| C | -0.88200 | 0.74254 | 0.27600 |
| P | 0.85874 | 0.49828 | 0.35793 |
| C | -3.49077 | 1.48472 | 0.32616 |
| C | -4.28181 | 1.53134 | -0.85183 |
| C | -3.97680 | 0.79387 | 1.46044 |
| C | -5.36199 | 0.66545 | -0.94148 |
| C | -5.05828 | -0.07380 | 1.28362 |
| C | -5.72689 | -0.20563 | 0.07899 |
| H | -5.94027 | 0.65210 | -1.85337 |

| | | | |
|---|----------|----------|----------|
| H | -5.40167 | -0.64696 | 2.13216 |
| C | -3.49597 | 1.01959 | 2.91317 |
| C | -4.04860 | 2.54741 | -1.98630 |
| C | -6.86545 | -1.19726 | -0.13568 |
| C | -2.74335 | 2.30237 | -2.74547 |
| H | -1.86295 | 2.49885 | -2.13001 |
| H | -2.67524 | 1.27315 | -3.10076 |
| H | -2.68668 | 2.97975 | -3.60280 |
| C | -4.04561 | 3.96207 | -1.38963 |
| H | -4.98722 | 4.16968 | -0.87508 |
| H | -3.23096 | 4.11040 | -0.67780 |
| H | -3.92316 | 4.70017 | -2.18722 |
| C | -5.17265 | 2.50761 | -3.02461 |
| H | -5.19555 | 1.56156 | -3.57047 |
| H | -6.15482 | 2.68035 | -2.57798 |
| H | -4.99914 | 3.30017 | -3.75592 |
| C | -2.50199 | -0.05001 | 3.37252 |
| H | -1.57110 | 0.00915 | 2.80804 |
| H | -2.26309 | 0.08675 | 4.43140 |
| H | -2.92034 | -1.05325 | 3.25442 |
| C | -2.87956 | 2.40488 | 3.11106 |
| H | -1.92552 | 2.53274 | 2.59177 |
| H | -3.55481 | 3.19366 | 2.77170 |
| H | -2.67517 | 2.56491 | 4.17319 |
| C | -4.70282 | 0.96929 | 3.86649 |
| H | -5.50134 | 1.63727 | 3.53621 |
| H | -5.11805 | -0.03362 | 3.97307 |
| H | -4.38318 | 1.28686 | 4.86197 |
| C | -7.10220 | -2.08067 | 1.08631 |
| H | -7.41118 | -1.49933 | 1.95904 |
| H | -7.90041 | -2.79455 | 0.87013 |
| H | -6.21017 | -2.65436 | 1.35125 |
| C | -6.52317 | -2.10224 | -1.32528 |
| H | -6.37950 | -1.52955 | -2.24310 |
| H | -5.60338 | -2.66292 | -1.14387 |
| H | -7.33268 | -2.81703 | -1.49739 |
| C | -8.16108 | -0.43391 | -0.43556 |
| H | -8.06997 | 0.18181 | -1.33249 |
| H | -8.98283 | -1.13719 | -0.59658 |
| H | -8.43159 | 0.22122 | 0.39640 |
| C | 2.28536 | 1.54062 | -0.14347 |
| C | 2.89369 | 1.26956 | -1.39770 |
| C | 3.08425 | 2.14468 | 0.87188 |
| C | 4.28375 | 1.20229 | -1.44056 |
| C | 4.46000 | 2.04202 | 0.75361 |
| C | 5.08882 | 1.46453 | -0.34557 |
| H | 4.74620 | 0.92342 | -2.37708 |
| H | 5.07404 | 2.44562 | 1.54946 |
| C | 2.18007 | 1.23891 | -2.76263 |
| C | 2.49749 | -0.00713 | -3.59267 |
| C | 2.72812 | 2.47188 | -3.51403 |
| H | 2.10491 | -0.90907 | -3.12537 |
| H | 2.03740 | 0.09106 | -4.57944 |
| H | 3.57050 | -0.13951 | -3.74241 |
| H | 2.52401 | 3.39189 | -2.96035 |
| H | 3.80396 | 2.40954 | -3.68151 |
| H | 2.23730 | 2.54422 | -4.48830 |
| C | 2.57080 | 3.08863 | 1.98056 |
| C | 3.22938 | 4.45564 | 1.69803 |
| C | 2.98764 | 2.65374 | 3.38850 |
| H | 2.98615 | 4.80483 | 0.69202 |
| H | 2.85639 | 5.19239 | 2.41495 |
| H | 4.31498 | 4.41901 | 1.78878 |
| H | 2.54004 | 1.70616 | 3.68720 |
| H | 4.07049 | 2.54319 | 3.46895 |
| H | 2.68004 | 3.41225 | 4.11339 |

