# Supporting Information available for

# Predicting viable isomers of [X,C,N] and [H,X,C,N] (X=Sn, Pb)

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RSC Advances

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**1. Theoretical methods**

GPESS: The GPESS platform includes isomer search and transition state search. The isomer search was based on the grid search program. The transition state search was divided into two types, one is the isomer conversion and the other is the isomer decomposition. For the interconversion TS search, the "QST2" algorithm was applied, which yet has a difficulty in placing atoms in the same atomic order between reactant and product (especially for molecules with many homo-atomic elements). This was treated in GPESS by automatic enumeration of all possible combinations. Besides, the decomposition TS search was considered directing to some relatively stable molecular fragments like $N_2$, $CO_2$ and NO.

**2.**

Table S1 Computed relative energies (in kcal/mol) at CCSD(T)/def2-QZVPP//B3LYP/def2-QZVPP+ZPVE and CCSD(T)/def2-QZVPP//PBE0/def2-QZVPP+ZPVE levels. "ZPVE" denote the zero-point vibrational energy.

| Species | CCSD(T)/def2-QZVPP//B3LYP/def2-QZVPP + ZPVE | CCSD(T)/def2-QZVPP//PBE0/def2-QZVPP + ZPVE | Error | Average error |
|---|---|---|---|---|
| SnCN $^2$1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| SnNC $^2$2 | 4.89 | 4.87 | -0.02 | 0.0004 |
| CSnN $^2$3 | 174.68 | 175.14 | 0.46 | 0.0093 |
| SnCN $^4$1 | 64.63 | 64.67 | 0.05 | 0.0009 |
| SnNC $^4$2 | 84.92 | 80.67 | -4.25 | 0.0849 |
| CSnN $^4$3 | 176.91 | 180.11 | 3.20 | 0.0640 |
| *c*-SnCN $^4$4 | 88.29 | 85.20 | -3.09 | 0.0617 |
| | | | | |
| PbCN $^2$1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| PbNC $^2$2 | 6.40 | 6.25 | -0.14 | 0.0029 |
| CPbN $^2$3 | 184.98 | 185.37 | 0.40 | 0.0079 |
| PbCN $^4$1 | 81.54 | 81.16 | -0.39 | 0.0077 |
| PbNC $^4$2 | 84.97 | 85.20 | 0.23 | 0.0045 |
| CPbN $^4$3 | 187.29 | 186.98 | -0.31 | 0.0061 |
| *c*-PbCN $^4$4 | 87.03 | 88.19 | 1.16 | 0.0232 |
| | | | | |
| HSnCN $^1$1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| HSnNC $^1$2 | 4.80 | 4.78 | -0.02 | 0.0004 |
| SnNCH $^1$3 | 34.86 | 34.87 | 0.02 | 0.0003 |
| NSnCH $^1$4 | 142.34 | 142.98 | 0.64 | 0.0127 |
| SnCNH $^1$5 | 30.82 | 30.85 | 0.03 | 0.0006 |
| CSnNH $^1$6 | 149.12 | 149.02 | -0.10 | 0.0020 |
| *c*-SnCHN $^1$7 | 14.49 | 14.59 | 0.10 | 0.0020 |
| *c*-SnCNH $^1$8 | 38.47 | 38.52 | 0.05 | 0.0010 |
| HSnCN $^3$1 | 35.69 | 35.77 | 0.08 | 0.0016 |
| HSnNC $^3$2 | 46.40 | 46.41 | 0.01 | 0.0002 |
| SnNCH $^3$3 | 20.53 | 20.89 | 0.36 | 0.0072 |

| | | | | |
|---|---|---|---|---|
| NSnCH $^{3}$4 | 137.57 | 137.47 | -0.10 | 0.0020 |
| HNCSn $^{3}$5 | 25.07 | 24.99 | -0.08 | 0.0016 |
| CSnNH $^{3}$6 | 131.81 | 131.81 | 0.00 | 0.0000 |
| *c*-SnCHN $^{3}$7 | 44.75 | 45.07 | 0.32 | 0.0064 |
| *c*-SnHNC $^{3}$8 | 51.83 | 51.88 | 0.05 | 0.0010 |
| CSn(H)N $^{3}$9 | 194.28 | 196.49 | 2.21 | 0.0442 |
| | | | | |
| HPbCN $^{1}$1 | 0.00 | 0.00 | 0.00 | 0.0000 |
| HPbNC $^{1}$2 | 5.89 | 5.85 | -0.04 | 0.0008 |
| PbNCH $^{1}$3 | 32.55 | 33.09 | 0.54 | 0.0107 |
| HCPbN $^{1}$4 | 149.65 | 150.26 | 0.61 | 0.0122 |
| HNCPb $^{1}$5 | 29.86 | 29.84 | -0.03 | 0.0005 |
| HNPbC $^{1}$6 | 151.76 | 152.21 | 0.46 | 0.0092 |
| *c*-PbCHN $^{1}$7 | 14.78 | 14.73 | -0.05 | 0.0010 |
| *c*-PbCHN $^{1}$8 | 37.30 | 37.12 | -0.18 | 0.0037 |
| CHPbN $^{1}$9 | 44.90 | 43.60 | -1.30 | 0.0260 |
| CHPbN $^{1}$10 | 58.30 | 58.73 | 0.43 | 0.0086 |
| PbNHC $^{1}$11 | 33.34 | 30.80 | -2.54 | 0.0508 |
| HPbCN $^{3}$1 | 47.29 | 47.26 | -0.02 | 0.0004 |
| HPbNC $^{3}$2 | 58.25 | 58.06 | -0.19 | 0.0038 |
| PbNCH $^{3}$3 | 14.39 | 14.70 | 0.31 | 0.0062 |
| NPbCH $^{3}$4 | 147.84 | 147.44 | -0.40 | 0.0080 |
| PbCNH $^{3}$5 | 20.50 | 20.95 | 0.45 | 0.0089 |
| CPbNH $^{3}$6 | 139.91 | 139.98 | 0.07 | 0.0014 |
| *c*-PbHNC $^{3}$7 | 61.22 | 61.03 | -0.19 | 0.0038 |
| CPb(H)N $^{3}$8 | 210.97 | 213.65 | 2.68 | 0.0536 |

**3.**

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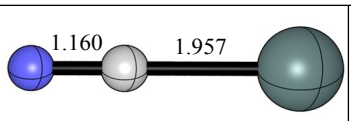
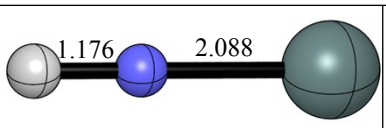
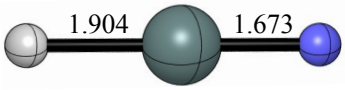
|  |  |  |
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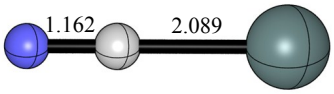
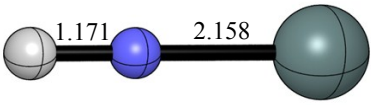
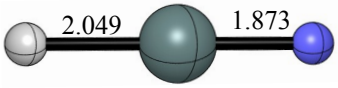
|  |  |  |
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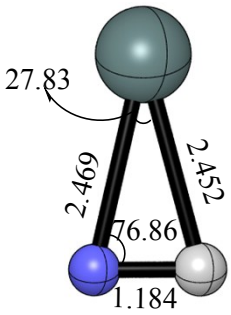
|  | | |
| $^{4}4$ | | |

Figure S1. Optimized geometries of isomers of the doublet and quartet neutral [Sn,C,N] at the B3LYP/def2-qzvpp level. Bond lengths are in angstroms and angles are in degrees.

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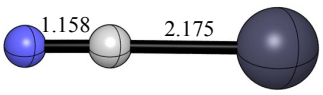
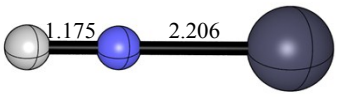
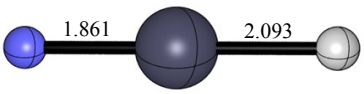
|  |  |  |
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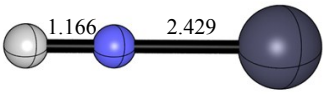
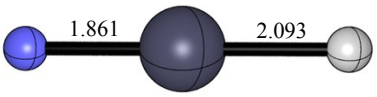
|  |  |  |
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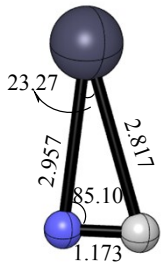
|  | | |
| $^{4}4$ | | |

Figure S2. Optimized geometries of isomers of the doublet and quartet neutral [Pb,C,N] at the B3LYP/def2-qzvpp level. Bond lengths are in angstroms and angles are in degrees.