| | | | |
|----|----------|----------|----------|
| C | 6.59339 | 1.23578 | -0.34170 |
| C | 7.31971 | 2.58073 | -0.21954 |
| C | 7.07084 | 0.53782 | -1.61224 |
| H | 7.05587 | 3.10356 | 0.70242 |
| H | 8.40118 | 2.42031 | -0.21149 |
| H | 7.07953 | 3.23650 | -1.06041 |
| H | 6.57337 | -0.42475 | -1.75187 |
| H | 6.90765 | 1.14948 | -2.50367 |
| H | 8.14422 | 0.34835 | -1.53981 |
| Cl | -2.36638 | -1.41904 | -2.34519 |
| Au | 2.89939 | -2.31662 | 0.16995 |
| Cl | 4.80257 | -3.28346 | 0.92914 |
| C | 1.07098 | 3.35829 | 1.92814 |
| H | 0.76334 | 3.69676 | 0.93675 |
| H | 0.45056 | 2.50549 | 2.19555 |
| H | 0.82501 | 4.15267 | 2.63733 |
| C | 0.67148 | 1.43517 | -2.69504 |
| H | 0.13209 | 0.56454 | -2.32436 |
| H | 0.41482 | 2.30309 | -2.08280 |
| H | 0.29437 | 1.62211 | -3.70342 |
| C | 6.95052 | 0.34851 | 0.85794 |
| H | 6.67343 | 0.81906 | 1.80402 |
| H | 6.44528 | -0.61873 | 0.80183 |
| H | 8.02928 | 0.17109 | 0.87862 |
| Pb | -1.71288 | -1.50255 | 0.07826 |
| S | 1.03134 | -1.30644 | -0.66203 |
| C | 1.19474 | -0.00298 | 2.07420 |
| H | 2.25426 | -0.24155 | 2.17097 |
| H | 0.90162 | 0.75180 | 2.79843 |
| H | 0.62159 | -0.91335 | 2.25175 |

Coordination through P(sp²) atom

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.75718 | 0.09420 | 0.83287 |
| C | 0.48732 | -0.28988 | -0.73305 |
| P | -1.02087 | -0.13508 | -1.61567 |
| Pb | 1.89471 | -0.71218 | -2.65428 |
| Cl | 0.97899 | -3.03265 | -2.83156 |
| C | -2.32983 | 0.84599 | -0.86911 |
| H | -3.19280 | 0.83465 | -1.53802 |
| H | -2.60971 | 0.42598 | 0.09953 |
| H | -1.98548 | 1.87239 | -0.73948 |
| Au | -0.52453 | 0.84010 | 2.46611 |
| Cl | -1.86223 | 1.60882 | 4.11644 |
| H | 2.13550 | -0.11927 | 1.05756 |
| H | -1.54616 | -1.44046 | -1.67387 |
| S | -0.48176 | 0.52103 | -3.42556 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.80617 | 0.17056 | 0.78812 |
| C | 0.46042 | -0.18271 | -0.76762 |
| P | -1.14381 | -0.21203 | -1.48928 |
| Pb | 1.74416 | -0.62114 | -2.76015 |
| Cl | 1.39102 | -3.10101 | -2.52252 |
| C | -2.28180 | 1.03953 | -0.86777 |
| H | -3.21644 | 0.96636 | -1.42776 |
| H | -2.47639 | 0.88650 | 0.19614 |
| H | -1.84754 | 2.02714 | -1.02303 |
| C | -1.89032 | -1.81097 | -1.13366 |
| H | -2.06898 | -1.90354 | -0.06008 |
| H | -2.83168 | -1.89384 | -1.68018 |
| H | -1.20145 | -2.58918 | -1.46764 |
| C | 2.58305 | 0.05881 | 1.11958 |
| H | 3.13771 | -0.23851 | 0.23002 |

| | | | |
|----|----------|----------|----------|
| H | 2.94143 | 1.02497 | 1.48205 |
| H | 2.74262 | -0.67380 | 1.91432 |
| Au | -0.53742 | 0.71651 | 2.46035 |
| Cl | -1.94807 | 1.26301 | 4.14493 |
| S | -0.82784 | 0.03906 | -3.46053 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.74025 | 0.17411 | 0.81752 |
| C | 0.47854 | -0.11919 | -0.77291 |
| P | -1.12410 | -0.24991 | -1.51087 |
| Pb | 1.82239 | 0.07084 | -2.78429 |
| Cl | 2.43806 | -2.36620 | -2.92968 |
| C | -2.27890 | 0.99234 | -0.88541 |
| H | -3.19265 | 0.96195 | -1.47996 |
| H | -2.50963 | 0.83099 | 0.16898 |
| H | -1.81298 | 1.97061 | -1.00588 |
| Au | -0.73899 | 0.53616 | 2.43992 |
| Cl | -2.27507 | 0.92651 | 4.06386 |
| C | 2.51954 | 0.19166 | 1.34134 |
| C | 2.67483 | -0.98619 | 2.31040 |
| C | 3.48858 | 0.04562 | 0.18115 |
| C | 2.76013 | 1.50677 | 2.08511 |
| H | 1.96532 | -0.92640 | 3.13935 |
| H | 2.53776 | -1.94479 | 1.80489 |
| H | 3.68444 | -0.96586 | 2.73188 |
| H | 3.44093 | 0.90637 | -0.49215 |
| H | 4.51032 | 0.00585 | 0.57116 |
| H | 3.31968 | -0.87406 | -0.38470 |
| H | 3.77410 | 1.50349 | 2.49607 |
| H | 2.66611 | 2.37079 | 1.42279 |
| H | 2.06214 | 1.63623 | 2.91571 |
| C | -1.88765 | -1.92006 | -1.22553 |
| C | -3.22383 | -1.94514 | -1.96979 |
| C | -0.95779 | -2.98814 | -1.79289 |
| C | -2.11154 | -2.15968 | 0.26434 |
| H | -3.95519 | -1.26174 | -1.53326 |
| H | -3.10223 | -1.70536 | -3.02818 |
| H | -3.63714 | -2.95517 | -1.90088 |
| H | 0.01632 | -2.99139 | -1.30174 |
| H | -1.42047 | -3.96745 | -1.64005 |
| H | -0.78889 | -2.85313 | -2.86190 |
| H | -2.58451 | -3.13829 | 0.38795 |
| H | -1.17373 | -2.17856 | 0.82176 |
| H | -2.77061 | -1.41969 | 0.72258 |
| S | -0.83148 | 0.07077 | -3.48191 |