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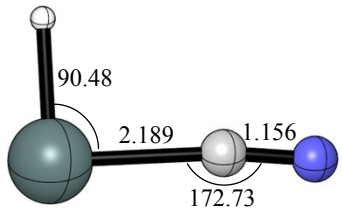
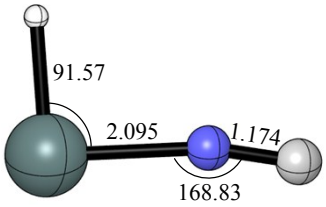
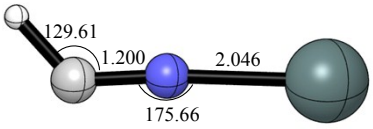
|  |  |  |
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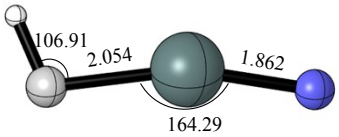
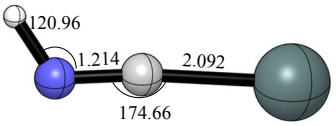
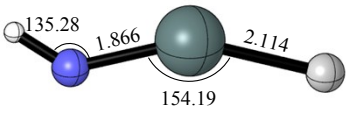
|  |  |  |
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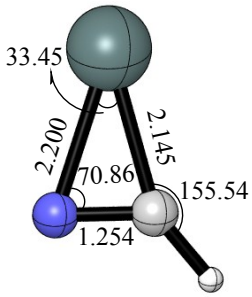
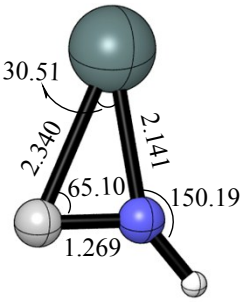
|  |  | |
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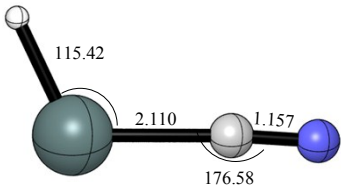
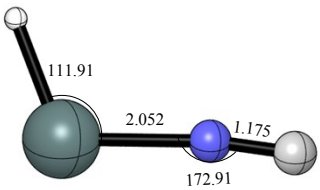
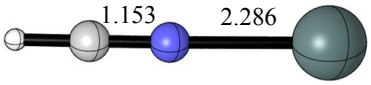
|  |  |  |
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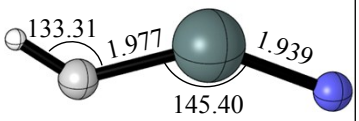
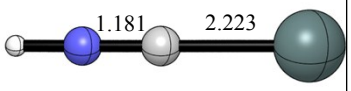
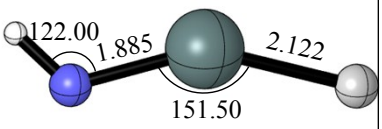
|  |  |  |
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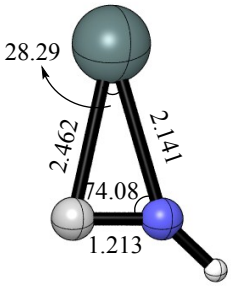
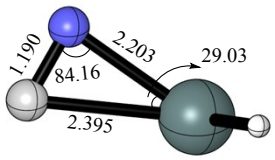
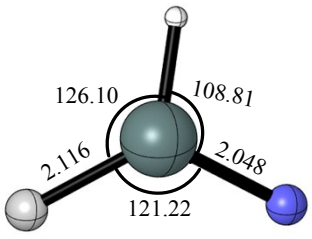
|  |  |  |
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Figure S3. Optimized geometries of isomers of the singlet and triplet neutral [H,Sn,C,N] at the B3LYP/def2-qzvpp level. Bond lengths are in angstroms and angles are in degrees.

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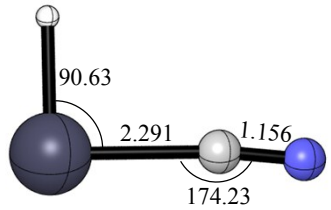
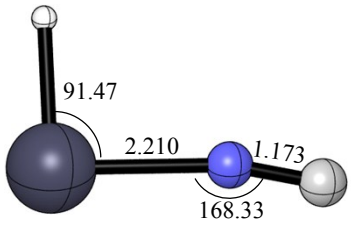
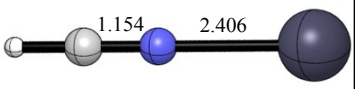
|  |  |  |
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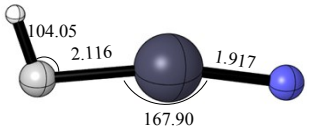
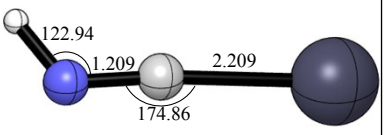
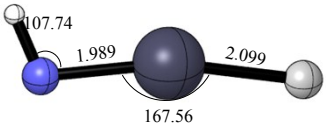
|  |  |  |
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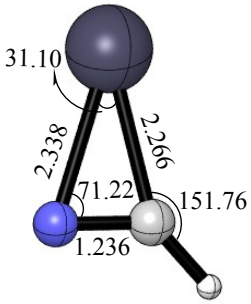
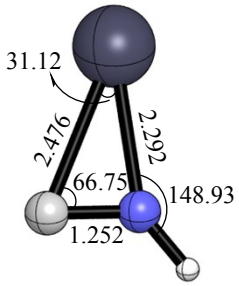
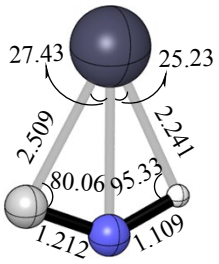
|  |  |  |
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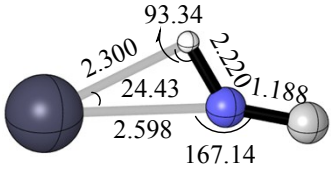
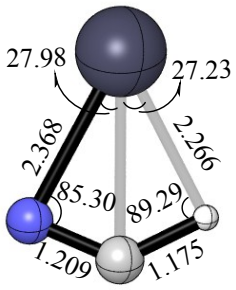
|  |  | |
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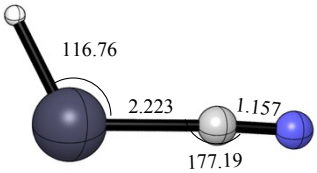
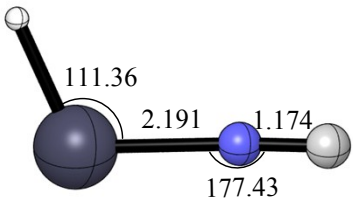
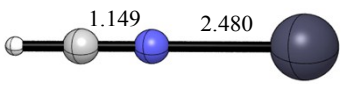
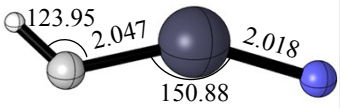
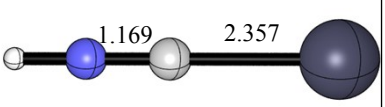
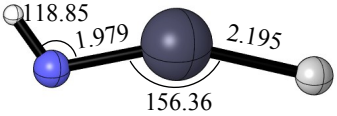
|  |  |  |
| $^{3}1$ | $^{3}2$ | $^{3}3$ |



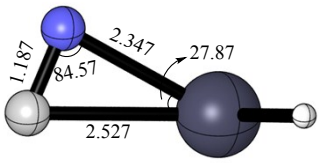

$^{3}$4



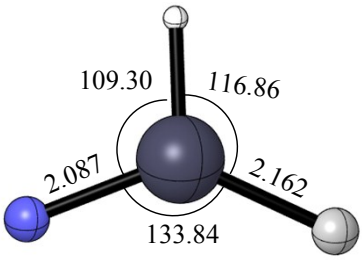

$^{3}$5




$^{3}$6




$^{3}$7




$^{3}$8

Figure S4. Optimized geometries of isomers of the singlet and triplet neutral [H,Pb,C,N] at the B3LYP/def2-qzvpp level. Bond lengths are in angstroms and angles are in degrees.

**5.**

Table S2 Charge analysis (q, |e|) of $^{2}$XCN and $^{2}$XNC (X=Sn, Pb) at the B3LYP/def2-QZVPP level.

| Speices | q(X) | | |
|---|---|---|---|
| | NPA | Hirshfeld | ADCH |
| SiCN $^{2}$1 | 0.647 | 0.260 | 0.208 |
| GeCN $^{2}$1 | 0.626 | 0.292 | 0.251 |
| SnCN $^{2}$1 | 0.670 | 0.340 | 0.308 |
| PbCN $^{2}$1 | 0.672 | 0.378 | 0.356 |
| SiNC $^{2}$2 | 0.771 | 0.248 | 0.191 |
| GeNC $^{2}$2 | 0.743 | 0.298 | 0.257 |
| SnNC $^{2}$2 | 0.785 | 0.360 | 0.327 |
| PbNC $^{2}$2 | 0.789 | 0.411 | 0.402 |

Table S3 Charge analysis (q, |e|) of $^{1}$HXCN and $^{1}$HXNC (X=Sn, Pb) at the B3LYP/def2-QZVPP level.

| Speices | q(X) | | | q(H) | | |
|---|---|---|---|---|---|---|
| | NPA | Hirshfeld | ADCH | NPA | Hirshfeld | ADCH |
| HSiCN $^{1}$1 | 0.814 | 0.331 | 0.151 | -0.271 | -0.087 | 0.032 |
| HGeCN $^{2}$1 | 0.791 | 0.372 | 0.233 | -0.262 | -0.095 | 0.000 |
| HSnCN $^{1}$1 | 0.670 | 0.449 | 0.341 | -0.335 | -0.123 | -0.053 |
| HPbCN $^{1}$1 | 0.946 | 0.503 | 0.458 | -0.341 | -0.138 | -0.106 |
| HSiNC $^{1}$2 | 0.985 | 0.335 | 0.142 | -0.303 | -0.099 | 0.030 |
| HGeNC $^{1}$2 | 0.965 | 0.398 | 0.264 | -0.293 | -0.105 | -0.005 |
| HSnNC $^{1}$2 | 0.672 | 0.484 | 0.386 | -0.363 | -0.131 | -0.058 |
| HPbNC $^{1}$2 | 1.113 | 0.548 | 0.519 | -0.370 | -0.145 | -0.112 |

**5.**

Table S4 Relative (kcal/mol) energies of doublet/quartet [X,C,N] and singlet/triplet [H，X,C,N] (X=Sn, Pb) structures and transition states at B3LYP/def2-qzvpp and single-point CCSD(T)/def2-qzvpp//B3LYP/ def2-qzvpp with inclusion of B3LYP/def2-qzvpp zero-point vibrational energies (ZPVE). We have also performed the T1 diagnostics of the relevant structures.

| Species | SP+ZPVE | T1 diagnostics |
|---|---|---|
| SnCN $^{2}$1 | 0.00 | 0.020910 |
| SnNC $^{2}$2 | 4.89 | 0.017288 |
| CSnN $^{2}$3 | 174.68 | 0.074056 |
| $^{2}$ts1/2($^{2}$A') | 12.89 | 0.019953 |
| $^{2}$ts1/2($^{2}$A'') | 11.31 | 0.017178 |
| $^{2}$ts2/3 | 174.31 | 0.103724 |
| SnCN $^{4}$1 | 64.63 | 0.033058 |
| SnNC $^{4}$2 | 84.92 | 0.062725 |
| CSnN $^{4}$3 | 176.91 | 0.075432 |
| *c*-SnCN $^{4}$4 | 88.29 | 0.048961 |
| $^{4}$ts1/4 | 91.65 | 0.058735 |
| $^{4}$ts2/4 | 87.91 | 0.053939 |
| $^{4}$ts3/4 | 189.98 | 0.074052 |
| $^{3}$Sn+CN | 94.44 | |
| $^{3}$C+$^{2}$SnN | 255.56 | |
| $^{4}$N+$^{3}$SnC | 201.78 | |
| | | |
| PbCN $^{2}$1 | 0.00 | 0.016669 |
| PbNC $^{2}$2 | 6.40 | 0.014678 |
| CPbN $^{2}$3 | 184.98 | 0.064738 |
| $^{2}$ts1/2($^{2}$A') | 11.21 | 0.016513 |
| $^{2}$ts1/2($^{2}$A'') | 10.05 | 0.014451 |
| $^{4}$ts2/3 | 199.76 | 0.059523 |
| PbCN $^{4}$1 | 81.54 | 0.039748 |
| PbNC $^{4}$2 | 84.97 | 0.057624 |
| CPbN $^{4}$3 | 187.29 | 0.045168 |
| *c*-PbCN $^{4}$4 | 87.03 | 0.065802 |
| $^{4}$ts1/4 | 90.81 | 0.087195 |
| $^{4}$ts2/4 | 87.72 | 0.053939 |
| $^{4}$ts3/4 | 195.70 | 0.043516 |
| $^{3}$Pb+$^{2}$CN | 92.27 | |
| $^{3}$C+$^{2}$PbN | 239.86 | |
| $^{4}$N+$^{3}$PbC | 196.87 | |
| | | |
| HSnCN $^{1}$1 | 0.00 | 0.015488 |

| | | |
|---|---|---|
| HSnNC $^{1}$2 | 4.80 | 0.016519 |
| SnNCH $^{1}$3 | 34.86 | 0.023648 |
| NSnCH $^{1}$4 | 142.34 | 0.055991 |
| SnCNH $^{1}$5 | 30.82 | 0.021294 |
| CSnNH $^{1}$6 | 149.12 | 0.038119 |
| *c*-SnCHN $^{1}$7 | 14.49 | 0.017605 |
| *c*-SnCNH $^{1}$8 | 38.47 | 0.019142 |
| $^{1}$ts1/2 | 11.68 | 0.016984 |
| $^{1}$ts1/5 | 69.01 | 0.032203 |
| $^{1}$ts1/7 | 51.68 | 0.015046 |
| $^{1}$ts1/8 | 54.89 | 0.021183 |
| $^{1}$ts2/3 | 81.02 | 0.027609 |
| $^{1}$ts2/7 | 148.10 | 0.106016 |
| $^{1}$ts2/7* | 38.90 | 0.022693 |
| $^{1}$ts2/8 | 64.61 | 0.017778 |
| $^{1}$ts3/7 | 46.14 | 0.027845 |
| $^{1}$ts4/6 | 192.66 | 0.130865 |
| $^{1}$ts4/7 | 168.67 | 0.101718 |
| $^{1}$ts5/8 | 53.10 | 0.025387 |
| $^{1}$ts6/8 | 150.71 | 0.061488 |
| $^{1}$ts7/8 | 76.30 | 0.021286 |
| $^{1}$Sn+HCN | 50.12 | |
| $^{1}$Sn+HNC | 64.40 | |
| HSnCN $^{3}$1 | 35.69 | 0.024380 |
| HSnNC $^{3}$2 | 46.40 | 0.020783 |
| SnNCH $^{3}$3 | 20.53 | 0.025424 |
| NSnCH $^{3}$4 | 137.57 | 0.063966 |
| HNCSn $^{3}$5 | 25.07 | 0.022733 |
| CSnNH $^{3}$6 | 131.81 | 0.089649 |
| *c*-SnCHN $^{3}$7 | 44.75 | 0.022227 |
| *c*-SnHNC $^{3}$8 | 51.83 | 0.021422 |
| CSn(H)N $^{3}$9 | 194.28 | 0.096351 |
| $^{3}$ts1/3 | 58.50 | 0.032684 |
| $^{3}$ts1/8 | 53.01 | 0.022197 |
| $^{3}$ts2/3 | 65.04 | 0.025180 |
| $^{3}$ts2/7 | 67.78 | 0.022420 |
| $^{3}$ts2/8 | 51.96 | 0.021025 |
| $^{3}$ts3/5 | 60.48 | 0.029897 |
| $^{3}$ts4/9 | 194.96 | 0.070548 |
| $^{3}$ts5/7 | 48.82 | 0.020075 |
| $^{3}$ts6/9 | 205.60 | 0.088033 |
| $^{3}$ts6/7 | 142.41 | 0.057099 |
| $^{3}$ts8/9 | 196.46 | 0.090130 |

| | | |
|---|---|---|
| $^{3}$Sn+HCN | 31.57 | |
| $^{3}$Sn+HNC | 45.84 | |
| $^{2}$CH+$^{2}$SnN | 187.79 | |
| $^{3}$NH+$^{3}$SnC | 187.48 | |
| $^{2}$H+$^{2}$CSnN | 237.32 | |
| HSn+CN | 97.30 | |
| $^{2}$H+$^{2}$SnCN | 62.63 | |
| $^{2}$H+$^{2}$SnNC | 67.52 | |
| | | |
| HPbCN $^{1}$1 | 0.00 | 0.014245 |
| HPbNC $^{1}$2 | 5.89 | 0.015083 |
| PbNCH $^{1}$3 | 32.55 | 0.015305 |
| HCPbN $^{1}$4 | 149.65 | 0.049274 |
| HNCPb $^{1}$5 | 29.86 | 0.022209 |
| HNPbC $^{1}$6 | 151.76 | 0.042286 |
| *c*-PbCHN $^{1}$7 | 14.78 | 0.013927 |
| *c*-PbCHN $^{1}$8 | 37.30 | 0.019809 |
| CHPbN $^{1}$9 | 44.90 | 0.019238 |
| CHPbN $^{1}$10 | 58.30 | 0.020286 |
| PbNHC $^{1}$11 | 33.34 | 0.019075 |
| $^{1}$Pb+HNC | 58.30 | |
| $^{1}$Pb+HCN | 44.01 | |
| $^{1}$ts1/2 | 9.63 | 0.015209 |
| $^{1}$ts1/5 | 65.43 | 0.028527 |
| $^{1}$ts1/7 | 44.03 | 0.013475 |
| $^{1}$ts2/11 | 29.65 | 0.015507 |
| $^{1}$ts2/9 | 42.23 | 0.016548 |
| $^{1}$ts3/10 | 75.38 | 0.021055 |
| $^{1}$ts3/7 | 37.76 | 0.012472 |
| $^{1}$ts4/6 | 203.56 | 0.112200 |
| $^{1}$ts4/7 | 159.70 | 0.090438 |
| $^{1}$ts5/8 | 49.67 | 0.037089 |
| $^{1}$ts6/8 | 159.95 | 0.056816 |
| $^{1}$ts7/11 | 34.06 | 0.020461 |
| $^{1}$ts7/8 | 73.22 | 0.024633 |
| $^{1}$ts8/10 | 57.52 | 0.016991 |
| $^{1}$ts8/9 | 48.60 | 0.017335 |
| HPbCN $^{3}$1 | 47.29 | 0.019888 |
| HPbNC $^{3}$2 | 58.25 | 0.018580 |
| PbNCH $^{3}$3 | 14.39 | 0.016882 |
| NPbCH $^{3}$4 | 147.84 | 0.057635 |
| PbCNH $^{3}$5 | 20.50 | 0.016727 |
| CPbNH $^{3}$6 | 139.91 | 0.068879 |

| | | |
|---|---|---|
| *c*-PbHNC $^{3}$7 | 61.22 | 0.018547 |
| CPb(H)N $^{3}$8 | 210.97 | 0.059222 |
| $^{3}$ts1/3 | 55.92 | 0.021741 |
| $^{3}$ts1/5 | 53.35 | 0.023508 |
| $^{3}$ts1/7 | 61.50 | 0.019765 |
| $^{3}$ts1/8 | 209.49 | 0.062674 |
| $^{3}$ts2/7 | 61.49 | 0.018011 |
| $^{3}$ts3/5 | 66.64 | 0.017658 |
| $^{3}$ts4/8 | 210.30 | 0.062718 |
| $^{3}$ts6/8 | 220.54 | 0.035097 |
| $^{3}$ts7/8 | 206.23 | 0.127857 |
| $^{3}$Pb+HCN | 25.36 | |
| $^{3}$Pb+HNC | 39.63 | |
| $^{2}$CH+$^{2}$PbN | 190.76 | |
| $^{3}$NH+$^{3}$PbC | 178.53 | |
| $^{2}$H+$^{2}$CPbN | 243.57 | |
| HPb+CN | 93.96 | |
| $^{2}$H+$^{2}$PbCN | 58.60 | |
| $^{2}$H+$^{2}$PbNC | 64.99 | |

**6.**

Table S5 Harmonic vibrational frequencies ($cm^{-1}$), infrared intensities (km/mol) (in parentheses), dipole moment (Debye), and rotational constants (GHZ) of doublet/doublet [Sn,C,N] and [Pb,C,N] at the B3LYP/def2-qzvpp level.

| Species | Frequencies (infrared intensity) | Dipole moments (Debye) | Rotational constants (GHZ) | | |
|---|---|---|---|---|---|
| SnCN $^2$1 | 159(3), 219(0), 370(65), 2210(19) | 4.7742 | 2.87844 | | |
| SnNC $^2$2 | 140(0), 401(92), 2090(328) | 4.7679 | 3.23304 | | |
| CSnN $^2$3 | 104(12), 523(71), 793(14) | 2.0840 | 4.99979 | | |
| SnCN $^4$1 | 273(0), 273(0), 375(0), 2140(14) | 3.7183 | 3.04861 | | |
| SnNC $^4$2 | 212(10), 212(10), 247(37), 2030(195) | 0.0314 | 3.08090 | | |
| CSnN $^4$3 | 172(27), 172(27), 491(5), 718(7) | 1.6623 | 5.07940 | | |
| *c*-SnCN $^4$4 | 136(43), 200(16), 1921(107) | 1.2570 | 55.8282357 | 4.1594252 | 3.8710189 |
| PbCN $^2$1 | 150(1), 323(66), 2214(21) | 5.6974 | 2.4846333 | | |
| PbNC $^2$2 | 45(0), 110(0), 343(90), 2100(345) | 5.9103 | 2.7550782 | | |
| CPbN $^2$3 | 115(12), 487(63), 727(4) | 2.0090 | 4.7709116 | | |
| PbCN $^4$1 | 234(0), 234(0), 236(6), 2060(44) | 2.7677 | 2.5200082 | | |
| PbNC $^4$2 | 179(4), 183(16), 193(16), 2047(682) | 1.5485 | 2.3803909 | | |
| CPbN $^4$3 | 43(19), 58(11), 450(12), 2060(44) | 0.3162 | 4.3541923 | | |
| *c*-PbCN $^4$4 | 109(3), 179(23), 2008(170) | 1.0635 | 57.5444298 | 2.7430372 | 2.6182309 |