R = Ph

| | | | |
|----|----------|----------|----------|
| P | 0.74735 | 0.39098 | 0.56981 |
| C | 0.53343 | -0.35643 | -0.86909 |
| P | -0.98526 | -0.57674 | -1.72618 |
| Pb | 2.07793 | -1.01663 | -2.58150 |
| Cl | 2.09301 | -3.44872 | -1.92452 |
| C | -2.10176 | 0.83577 | -1.61552 |
| H | -2.99064 | 0.61980 | -2.21089 |
| H | -2.38863 | 1.03732 | -0.58194 |
| H | -1.59179 | 1.70800 | -2.02533 |
| Au | -0.70776 | 1.47999 | 1.84043 |
| Cl | -2.24930 | 2.56564 | 3.09771 |
| C | 2.45103 | 0.26770 | 1.10859 |
| C | 2.98340 | 1.29734 | 1.88526 |
| C | 3.23686 | -0.84344 | 0.79102 |
| C | 4.30242 | 1.23716 | 2.30334 |
| H | 2.36271 | 2.14499 | 2.15709 |
| C | 4.55183 | -0.89968 | 1.22175 |
| H | 2.80901 | -1.68148 | 0.24893 |
| C | 5.08679 | 0.14205 | 1.96870 |

| | | | |
|---|----------|----------|----------|
| H | 4.71663 | 2.04334 | 2.89726 |
| H | 5.15553 | -1.76791 | 0.98458 |
| H | 6.11609 | 0.09225 | 2.30502 |
| C | -1.85913 | -1.98629 | -1.01025 |
| C | -2.56190 | -1.83167 | 0.18515 |
| C | -1.79714 | -3.23159 | -1.62559 |
| C | -3.20890 | -2.91757 | 0.74917 |
| H | -2.60331 | -0.87167 | 0.68849 |
| C | -2.44508 | -4.31538 | -1.05278 |
| H | -1.23731 | -3.34779 | -2.54581 |
| C | -3.15151 | -4.15914 | 0.12956 |
| H | -3.75685 | -2.79317 | 1.67576 |
| H | -2.39201 | -5.28536 | -1.53284 |
| H | -3.65763 | -5.00819 | 0.57468 |
| S | -0.46829 | -0.89558 | -3.64185 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.72674 | 0.58618 | 0.93302 |
| C | 0.42157 | -0.42753 | -0.31504 |
| P | -0.97773 | -0.57477 | -1.37535 |
| Pb | 2.19508 | -1.11751 | -1.76093 |
| Cl | 1.64731 | -3.56963 | -1.57751 |
| Au | -0.60250 | 1.96865 | 2.04899 |
| Cl | -1.98004 | 3.37636 | 3.17328 |
| C | 2.48657 | 0.48978 | 1.33493 |
| C | 3.31640 | 1.57866 | 1.01860 |
| C | 3.00531 | -0.64671 | 1.97800 |
| C | 4.66660 | 1.49605 | 1.32953 |
| C | 4.36373 | -0.67610 | 2.26907 |
| C | 5.21117 | 0.37736 | 1.94913 |
| H | 5.31117 | 2.33460 | 1.08387 |
| H | 4.76896 | -1.54893 | 2.77178 |
| C | -1.85127 | -2.15592 | -1.10560 |
| C | -2.25118 | -2.46613 | 0.21285 |
| C | -2.18306 | -3.04371 | -2.15402 |
| C | -2.93523 | -3.65089 | 0.45541 |
| C | -2.86686 | -4.21267 | -1.84192 |
| C | -3.24269 | -4.54873 | -0.55153 |
| H | -3.23841 | -3.86961 | 1.47466 |
| H | -3.11777 | -4.88680 | -2.65466 |
| C | 2.77800 | 2.81239 | 0.35763 |
| H | 2.27895 | 2.58209 | -0.58847 |
| H | 2.04131 | 3.31571 | 0.99145 |
| H | 3.57981 | 3.52090 | 0.14852 |
| C | 2.14155 | -1.80896 | 2.36971 |
| H | 1.24909 | -1.47680 | 2.90846 |
| H | 1.80247 | -2.37795 | 1.49924 |
| H | 2.69052 | -2.48973 | 3.02078 |
| C | 6.67614 | 0.30314 | 2.24916 |
| H | 7.22239 | -0.11964 | 1.40011 |
| H | 7.09307 | 1.29232 | 2.44558 |
| H | 6.87386 | -0.33267 | 3.11357 |
| C | -1.97671 | -1.61403 | 1.41725 |
| H | -2.68576 | -1.85617 | 2.20949 |
| H | -0.97243 | -1.80247 | 1.80355 |
| H | -2.05058 | -0.54243 | 1.23824 |
| C | -1.86598 | -2.84324 | -3.60741 |
| H | -2.18724 | -1.87229 | -3.98358 |
| H | -0.79377 | -2.91903 | -3.79282 |
| H | -2.36791 | -3.61485 | -4.19220 |
| C | -3.94332 | -5.83802 | -0.25964 |
| H | -4.60716 | -6.12469 | -1.07731 |
| H | -3.21687 | -6.64641 | -0.13089 |
| H | -4.53093 | -5.77475 | 0.65756 |
| C | -2.23475 | 0.71789 | -1.22002 |
| H | -2.80333 | 0.63517 | -0.29439 |

| | | | |
|---|----------|----------|----------|
| H | -1.74845 | 1.69247 | -1.27244 |
| H | -2.91526 | 0.60925 | -2.06742 |
| S | -0.05475 | -0.29251 | -3.14914 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | -0.84475 | 1.09382 | 0.09400 |
| C | -0.20042 | -0.37871 | 0.41048 |
| P | 1.41168 | -1.06356 | 0.61741 |
| Cl | -2.12530 | -2.61148 | -2.08067 |
| C | 3.07844 | -0.42702 | 0.14677 |
| C | 3.63505 | -0.89056 | -1.08142 |
| C | 3.97259 | 0.02424 | 1.15654 |
| C | 4.97439 | -1.25196 | -1.08634 |
| C | 5.30113 | -0.38589 | 1.07771 |
| C | 5.80950 | -1.11096 | 0.01337 |
| H | 5.38512 | -1.65452 | -2.00366 |
| H | 5.96639 | -0.10018 | 1.88051 |
| C | -2.65740 | 0.87193 | 0.14150 |
| C | -3.40742 | 0.76616 | -1.05888 |
| C | -3.25932 | 0.53754 | 1.38240 |
| C | -4.62553 | 0.09548 | -0.99674 |
| C | -4.46638 | -0.15280 | 1.34737 |
| C | -5.14214 | -0.44065 | 0.17150 |
| H | -5.17874 | -0.04161 | -1.91036 |
| H | -4.90514 | -0.46799 | 2.28488 |
| C | -3.01530 | 1.42663 | -2.39480 |
| C | -2.75975 | 0.94691 | 2.78682 |
| C | -6.41964 | -1.27300 | 0.20431 |
| C | 3.68668 | 1.09094 | 2.23742 |
| C | 2.96231 | -0.84861 | -2.46881 |
| C | 7.23449 | -1.64814 | -0.02532 |
| C | -3.95394 | 1.49688 | 3.58943 |
| H | -3.59564 | 1.87386 | 4.55041 |
| H | -4.43666 | 2.32148 | 3.06014 |
| H | -4.71112 | 0.74296 | 3.80389 |
| C | -1.72821 | 2.07434 | 2.78426 |
| H | -0.74073 | 1.75758 | 2.44693 |
| H | -2.04770 | 2.92011 | 2.17105 |
| H | -1.59509 | 2.43870 | 3.80640 |
| C | -2.18559 | -0.25727 | 3.53815 |
| H | -2.91179 | -1.07143 | 3.59973 |
| H | -1.28885 | -0.63329 | 3.04204 |
| H | -1.91386 | 0.02822 | 4.55860 |
| C | -7.46935 | -0.57554 | 1.07721 |
| H | -8.38758 | -1.16857 | 1.10560 |
| H | -7.12531 | -0.44702 | 2.10561 |
| H | -7.71487 | 0.41216 | 0.67944 |
| C | -7.01146 | -1.48109 | -1.18722 |
| H | -7.90489 | -2.10548 | -1.11174 |
| H | -7.31008 | -0.53657 | -1.64902 |
| H | -6.30876 | -1.98579 | -1.85446 |
| C | -6.09724 | -2.65013 | 0.79743 |
| H | -5.36121 | -3.17503 | 0.18324 |
| H | -5.70006 | -2.57139 | 1.81198 |
| H | -7.00215 | -3.26247 | 0.84037 |
| C | -4.03962 | 1.14367 | -3.49810 |
| H | -5.03728 | 1.51080 | -3.24656 |
| H | -3.72216 | 1.66588 | -4.40308 |
| H | -4.10124 | 0.07902 | -3.73605 |
| C | -2.99961 | 2.94654 | -2.17948 |
| H | -3.97934 | 3.30169 | -1.84967 |
| H | -2.26281 | 3.25117 | -1.43271 |
| H | -2.74846 | 3.45398 | -3.11462 |
| C | -1.66755 | 0.95541 | -2.94328 |
| H | -0.82052 | 1.28853 | -2.34173 |
| H | -1.62913 | -0.13154 | -3.02237 |