Table S6 Harmonic vibrational frequencies ($cm^{-1}$), infrared intensities (km/mol) (in parentheses), dipole moment (Debye), and rotational constants (GHZ) of singlet/triplet [H,Sn,C,N] and [H,Pb,C,N] at the B3LYP/def2-qzvpp level.

| Species | Frequencies (infrared intensity) | Dipole moments (Debye) | Rotational constants (GHZ) | | |
|---|---|---|---|---|---|
| HSnCN $^{1}$1 | 164(4), 203(3), 3737(69), 626(55), 1746(361), 2246(39) | 4.7842 | 158.4060773 | 2.8550646 | 2.8045168 |
| HSnNC $^{1}$2 | 94(2), 131(1), 410(98), 629(50), 1735(414), 2117(373) | 4.8126 | 152.0822952 | 3.2327890 | 3.1655005 |
| SnNCH $^{1}$3 | 170(2), 285(40), 351(110),767(1120), 1802(611), 3031(33) | 1.0547 | 865.2329686 | 3.0541690 | 3.0434260 |
| NSnCH $^{1}$4 | 122(11), 143(7), 528(22), 793(5), 808(40), 2976(16) | 3.3513 | 241.8777821 | 4.8760432 | 4.7796889 |
| SnCNH $^{1}$5 | 206(1), 286(41), 390(1), 905(526), 1823(531), 3360(16) | 1.1647 | 763.8556690 | 2.7858281 | 2.7757050 |
| CSnNH $^{1}$6 | 92(12), 293(115), 464(115),546(29), 796(37), 3592(82) | 2.0901 | 120.3884692 | 4.8403120 | 4.6532254 |
| *c*-SnCHN $^{1}$7 | 405(15), 552(50), 758(30), 1064(131), 1600(93), 2998(59) | 2.3879 | 42.1832507 | 5.1225551 | 4.5678543 |
| *c*-SnCNH $^{1}$8 | 359(1), 497(48), 641(65), 1060(64), 1503(124), 3361(5) | 2.5539 | 42.5527581 | 4.8671160 | 4.3675614 |
| HCNSn $^{3}$1 | 204(2), 251(0), 400(31), 496(18), 1719(31), 2220(4) | 4.3600 | 211.1244519 | 2.9859452 | 2.9443037 |
| HNCSn $^{3}$2 | 124(0), 164(0), 427(46), 465(11), 1625(15), 2100(234) | 4.3352 | 193.9186054 | 3.2975964 | 3.2424583 |
| SnNCH $^{3}$3 | 189(30), 201(6), 598(19), 602(26), 2067(571), 3435(513) | 3.9622 | 291333.4488043 | 2.6074545 | 2.6074311 |
| NSnCH $^{3}$4 | 104(5), 306(15), 577(59), 613(82), 675(41), 3159(2) | 2.8155 | 70.2637648 | 5.1124139 | 4.7656628 |
| SnCNH $^{3}$5 | 230(49), 243(12), 279(207), 397(350), 1943(1001), 3681(338) | 2.4091 | 2122.9149338 | 2.6465634 | 2.6432681 |
| CSnNH $^{3}$6 | 82(9), 211(56), 483(1), 578(120), 773(11), 3515(37) | 2.3900 | 96.6928520 | 4.8559605 | 4.6237535 |
| *c*-SnCHN $^{3}$7 | 189(12), 196(29), 455(90), 695(184), 1753(305), 3052(59) | 1.8627 | 46.2546401 | 3.8522885 | 3.5561194 |
| *c*-NHSnC $^{3}$8 | 147(9), 209(1), 376(36), 438(10), 1591(14), 1945(7) | 3.3425 | 44.0065826 | 4.6542780 | 4.3940424 |
| NSnCH $^{3}$9 | 77(11), 173(17), 363(16), 521(38), 534(25), 1816(127) | 2.1078 | 19.6859487 | 5.8964081 | 4.5615705 |
| HPbCN $^{1}$1 | 150(2),183(3), 329(67), 562(42), 1629(445), 2242(38) | 5.7488 | 145.7645480 | 2.4689069 | 2.4277859 |
| HPbNC $^{1}$2 | 62(2), 103(2), 358(90), 554(39), 1616(486),2118(367) | 5.9723 | 139.0559261 | 2.7667664 | 2.7127906 |
| PbNCH $^{1}$3 | 148(22), 204(4), 254(33), 801(23), 2075(644), 3438(536) | 3.2505 | 551891.37741 | 0.10698 | 0.10698 |

| | | | | | |
|---|---|---|---|---|---|
| HCPbN $^{1}$4 | 132(10), 145(4), 489(22), 734(4), 865(24), 2943(27) | 3.1987 | 294.0896744 | 4.5825580 | 4.5122473 |
| HNCPb $^{1}$5 | 190(4), 259(46), 326(3), 843(625), 1836(669), 3380(19) | 1.2179 | 804.2800496 | 2.3828401 | 2.3758013 |
| HNPbC $^{1}$6 | 101(6), 130(6), 533(24, 650(16), 909(37), 3397(17) | 1.6083 | 303.1188083 | 4.4845332 | 4.4191534 |
| *c*-PbCHN $^{1}$7 | 170(2), 221(0), 335(37), 393(5), 1341(7),2214(12) | 4.9044 | 190.1130301 | 2.5635217 | 2.5294146 |
| *c*-PbCHN $^{1}$8 | 295(1), 437(54), 599(72), 983(99， 1571（196),3383(11) | 2.6518 | 43.5624126 | 3.9126136 | 3.5901589 |
| CHPbN $^{1}$9 | 229(7), 444(21), 655(4), 775(660), 1749(259), 2158(219) | 3.7619 | 45.00220 | 3.49389 | 3.24217 |
| CHPbN $^{1}$10 | 87(18), 107(1), 189(46), 823(273), 1918(57), 250(1890) | 3.4663 | 365.7808763 | 2.1152633 | 2.1031014 |
| PbNHC $^{1}$11 | 175(181), 431(181), 516(705), 775(6), 1832(330), 2598(96) | 3.3060 | 43.2963678 | 3.5211683 | 3.2563397 |
| HPbCN $^{3}$1 | 170(2), 221(0), 335(37), 393(5), 1341(7), 2214(12) | 4.9044 | 190.1130301 | 2.5635217 | 2.5294146 |
| HPbNC $^{3}$2 | 89(0), 130(0), 328(20), 334(12), 1103(27), 2093(133) | 5.0574 | 164.8698876 | 2.7692292 | 2.7234843 |
| PbNCH $^{3}$3 | 161(31), 171(2), 671(22), 673(26), 2125(354), 3436(425) | 3.8916 | 1427740.8915008 | 2.1315915 | 2.1315883 |
| NPbCH $^{3}$4 | 105(7), 259(21), 517(37), 533(74), 696(98), 3093 (10) | 2.5682 | 83.5155922 | 4.6597915 | 4.4135362 |
| PbCNH $^{3}$5 | 149(130), 149(130), 208(5), 208(5), 236(3), 2024(1035), 3822(934) | 3.1624 | 0.0000000 | 2.1722489 | 2.1722489 |
| CPbNH $^{3}$6 | 71(11), 173(47), 431(3), 628(88), 729(19), 3446(20) | 2.2669 | 115.2486825 | 4.4170551 | 4.2540145 |
| *c*-PbHNC $^{3}$7 | 103(8), 156(1), 297(2), 320(39), 1058(16), 197(9) | 4.2260 | 42.5414493 | 3.8068986 | 3.6386664 |
| CPb(H)N $^{3}$8 | 76(14), 209(5), 258(9), 477(95), 510(2), 1702(134) | 1.6524 | 25.9536307 | 5.0991843 | 4.2618470 |

**7.**

Table S7 Selected standard bond distances (r) (in Å) of reference molecules.

| X | r(X-C) | r(X=C) | r(X-N) | r(X=N) |
|---|---|---|---|---|
| | $XH_3$-$CH_3$ | $XH_2$=$CH_2$ | $XH_3$-$NH_2$ | $XH_2$=NH |
| C | 1.527 | 1.324 | 1.436 | 1.263 |
| Si | 1.877 | 1.701 | 1.738 | 1.593 |
| Ge | 1.965 | 1.775 | 1.853 | 1.710 |
| Sn | 2.159 | 1.960 | 2.049 | 1.909 |
| Pb | 2.242 | 2.017 | 2.161 | 1.997 |

**8.**

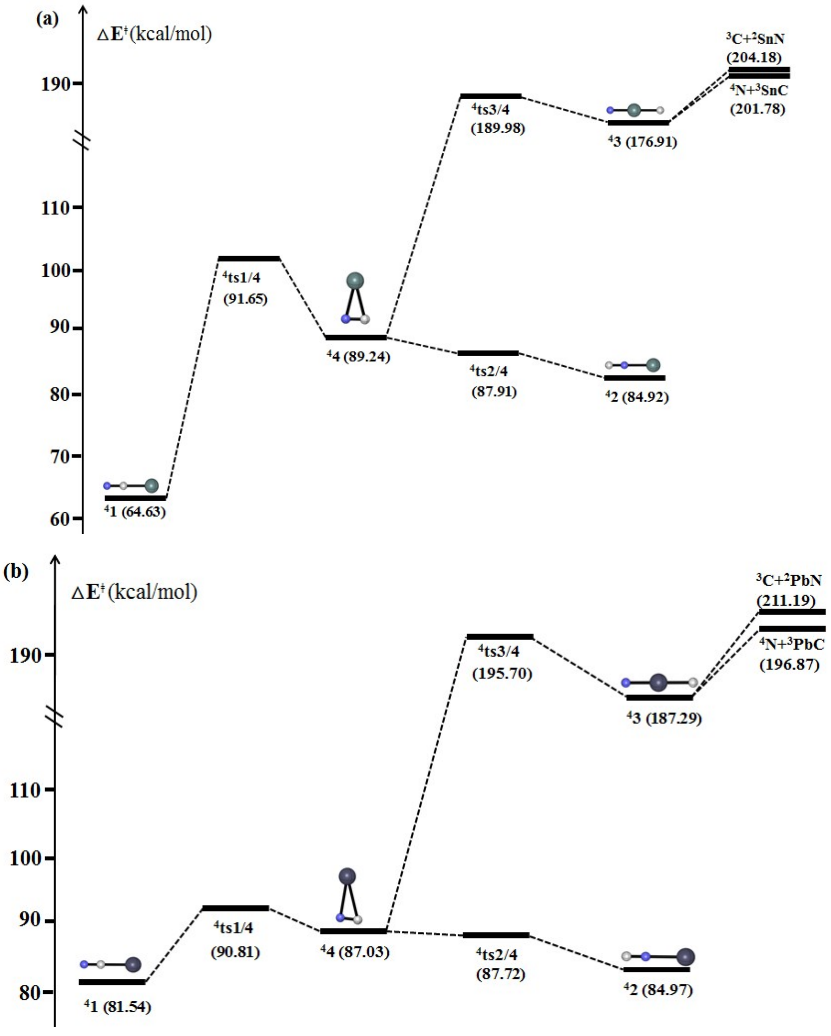



Fig. S5 Schematic potential energy surfaces of quartet [X,C,N] (X=Sn, Pb) at the level of CCSD(T)/def2-QZVPP//B3LYP/def2-QZVPP+ZPVE in the parentheses.