| | | | |
|----|----------|----------|----------|
| H | -1.51474 | 1.38686 | -3.93661 |
| C | 2.31908 | 1.75306 | 2.11853 |
| H | 2.20329 | 2.21344 | 1.13533 |
| H | 1.46927 | 1.09407 | 2.27701 |
| H | 2.24018 | 2.55312 | 2.85849 |
| C | 4.68506 | 2.24030 | 1.97319 |
| H | 4.46497 | 3.06786 | 2.65269 |
| H | 5.72055 | 1.94150 | 2.13647 |
| H | 4.59167 | 2.61141 | 0.95069 |
| C | 3.93564 | 0.58956 | 3.66391 |
| H | 4.94903 | 0.19892 | 3.77658 |
| H | 3.82432 | 1.41966 | 4.36657 |
| H | 3.24587 | -0.19727 | 3.96700 |
| C | 1.53588 | -0.31820 | -2.47507 |
| H | 1.23606 | -0.13179 | -3.50905 |
| H | 0.81564 | -1.02308 | -2.06328 |
| H | 1.46535 | 0.63269 | -1.94048 |
| C | 2.99939 | -2.19790 | -3.19066 |
| H | 2.40185 | -2.94184 | -2.66458 |
| H | 2.58864 | -2.08029 | -4.19691 |
| H | 4.01624 | -2.58204 | -3.29448 |
| C | 3.78728 | 0.16948 | -3.28494 |
| H | 3.78220 | 1.15183 | -2.80642 |
| H | 4.82533 | -0.13996 | -3.41262 |
| H | 3.34284 | 0.27441 | -4.27819 |
| C | 7.97949 | -1.40650 | 1.28476 |
| H | 8.10986 | -0.34106 | 1.49085 |
| H | 7.46375 | -1.86211 | 2.13392 |
| H | 8.97570 | -1.85095 | 1.22467 |
| C | 8.01318 | -0.96681 | -1.15699 |
| H | 7.55903 | -1.15272 | -2.13215 |
| H | 8.05683 | 0.11465 | -1.00713 |
| H | 9.03758 | -1.34796 | -1.18910 |
| C | 7.18517 | -3.15927 | -0.28114 |
| H | 6.64648 | -3.67436 | 0.51789 |
| H | 6.68691 | -3.39325 | -1.22386 |
| H | 8.19914 | -3.56599 | -0.32658 |
| Au | 0.17041 | 3.03199 | -0.34479 |
| Cl | 1.23666 | 4.99539 | -0.76720 |
| Pb | -1.43076 | -2.49094 | 0.34192 |
| S | 1.22460 | -2.92095 | -0.18593 |
| C | 1.50976 | -1.45199 | 2.39539 |
| H | 2.44404 | -1.98767 | 2.56632 |
| H | 1.43451 | -0.59662 | 3.05865 |
| H | 0.68488 | -2.13634 | 2.59638 |

Coordination through $\pi(C=P)$ bond

R= H

| | | | |
|----|----------|----------|----------|
| P | 0.71190 | 0.02870 | 0.95480 |
| C | 0.45534 | 0.14994 | -0.74532 |
| P | -1.12538 | -0.01599 | -1.52261 |
| Pb | 1.72936 | -0.11019 | -2.80305 |
| Cl | 1.22184 | -2.57029 | -2.76297 |
| C | -2.54588 | 0.69910 | -0.67541 |
| H | -3.45295 | 0.43910 | -1.22450 |
| H | -2.60502 | 0.30165 | 0.34060 |
| H | -2.43912 | 1.78403 | -0.64370 |
| Au | 0.75511 | 2.17804 | -0.08335 |
| Cl | 1.00332 | 4.41659 | -0.07816 |
| H | -1.37607 | -1.40197 | -1.50561 |
| H | 2.13478 | -0.11128 | 0.94769 |
| S | -0.89044 | 0.66737 | -3.38259 |

R = Me

| | | | |
|----|----------|----------|----------|
| P | 0.77593 | 0.11547 | 0.85041 |
| C | 0.38322 | 0.23386 | -0.81850 |
| P | -1.23940 | -0.09104 | -1.45939 |
| Pb | 1.57510 | 0.02904 | -2.92687 |
| Cl | 1.69411 | -2.48431 | -2.66900 |
| C | -2.57875 | 0.84934 | -0.69683 |
| H | -3.52692 | 0.53548 | -1.13857 |
| H | -2.59607 | 0.66389 | 0.37956 |
| H | -2.42993 | 1.91294 | -0.88387 |
| C | -1.60580 | -1.82404 | -1.13002 |
| H | -1.70095 | -1.98595 | -0.05393 |
| H | -2.53703 | -2.09032 | -1.63308 |
| H | -0.78910 | -2.42911 | -1.52918 |
| C | 2.59783 | -0.10104 | 0.89264 |
| H | 3.10398 | 0.26685 | 0.00013 |
| H | 3.00229 | 0.39441 | 1.77756 |
| H | 2.78690 | -1.17525 | 0.99054 |
| Au | 0.59596 | 2.27871 | -0.17483 |
| Cl | 0.71870 | 4.53031 | -0.12203 |
| S | -1.12621 | 0.27723 | -3.42988 |

R = t-Bu

| | | | |
|----|----------|----------|----------|
| P | 0.66781 | 0.16455 | 0.74397 |
| C | 0.35330 | 0.28551 | -0.94322 |
| P | -1.24373 | -0.12621 | -1.63615 |
| Pb | 1.57779 | 0.63070 | -3.03908 |
| Cl | 2.50096 | -1.71395 | -3.26036 |
| C | -2.59386 | 0.86952 | -0.95208 |
| H | -3.54417 | 0.53134 | -1.36860 |
| H | -2.61651 | 0.79322 | 0.13594 |
| H | -2.43515 | 1.90874 | -1.24063 |
| Au | 0.34824 | 2.33850 | -0.22240 |
| Cl | 0.29712 | 4.59095 | -0.08066 |
| C | 2.51430 | 0.09591 | 1.05225 |
| C | 2.77073 | -1.38455 | 1.36130 |
| C | 3.41676 | 0.55117 | -0.07938 |
| C | 2.75442 | 0.93607 | 2.30720 |
| H | 2.12380 | -1.75461 | 2.16200 |
| H | 2.62545 | -2.01009 | 0.47694 |
| H | 3.80706 | -1.50806 | 1.69159 |
| H | 3.20930 | 1.58261 | -0.37776 |
| H | 4.46096 | 0.51258 | 0.24897 |
| H | 3.33727 | -0.11155 | -0.94508 |
| H | 3.78345 | 0.79377 | 2.65141 |
| H | 2.60782 | 2.00138 | 2.11260 |
| H | 2.08705 | 0.64623 | 3.12382 |
| C | -1.69852 | -1.90087 | -1.30691 |
| C | -2.87561 | -2.25911 | -2.21542 |
| C | -0.51088 | -2.79768 | -1.64013 |
| C | -2.10368 | -2.07634 | 0.15583 |
| H | -3.76241 | -1.65453 | -2.01174 |
| H | -2.61694 | -2.15196 | -3.26949 |
| H | -3.14326 | -3.30393 | -2.03373 |
| H | 0.34285 | -2.61218 | -0.98705 |
| H | -0.81449 | -3.84059 | -1.51042 |
| H | -0.17294 | -2.66708 | -2.66880 |
| H | -2.29767 | -3.13782 | 0.33520 |
| H | -1.31847 | -1.76420 | 0.84815 |
| H | -3.01680 | -1.53052 | 0.40117 |
| S | -1.08330 | 0.22792 | -3.61244 |

R = Ph

| | | | |
|---|---------|---------|---------|
| P | 0.72375 | 0.37861 | 0.77424 |
|---|---------|---------|---------|

| | | | |
|----|----------|----------|----------|
| C | 0.24532 | 0.30548 | -0.87592 |
| P | -1.41206 | -0.02443 | -1.41272 |
| Pb | 1.31836 | 0.25181 | -3.06619 |
| Cl | 1.53097 | -2.26320 | -3.21166 |
| C | -2.69582 | 0.89906 | -0.53737 |
| H | -3.66994 | 0.58656 | -0.91791 |
| H | -2.64233 | 0.70123 | 0.53493 |
| H | -2.55454 | 1.96471 | -0.72092 |
| Au | 0.48533 | 2.42471 | -0.45387 |
| Cl | 0.59687 | 4.67019 | -0.65443 |
| C | -1.76789 | -1.76632 | -1.08052 |
| C | -1.92736 | -2.66716 | -2.12593 |
| C | -1.88431 | -2.20334 | 0.23925 |
| C | -2.21191 | -3.99706 | -1.85334 |
| H | -1.81703 | -2.32461 | -3.14755 |
| C | -2.16826 | -3.53145 | 0.50518 |
| H | -1.74338 | -1.51408 | 1.06554 |
| C | -2.33393 | -4.42853 | -0.54241 |
| H | -2.32926 | -4.69770 | -2.67149 |
| H | -2.25713 | -3.86834 | 1.53140 |
| H | -2.55306 | -5.46918 | -0.33226 |
| C | 2.52810 | 0.16789 | 0.74943 |
| C | 3.15953 | -0.74038 | -0.10179 |
| C | 3.28532 | 0.87120 | 1.68834 |
| C | 4.53374 | -0.91324 | -0.03386 |
| H | 2.57788 | -1.33785 | -0.79721 |
| C | 4.65922 | 0.70690 | 1.74000 |
| H | 2.79789 | 1.56197 | 2.36929 |
| C | 5.28444 | -0.18428 | 0.87777 |
| H | 5.01595 | -1.62523 | -0.69388 |
| H | 5.24379 | 1.27177 | 2.45691 |
| H | 6.35908 | -0.31866 | 0.92492 |
| S | -1.43805 | 0.40966 | -3.36943 |