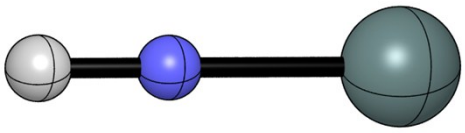
**9.** Table S8 Cartesian coordinates of doublet/doublet [X,C,N] and singlet/triplet [H,X,C,N] (X=Sn, Pb) structures and transition states at the B3LYP/def2-QZVP level of theory.

CNSn_doublet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | -2.756016 |
| C | 0.000000 | 0.000000 | -1.597546 |
| Sn | 0.000000 | 0.000000 | 0.577548 |

CNSn_doublet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000618 | -2.720656 | 0.000000 |
| N | -0.000529 | -1.544804 | 0.000000 |
| Sn | 0.000000 | 0.542751 | 0.000000 |

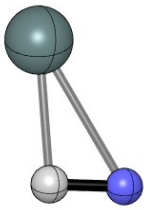


CNSn_doublet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.092172 | 2.098703 | 0.000000 |
| Sn | 0.000000 | 0.007437 | 0.000000 |
| N | -0.079005 | -1.852010 | 0.000000 |

CNSn_doublet_ts1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.588042 | -1.686478 | 0.000000 |
| N | -0.504036 | -2.109737 | 0.000000 |
| Sn | 0.000000 | 0.497741 | 0.000000 |

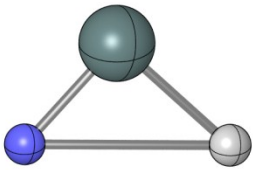


CNSn_doublet_ts2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.630082 | -1.873185 | 0.000000 |
| N | -0.540071 | -1.807291 | 0.000000 |
| Sn | 0.000000 | 0.477803 | 0.000000 |

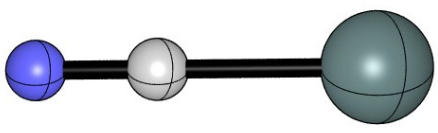
CNSn_doublet_ts3-B3LYP -def2-qzvpp

| | | | |
|---|---|---|---|
| C | 1.556792 | -1.190815 | 0.000000 |
| N | -1.334393 | -1.084525 | 0.000000 |
| Sn | 0.000000 | 0.294731 | 0.000000 |



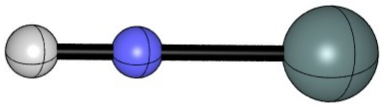
CNSn_quartet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | -2.691129 |
| C | 0.000000 | 0.000000 | -1.528984 |
| Sn | 0.000000 | 0.000000 | 0.560236 |



CNSn_quartet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | -2.772487 |
| N | 0.000000 | 0.000000 | -1.601565 |
| Sn | 0.000000 | 0.000000 | 0.556918 |

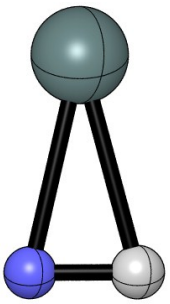


CNSn_quartet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | 2.062037 |
| Sn | 0.000000 | 0.000000 | 0.012975 |
| N | 0.000000 | 0.000000 | -1.860140 |

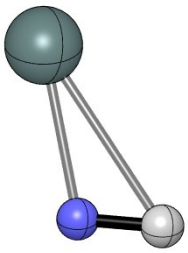
CNSn_quartet_4-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.637304 | -1.892375 | 0.000000 |
| N | -0.546261 | -1.897874 | 0.000000 |
| Sn | 0.000000 | 0.492787 | 0.000000 |



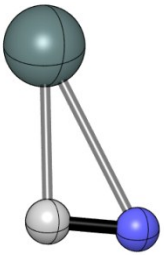
CNSn_quartet_ts1-B3LYP -def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.559448 | -2.378560 | 0.000000 |
| N | -0.479527 | -1.838474 | 0.000000 |
| Sn | 0.000000 | 0.542814 | 0.000000 |



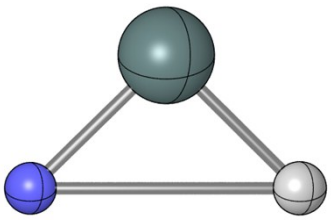
CNSn_quartet_ts2-B3LYP -def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.591310 | -1.751184 | 0.000000 |
| N | -0.506837 | -2.163287 | 0.000000 |
| Sn | 0.000000 | 0.513002 | 0.000000 |



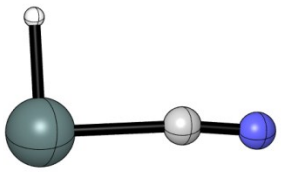
CNSn_quartet_ts3-B3LYP -def2-qzvpp

| | | | |
|---|---|---|---|
| C | 1.600614 | -1.031663 | 0.000000 |
| N | -1.371955 | -1.291029 | 0.000000 |
| Sn | 0.000000 | 0.304544 | 0.000000 |



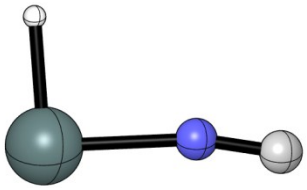
HCNSn_singlet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | -0.207592 | -2.764053 | 0.000000 |
| H | 1.773459 | 0.541982 | 0.000000 |
| C | -0.053385 | -1.618378 | 0.000000 |
| Sn | 0.000000 | 0.570333 | 0.000000 |



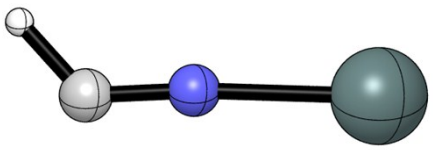
HCNSn_singlet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.777635 | 0.559912 | 0.000000 |
| Sn | 0.000000 | 0.532876 | 0.000000 |
| C | -0.266645 | -2.711190 | 0.000000 |
| N | -0.025395 | -1.562369 | 0.000000 |



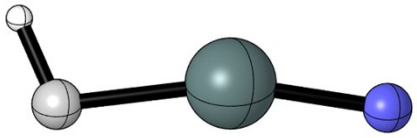
HCNSn_singlet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | -0.103730 | -2.651206 | 0.000000 |
| H | 0.679856 | -3.412676 | 0.000000 |
| N | -0.008211 | -1.455348 | 0.000000 |
| Sn | 0.000000 | 0.590147 | 0.000000 |



HCNSn_singlet_4-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 1.548113 | -1.299297 | 0.000000 |
| Sn | 0.000000 | 0.051243 | 0.000000 |
| H | 2.485746 | -0.713610 | 0.000000 |
| N | -1.682061 | 0.849605 | 0.000000 |



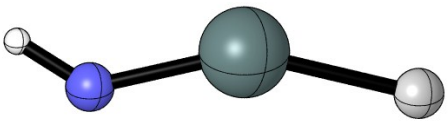
HCNSn_singlet_5-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 0.719009 | -3.286575 | 0.000000 |
| N | -0.106295 | -2.682846 | 0.000000 |
| Sn | 0.000000 | 0.618218 | 0.000000 |
| C | 0.004176 | -1.474070 | 0.000000 |



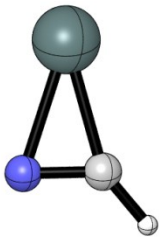
HCNSn_singlet_6-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -2.410340 | -1.071490 | 0.000000 |
| N | -1.401380 | -1.131560 | 0.000000 |
| Sn | 0.000000 | 0.100063 | 0.000000 |
| C | 2.036666 | 0.664879 | 0.000000 |



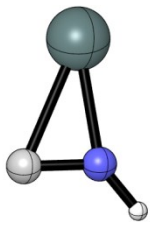
HCNSn_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.279053 | -2.436269 | 0.000000 |
| C | 0.575132 | -1.597957 | 0.000000 |
| N | -0.675692 | -1.625329 | 0.000000 |
| Sn | 0.000000 | 0.468026 | 0.000000 |



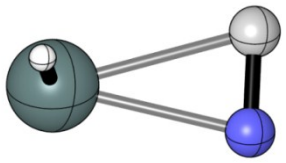
HCNSn_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.187993 | -2.349775 | 0.000000 |
| N | -0.491349 | -1.604745 | 0.000000 |
| C | 0.771239 | -1.729642 | 0.000000 |
| Sn | 0.000000 | 0.479217 | 0.000000 |



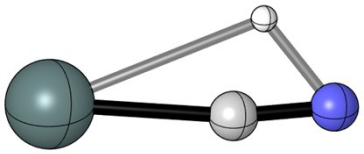
HCNSn_singlet_1_HCNSn_singlet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -0.562877 | 0.312820 | 1.711716 |
| C | 1.872139 | 0.618860 | -0.071718 |
| N | 1.815692 | -0.541700 | 0.073197 |
| Sn | -0.467596 | -0.004682 | -0.035876 |



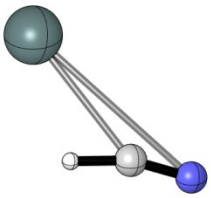
HCNSn_singlet_1_HCNSn_singlet_5-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| Sn | -0.617796 | 0.000854 | -0.000001 |
| H | 1.942136 | 1.020587 | 0.000024 |
| N | 2.783648 | -0.033018 | 0.000006 |
| C | 1.577019 | -0.138696 | 0.000001 |