R = Mes

| | | | |
|----|----------|----------|----------|
| P | 0.75184 | 0.40808 | 1.24836 |
| C | 0.09345 | 0.31669 | -0.34595 |
| P | -1.53544 | 0.01358 | -1.00002 |
| Pb | 1.32059 | 0.68983 | -2.41581 |
| Cl | 1.52042 | -1.70126 | -3.23796 |
| Au | 0.10219 | 2.43967 | 0.17351 |
| Cl | -0.12498 | 4.69364 | 0.13785 |
| C | -1.85174 | -1.78978 | -1.03537 |
| C | -2.02567 | -2.53272 | -2.22838 |
| C | -1.91791 | -2.46403 | 0.20524 |
| C | -2.18180 | -3.91092 | -2.13369 |
| C | -2.06462 | -3.84578 | 0.22715 |
| C | -2.18021 | -4.59576 | -0.92947 |
| H | -2.30811 | -4.47002 | -3.05515 |
| H | -2.09934 | -4.34424 | 1.19127 |
| C | 2.55333 | 0.25880 | 0.96092 |
| C | 3.03854 | -0.99883 | 0.54930 |
| C | 3.45265 | 1.28771 | 1.28651 |
| C | 4.40601 | -1.15847 | 0.36701 |
| C | 4.81142 | 1.07576 | 1.08448 |
| C | 5.30779 | -0.12821 | 0.60316 |
| H | 4.77701 | -2.12801 | 0.04829 |
| H | 5.50396 | 1.87670 | 1.32638 |
| C | 3.00584 | 2.60110 | 1.85540 |
| H | 2.67005 | 3.29453 | 1.07835 |
| H | 2.17491 | 2.48346 | 2.55600 |
| H | 3.82691 | 3.08217 | 2.38925 |
| C | 2.13858 | -2.18615 | 0.36251 |
| H | 1.38933 | -2.25456 | 1.15730 |
| H | 1.60592 | -2.15789 | -0.59110 |
| H | 2.72496 | -3.10574 | 0.38110 |

| | | | |
|---|----------|----------|----------|
| C | 6.77264 | -0.31698 | 0.35744 |
| H | 7.08231 | -1.34331 | 0.56323 |
| H | 7.01793 | -0.10733 | -0.68848 |
| H | 7.37090 | 0.35469 | 0.97529 |
| C | -1.91818 | -1.80324 | 1.55525 |
| H | -1.48239 | -2.47309 | 2.29802 |
| H | -1.36525 | -0.86856 | 1.60868 |
| H | -2.94563 | -1.60029 | 1.87425 |
| C | -2.29389 | -6.08686 | -0.88655 |
| H | -2.97071 | -6.45618 | -1.65937 |
| H | -1.31784 | -6.54975 | -1.06193 |
| H | -2.65411 | -6.43316 | 0.08338 |
| C | -2.08987 | -1.96934 | -3.61794 |
| H | -2.81748 | -1.16373 | -3.70781 |
| H | -1.12401 | -1.57708 | -3.93612 |
| H | -2.37402 | -2.76363 | -4.30915 |
| C | -2.94542 | 0.75980 | -0.13358 |
| H | -3.04889 | 0.40729 | 0.89004 |
| H | -2.81522 | 1.84275 | -0.14350 |
| H | -3.84477 | 0.50430 | -0.69870 |
| S | -1.41425 | 0.99806 | -2.75621 |

R = Mes*

| | | | |
|----|----------|----------|----------|
| P | 0.67171 | 0.04588 | 1.11078 |
| C | 0.41989 | 0.07081 | -0.60738 |
| P | -1.09329 | -0.05353 | -1.61641 |
| Pb | 2.09438 | 0.60238 | 2.37114 |
| Cl | 3.10065 | -1.50302 | -3.39810 |
| Au | 0.44919 | 2.18071 | -0.01555 |
| Cl | 0.27929 | 4.44037 | -0.21780 |
| C | 2.52413 | -0.02892 | 1.23754 |
| C | 3.22640 | -1.15954 | 0.73659 |
| C | 3.27627 | 1.09920 | 1.64729 |
| C | 4.53111 | -0.97928 | 0.29938 |
| C | 4.58794 | 1.20860 | 1.17814 |
| C | 5.21037 | 0.22842 | 0.42492 |
| H | 5.04664 | -1.82611 | -0.13443 |
| H | 5.14252 | 2.10048 | 1.43356 |
| C | 2.88326 | 2.13261 | 2.72549 |
| C | 2.76337 | -2.61971 | 0.90343 |
| C | 6.59996 | 0.39663 | -0.17915 |
| C | 3.83707 | 1.86373 | 3.90788 |
| H | 3.71444 | 0.84555 | 4.28602 |
| H | 4.88295 | 1.99392 | 3.62747 |
| H | 3.61526 | 2.55993 | 4.72140 |
| C | 3.08413 | 3.57699 | 2.25877 |
| H | 2.43449 | 3.82869 | 1.41938 |
| H | 2.84528 | 4.26060 | 3.07811 |
| H | 4.11516 | 3.77512 | 1.96165 |
| C | 1.47479 | 1.99999 | 3.29679 |
| H | 1.38867 | 2.65423 | 4.16859 |
| H | 0.69628 | 2.31380 | 2.59806 |
| H | 1.25786 | 0.98184 | 3.62866 |
| C | 3.05603 | -3.48275 | -0.32499 |
| H | 2.59919 | -3.07644 | -1.22562 |
| H | 4.12579 | -3.57772 | -0.51683 |
| H | 2.67030 | -4.49248 | -0.15921 |
| C | 3.58556 | -3.16455 | 2.08795 |
| H | 4.65647 | -3.11931 | 1.88333 |
| H | 3.39164 | -2.59244 | 2.99898 |
| H | 3.31663 | -4.20853 | 2.27443 |
| C | 1.29878 | -2.79977 | 1.28359 |
| H | 1.03635 | -2.24503 | 2.19039 |
| H | 0.61951 | -2.51480 | 0.48112 |
| H | 1.11517 | -3.85615 | 1.49929 |
| C | 7.21267 | 1.75563 | 0.14815 |