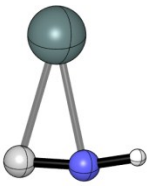
HCNSn_singlet_1_HCNSn_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.406114 | 1.116632 | 0.000010 |
| C | -2.151673 | 0.305183 | 0.000003 |
| N | -3.141279 | -0.282598 | -0.000002 |
| Sn | 0.726102 | -0.019391 | 0.000000 |



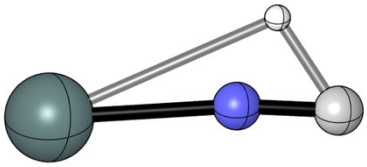
HCNSn_singlet_1_HCNSn_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.748380 | 1.441401 | 0.000003 |
| C | -1.833448 | -0.763815 | -0.000001 |
| N | -1.902668 | 0.443195 | 0.000001 |
| Sn | 0.521355 | 0.000782 | 0.000000 |



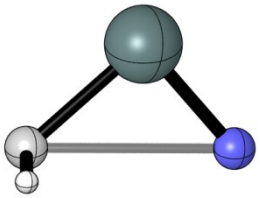
HCNSn_singlet_2_HCNSn_singlet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -2.192750 | 1.022629 | 0.000287 |
| C | -2.856460 | -0.133869 | 0.000128 |
| N | -1.641550 | -0.005269 | 0.000077 |
| Sn | 0.616447 | -0.003651 | -0.000032 |



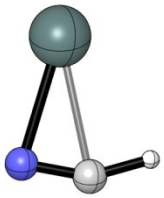
HCNSn_singlet_2_HCNSn_singlet_7-B3LYP-def2-qzvpp*

| | | | |
|---|---|---|---|
| H | 2.177984 | 0.754107 | 0.842813 |
| C | 1.861240 | 0.426311 | -0.167311 |
| N | -0.799752 | 1.532326 | -0.012795 |
| Sn | -0.154943 | -0.280765 | 0.005012 |



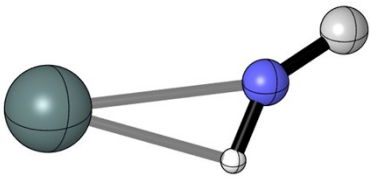
HCNSn_singlet_2_HCNSn_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.566438 | -1.629341 | 0.000000 |
| C | 0.516761 | -1.921844 | 0.000000 |
| N | -0.666715 | -1.704067 | 0.000000 |
| Sn | 0.000000 | 0.501777 | 0.000000 |



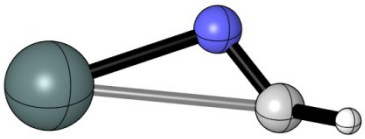
HCNSn_singlet_2_HCNSn_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.446218 | 1.054610 | 0.000053 |
| C | 3.122603 | -0.254001 | 0.000012 |
| N | 2.030327 | 0.186917 | -0.000016 |
| Sn | -0.687883 | -0.016780 | 0.000000 |



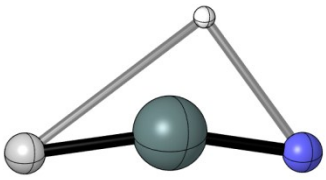
HCNSn_singlet_3_HCNSn_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 3.037883 | -0.717828 | 0.500849 |
| C | 2.214415 | -0.361045 | -0.126615 |
| N | 1.497941 | 0.598649 | 0.021037 |
| Sn | -0.536199 | -0.026129 | 0.002232 |



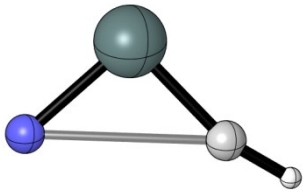
HCNSn_singlet_4_HCNSn_singlet_6-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | 1.880609 | -0.278411 | 0.000572 |
| Sn | -0.020323 | 0.032101 | -0.000187 |
| C | -2.109435 | -0.224275 | 0.000665 |
| H | 0.508513 | 1.689493 | 0.001367 |



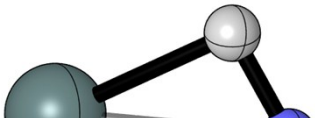
HCNSn_singlet_4_HCNSn_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 2.354125 | -1.687966 | 0.000000 |
| C | 1.406553 | -1.141230 | 0.000000 |
| N | -1.541920 | -1.043353 | 0.000000 |
| Sn | 0.000000 | 0.316776 | 0.000000 |



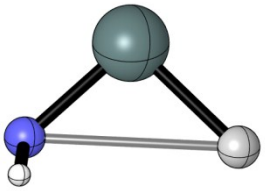
HCNSn_singlet_5_HCNSn_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 2.782444 | -0.706095 | 0.498074 |
| C | 1.544915 | 0.746682 | 0.015980 |



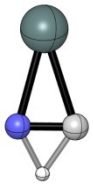
| | | | |
|---|---|---|---|
| N | 2.018050 | -0.389664 | -0.103700 |
| Sn | -0.523566 | -0.020927 | 0.002639 |

HCNSn_singlet_6_HCNSn_singlet_8-B3LYP-def2-qzvpp



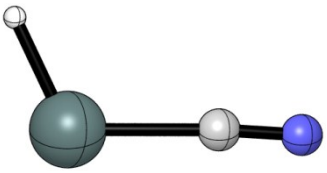
| | | | |
|---|---|---|---|
| H | 1.838838 | 1.222396 | 0.671078 |
| C | -1.209049 | 1.507089 | -0.024536 |
| N | 1.637830 | 0.604558 | -0.119835 |
| Sn | -0.120987 | -0.289937 | 0.006300 |

HCNSn_singlet_7_HCNSn_singlet_8-B3LYP-def2-qzvpp



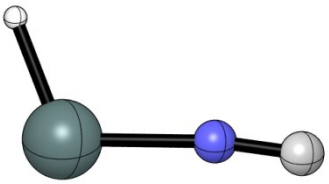
| | | | |
|---|---|---|---|
| H | -0.039416 | -2.740525 | 0.000000 |
| C | 0.693704 | -1.692190 | 0.000000 |
| N | -0.588972 | -1.680125 | 0.000000 |
| Sn | 0.000000 | 0.493091 | 0.000000 |

HCNSn_triplet_1-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 1.583789 | 1.237021 | 0.000000 |
| Sn | 0.000000 | 0.543530 | 0.000000 |
| C | -0.065371 | -1.565326 | 0.000000 |
| N | -0.170223 | -2.717369 | 0.000000 |

HCNSn_triplet_2-B3LYP-def2-qzvpp



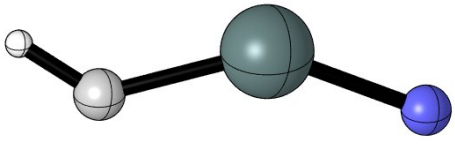
| | | | |
|---|---|---|---|
| H | 1.634337 | 1.130639 | 0.000000 |
| Sn | 0.000000 | 0.516090 | 0.000000 |
| N | -0.046595 | -1.535518 | 0.000000 |
| C | -0.218028 | -2.697752 | 0.000000 |

HCNSn_triplet_3-B3LYP-def2-qzvpp



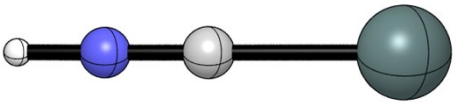
| | | | |
|---|---|---|---|
| H | -3.861355 | 0.021255 | 0.000175 |
| C | -2.796744 | 0.002555 | -0.000070 |
| N | -1.643452 | -0.009276 | 0.000040 |
| Sn | 0.642920 | 0.000567 | -0.000001 |

HCNSn_triplet_4-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 2.790939 | -0.372754 | 0.000000 |
| C | 1.773175 | -0.752686 | 0.000000 |
| Sn | 0.000000 | 0.120494 | 0.000000 |
| N | -1.918570 | -0.162260 | 0.000000 |

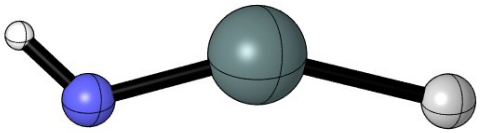
HCNSn_triplet_5-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| Sn | 0.000000 | 0.649549 | 0.000000 |
| C | -0.000781 | -1.573112 | 0.000000 |
| H | 0.004367 | -3.757076 | 0.000000 |
| N | 0.000045 | -2.754529 | 0.000000 |

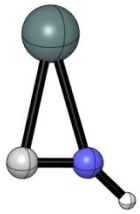
HCNSn_triplet_6-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -2.405577 | -0.805048 | 0.000000 |
| N | -1.436611 | -1.113445 | 0.000000 |
| Sn | 0.000000 | 0.106885 | 0.000000 |
| C | 2.076976 | 0.542486 | 0.000000 |



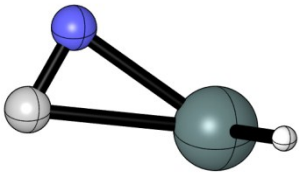
HCNSn_triplet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.135410 | -2.680986 | 0.000000 |
| N | -0.470463 | -1.916708 | 0.000000 |
| C | 0.738108 | -1.809289 | 0.000000 |
| Sn | 0.000000 | 0.539073 | 0.000000 |



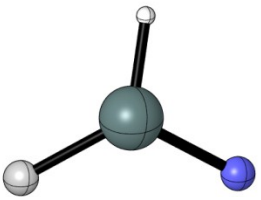
HCNSn_triplet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | -1.880883 | -0.598669 | 0.091737 |
| N | -1.686306 | 0.571494 | -0.007895 |
| Sn | 0.437774 | -0.012590 | -0.040281 |
| H | 1.200736 | 0.221047 | 1.518891 |



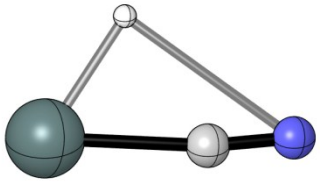
HCNSn_triplet_9-B3LYP-qzvpp-1

| | | | |
|---|---|---|---|
| H | 0.217825 | -1.821137 | 0.435630 |
| C | -1.859863 | 0.875727 | 0.062636 |
| N | 1.767469 | 0.801013 | 0.046200 |
| Sn | -0.028619 | -0.180806 | -0.022697 |



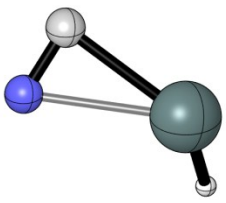
HCNSn_triplet_1_HCNSn_triplet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| Sn | -0.590478 | -0.017326 | -0.000021 |
| C | 1.607001 | -0.115930 | 0.000059 |
| N | 2.770582 | -0.009741 | 0.000099 |
| H | 0.487829 | 1.630066 | -0.000004 |

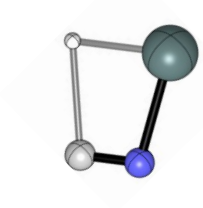


HCNSn_triplet_1_HCNSn_triplet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.090942 | 1.290991 | 0.927605 |
| Sn | 0.453030 | -0.025541 | -0.026113 |
| C | -1.696578 | -0.592621 | 0.215753 |
| N | -1.937570 | 0.505967 | -0.130928 |

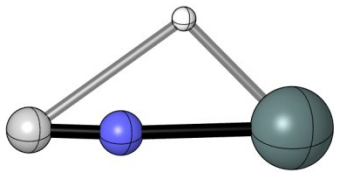


HCNSn_triplet_2_HCNSn_triplet_3-B3LYP-def2-qzvpp



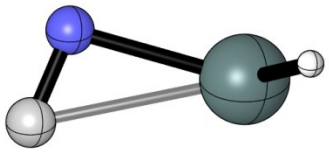
| | | | |
|---|---|---|---|
| H | -0.320080 | 1.734354 | 0.000027 |
| C | -2.146433 | 0.470337 | -0.000002 |
| N | -1.648009 | -0.591138 | -0.000021 |
| Sn | 0.494695 | -0.008368 | 0.000003 |

HCNSn_triplet_2_HCNSn_triplet_7-B3LYP-def2-qzvpp



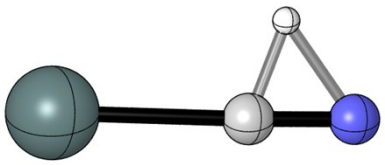
| | | | |
|---|---|---|---|
| H | -0.813172 | 1.391791 | 0.000002 |
| C | -2.811268 | -0.037840 | 0.000011 |
| N | -1.626245 | -0.075751 | 0.000006 |
| Sn | 0.581290 | -0.012690 | -0.000002 |

HCNSn_triplet_2_HCNSn_triplet_8-B3LYP-def2-qzvpp



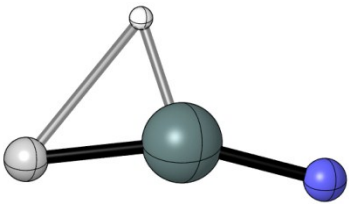
| | | | |
|---|---|---|---|
| H | 1.204904 | 0.163173 | 1.532270 |
| Sn | 0.451925 | -0.018637 | -0.039587 |
| C | -2.080366 | -0.527835 | 0.082299 |
| N | -1.616997 | 0.562243 | -0.006675 |

HCNSn_triplet_3_HCNSn_triplet_5-B3LYP-def2-qzvpp



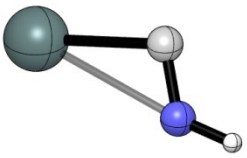
| | | | |
|---|---|---|---|
| Sn | -0.627731 | -0.001733 | -0.000002 |
| H | 2.037158 | 1.051528 | 0.000025 |
| N | 2.815432 | -0.076364 | 0.000006 |
| C | 1.606899 | -0.071725 | 0.000003 |

HCNSn_triplet_4_HCNSn_triplet_9-B3LYP-def2-qzvpp



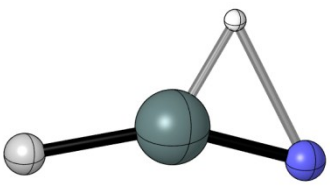
| | | | |
|---|---|---|---|
| H | -0.720285 | 1.654480 | 0.000001 |
| N | 1.931400 | -0.255794 | 0.000000 |
| Sn | -0.009614 | 0.048244 | 0.000000 |
| C | -2.053139 | -0.379352 | 0.000000 |

HCNSn_triplet_5_HCNSn_triplet_7-B3LYP-def2-qzvpp



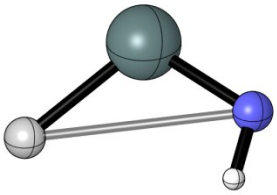
| | | | |
|---|---|---|---|
| Sn | 0.000000 | 0.568661 | 0.000000 |
| C | 0.619650 | -1.612954 | 0.000000 |
| N | -0.455417 | -2.217100 | 0.000000 |
| H | -0.529980 | -3.235632 | 0.000000 |

HCNSn_triplet_6_HCNSn_triplet_9-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 0.870376 | 1.581849 | 0.000178 |
| N | 1.869456 | -0.410206 | 0.000042 |
| Sn | -0.023725 | 0.064010 | -0.000016 |
| C | -2.128390 | -0.318485 | 0.000057 |

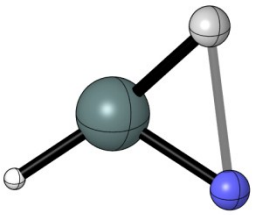
HCNSn_triplet_6_HCNSn_triplet_7-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 1.440093 | 1.753694 | 0.000327 |
| C | -1.669617 | 1.180302 | 0.000098 |
| N | 1.628871 | 0.745861 | 0.000168 |
| Sn | -0.056490 | -0.281131 | -0.000042 |

HCNSn_triplet_8_HCNSn_triplet_9-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.670574 | -0.741496 | 0.687306 |
| C | 1.341715 | 1.267126 | 0.081374 |
| N | 1.373841 | -1.149976 | 0.009869 |
| Sn | -0.319932 | 0.023771 | -0.024893 |

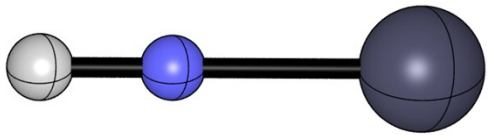


CNPb_doublet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | -0.008848 | -3.039857 | 0.000000 |
| C | 0.010322 | -1.881774 | 0.000000 |
| Pb | 0.000000 | 0.397191 | 0.000000 |

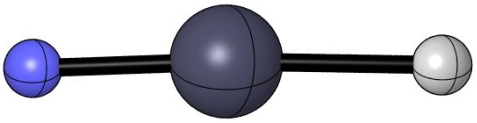
CNPb_doublet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | -3.004326 |
| N | 0.000000 | 0.000000 | -1.829789 |
| Pb | 0.000000 | 0.000000 | 0.376030 |



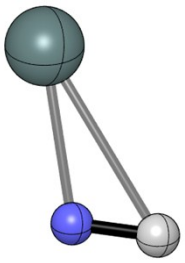
CNPb_doublet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 1.668569 | 1.335678 | 0.000000 |
| Pb | 0.000000 | 0.010349 | 0.000000 |
| N | -1.430202 | -1.266097 | 0.000000 |



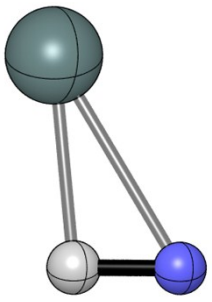
CNPb_doublet_ts1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.591949 | -1.943678 | 0.000000 |
| N | -0.507385 | -2.347028 | 0.000000 |
| Pb | 0.000000 | 0.342576 | 0.000000 |



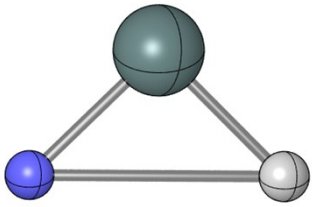
CNPb_doublet_ts2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.628841 | -2.141659 | 0.000000 |
| N | -0.539006 | -2.034675 | 0.000000 |
| Pb | 0.000000 | 0.330399 | 0.000000 |



CNPb_doublet_ts3-def2-qzvpp-B3LYP

| | | | |
|---|---|---|---|
| C | 1.506304 | -1.496854 | 0.000000 |
| N | -1.291118 | -1.321775 | 0.000000 |
| Pb | 0.000000 | 0.222360 | 0.000000 |

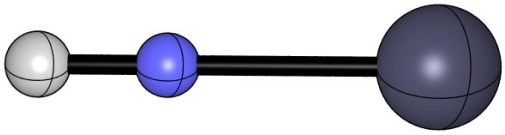


CNPb_quartet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | -3.025077 |
| C | 0.000000 | 0.000000 | -1.856929 |
| Pb | 0.000000 | 0.000000 | 0.394111 |

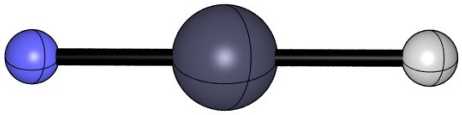
CNPb_quartet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | -3.189310 |
| N | 0.000000 | 0.000000 | -2.023152 |
| Pb | 0.000000 | 0.000000 | 0.406072 |



CNPb_quartet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | 2.189949 |
| Pb | 0.000000 | 0.000000 | 0.014207 |
| N | 0.000000 | 0.000000 | -2.043518 |



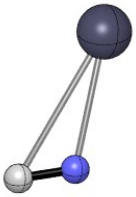
CNPb_quartet_4-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | -0.538206 | -2.378642 | 0.000000 |
| C | 0.627907 | -2.503517 | 0.000000 |
| Pb | 0.000000 | 0.386239 | 0.000000 |

CNPb_quartet_ts1-def2-qzvpp-B3LYP

| | | | |
|---|---|---|---|
| C | 0.499330 | -2.432927 | 0.000000 |
| N | -0.427997 | -3.136244 | 0.000000 |
| Pb | 0.000000 | 0.445747 | 0.000000 |

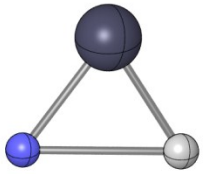
CNPb_quartet_ts2-def2-qzvpp-B3LYP



| | | | |
|---|---|---|---|
| C | 0.540907 | -2.983648 | 0.000000 |
| N | -0.463635 | -2.397541 | 0.000000 |
| Pb | 0.000000 | 0.422984 | 0.000000 |