| | | | |
|---|----------|----------|----------|
| H | 6.59517 | 2.57894 | -0.21945 |
| H | 7.36138 | 1.88899 | 1.22306 |
| H | 8.19087 | 1.83829 | -0.33144 |
| C | 6.48752 | 0.26917 | -1.70332 |
| H | 7.47804 | 0.34031 | -2.16159 |
| H | 6.03985 | -0.68029 | -2.00306 |
| H | 5.86826 | 1.06998 | -2.11614 |
| C | 7.53954 | -0.69210 | 0.35242 |
| H | 7.62124 | -0.64282 | 1.44123 |
| H | 7.19898 | -1.69367 | 0.08367 |
| H | 8.53936 | -0.56040 | -0.07007 |
| C | -2.34181 | -1.44259 | -1.66568 |
| C | -2.32116 | -2.33186 | -2.78002 |
| C | -3.58667 | -1.26056 | -1.00058 |
| C | -3.52544 | -2.60525 | -3.41372 |
| C | -1.13202 | -3.20492 | -3.22215 |
| C | -4.75310 | -1.59272 | -1.68420 |
| C | -3.78600 | -0.92527 | 0.49153 |
| C | -4.75481 | -2.16379 | -2.94629 |
| H | -3.49421 | -3.21834 | -4.30595 |
| C | -0.72275 | -3.00461 | -4.68272 |
| C | -1.60646 | -4.66569 | -3.05993 |
| C | 0.07241 | -3.07197 | -2.30744 |
| H | -5.69773 | -1.40197 | -1.19399 |
| C | -2.49829 | -0.65451 | 1.25173 |
| C | -4.37131 | -2.20936 | 1.11665 |
| C | -4.78013 | 0.21352 | 0.73977 |
| C | -6.02377 | -2.40579 | -3.75307 |
| H | 0.02340 | -3.75553 | -4.95488 |
| H | -1.57424 | -3.12171 | -5.35738 |
| H | -0.28648 | -2.02148 | -4.84501 |
| H | -2.40271 | -4.92961 | -3.75694 |
| H | -0.76215 | -5.33336 | -3.25126 |
| H | -1.96669 | -4.85439 | -2.04548 |
| H | 0.53327 | -2.08821 | -2.34524 |
| H | -0.20336 | -3.30829 | -1.27758 |
| H | 0.84319 | -3.77880 | -2.61976 |
| H | -1.76468 | -1.44466 | 1.08076 |
| H | -2.03607 | 0.30136 | 1.01182 |
| H | -2.70518 | -0.62958 | 2.32427 |
| H | -4.50751 | -2.06075 | 2.19151 |
| H | -5.33759 | -2.47286 | 0.68545 |
| H | -3.69513 | -3.05521 | 0.97189 |
| H | -5.76475 | -0.00314 | 0.32244 |
| H | -4.90735 | 0.35574 | 1.81612 |
| H | -4.44583 | 1.16188 | 0.31766 |
| C | -7.26169 | -1.83218 | -3.06884 |
| C | -6.23399 | -3.91195 | -3.94938 |
| C | -5.87197 | -1.73215 | -5.12217 |
| H | -7.46561 | -2.32286 | -2.11361 |
| H | -7.16533 | -0.75806 | -2.89151 |
| H | -8.13508 | -1.98597 | -3.70688 |
| H | -5.40313 | -4.37140 | -4.48818 |
| H | -6.33510 | -4.42218 | -2.98834 |
| H | -7.14484 | -4.09093 | -4.52731 |
| H | -5.73649 | -0.65325 | -5.01491 |
| H | -5.01340 | -2.12313 | -5.67155 |
| H | -6.76602 | -1.90502 | -5.72747 |
| S | -0.37611 | 0.24405 | -3.48899 |
| C | -2.21269 | 1.37576 | -1.42878 |
| H | -2.61537 | 1.49980 | -0.42841 |
| H | -1.66084 | 2.26999 | -1.71735 |
| H | -3.02664 | 1.22274 | -2.13958 |