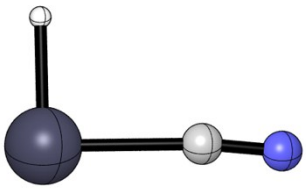
CNPb_quartet_ts3-def2-qzvpp-B3LYP

| | | | |
|---|---|---|---|
| C | 1.417358 | -1.492894 | 0.000000 |
| N | -1.214879 | -1.762382 | 0.000000 |
| Pb | 0.000000 | 0.259683 | 0.000000 |



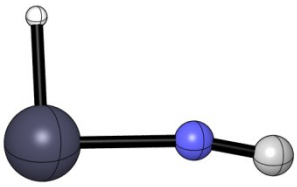
HCNPb_singlet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | -0.210242 | -3.043361 | 0.000000 |
| H | 1.847547 | 0.363927 | 0.000000 |
| C | -0.062642 | -1.896487 | 0.000000 |
| Pb | 0.000000 | 0.394128 | 0.000000 |



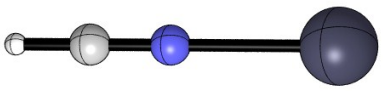
HCNPb_singlet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.851963 | 0.404534 | 0.000000 |
| Pb | 0.000000 | 0.370471 | 0.000000 |
| N | -0.026550 | -1.838990 | 0.000000 |
| C | -0.277685 | -2.985033 | 0.000000 |



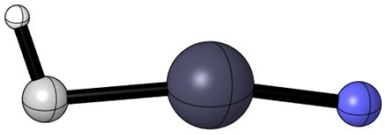
HCNPb_singlet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| C | 0.001002 | -3.113953 | 0.000000 |
| H | 0.003050 | -4.178537 | 0.000000 |
| N | -0.001295 | -1.959713 | 0.000000 |
| Pb | 0.000000 | 0.446101 | 0.000000 |



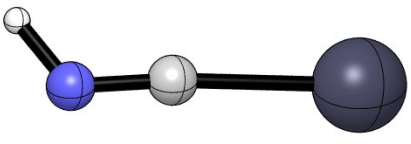
HCNPb_singlet_4-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 2.386699 | -1.044619 | 0.000000 |
| Pb | 0.000000 | 0.027289 | 0.000000 |
| C | 1.403542 | -1.556419 | 0.000000 |
| N | -1.543993 | 1.163635 | 0.000000 |



HCNPb_singlet_5-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| N | -0.103102 | -2.984544 | 0.000000 |
| H | 0.701466 | -3.613050 | 0.000000 |
| C | 0.003374 | -1.780359 | 0.000000 |
| Pb | 0.000000 | 0.429110 | 0.000000 |



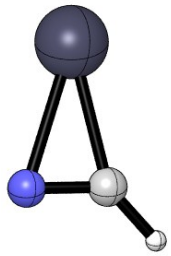
HCNPb_singlet_6-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.823972 | -1.666088 | 0.000000 |

| | | | |
|---|---|---|---|
| N | -0.803674 | -1.774993 | 0.000000 |
| Pb | 0.000000 | 0.044752 | 0.000000 |
| C | 1.241615 | 1.736897 | 0.000000 |

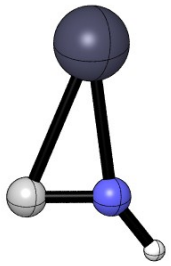
HCNPb_singlet_7-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.306421 | -2.667461 | 0.000000 |
| C | 0.564753 | -1.862827 | 0.000000 |
| N | -0.670705 | -1.908334 | 0.000000 |
| Pb | 0.000000 | 0.331741 | 0.000000 |



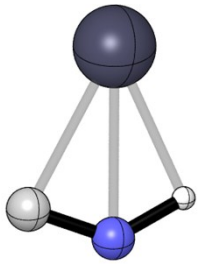
HCNPb_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.182571 | -2.640033 | 0.000000 |
| N | -0.484194 | -1.898167 | 0.000000 |
| C | 0.761988 | -2.014280 | 0.000000 |
| Pb | 0.000000 | 0.341620 | 0.000000 |



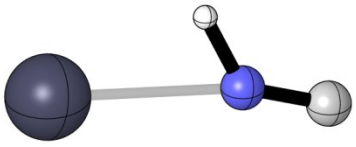
HCNPb_singlet_9-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.296183 | -1.473066 | 0.000000 |
| N | 0.454904 | -2.195941 | 0.000000 |
| C | -0.746752 | -2.040384 | 0.000000 |
| Pb | 0.000000 | 0.354719 | 0.000000 |



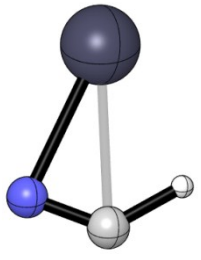
HCNPb_singlet_10-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.619161 | 1.010947 | 0.000152 |
| C | 3.316895 | -0.152692 | 0.000005 |
| N | 2.150860 | 0.074792 | 0.000120 |
| Pb | -0.446056 | -0.007541 | -0.000012 |

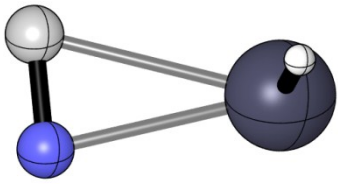


HCNPb_singlet_11-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.448633 | -1.443285 | 0.000000 |
| Pb | 0.000000 | 0.341568 | 0.000000 |
| C | 0.526875 | -2.172731 | 0.000000 |
| N | -0.658555 | -1.932700 | 0.000000 |



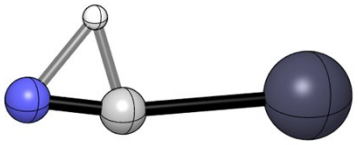
HCNPb_singlet_1_HCNPb_singlet_2-B3LYP-def2-



qzvpp

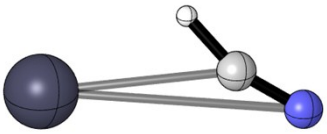
| | | | |
|---|---|---|---|
| H | 0.433988 | 0.351295 | 1.793598 |
| C | -2.142993 | 0.610213 | -0.083351 |
| N | -2.035913 | -0.544449 | 0.086477 |
| Pb | 0.325309 | -0.002456 | -0.023156 |

HCNPb_singlet_1_HCNPb_singlet_5-B3LYP-def2-qzvpp



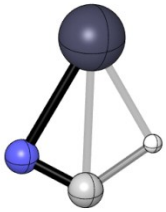
| | | | |
|---|---|---|---|
| H | 1.015855 | -2.236687 | 0.000000 |
| C | -0.160453 | -1.901094 | 0.000000 |
| N | -0.007591 | -3.097180 | 0.000000 |
| Pb | 0.000000 | 0.430774 | 0.000000 |

HCNPb_singlet_1_HCNPb_singlet_7-B3LYP-def2-qzvpp



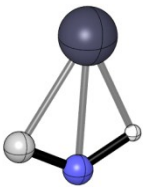
| | | | |
|---|---|---|---|
| H | 1.682630 | 1.111656 | 0.000011 |
| C | 2.422241 | 0.293298 | -0.000005 |
| N | 3.423519 | -0.275242 | 0.000002 |
| Pb | -0.490009 | -0.011521 | 0.000000 |

HCNPb_singlet_2_HCNPb_singlet_11-B3LYP-def2-qzvpp



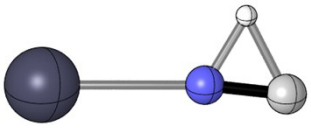
| | | | |
|---|---|---|---|
| H | 1.430074 | -1.127425 | 0.000000 |
| C | 0.526477 | -2.161799 | 0.000000 |
| N | -0.655562 | -1.886685 | 0.000000 |
| Pb | 0.000000 | 0.332988 | 0.000000 |

HCNPb_singlet_2_HCNPb_singlet_9-B3LYP-def2-qzvpp



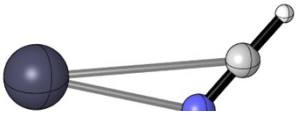
| | | | |
|---|---|---|---|
| H | -1.241733 | 1.310059 | 0.000025 |
| C | -2.005317 | -0.730340 | -0.000015 |
| N | -2.164484 | 0.467946 | 0.000008 |
| Pb | 0.346647 | -0.002483 | 0.000000 |

HCNPb_singlet_3_HCNPb_singlet_10-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 2.589562 | 1.019495 | 0.000011 |
| C | 3.180179 | -0.138351 | 0.000014 |
| N | 1.974186 | -0.004874 | -0.000020 |
| Pb | -0.432804 | -0.001894 | 0.000001 |

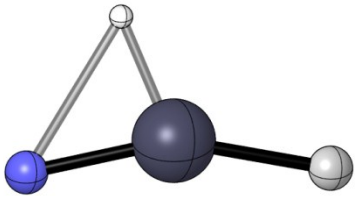
HCNPb_singlet_3_HCNPb_singlet_7-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 3.770299 | 1.091928 | 0.000037 |

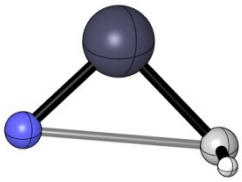
| | | | |
|---|---|---|---|
| C | 3.058967 | 0.296970 | -0.000012 |
| N | 2.303276 | -0.562609 | 0.000005 |
| Pb | -0.466427 | 0.012982 | 0.000000 |

HCNPb_singlet_4_HCNPb_singlet_6-B3LYP-def2-qzvpp



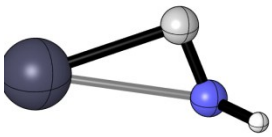
| | | | |
|---|---|---|---|
| N | -1.945293 | -0.386066 | 0.000111 |
| C | 2.110719 | -0.329121 | 0.000107 |
| H | -0.681180 | 1.686186 | -0.000071 |
| Pb | 0.019926 | 0.036476 | -0.000016 |

HCNPb_singlet_4_HCNPb_singlet_7-B3LYP-def2-qzvpp



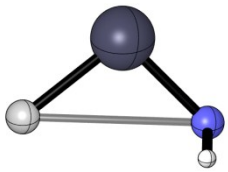
| | | | |
|---|---|---|---|
| H | -2.348946 | 0.677765 | 0.865180 |
| C | -2.048416 | 0.400146 | -0.167674 |
| N | 0.681026 | 1.753295 | -0.011592 |
| Pb | 0.120393 | -0.187216 | 0.002707 |

HCNPb_singlet_5_HCNPb_singlet_8-B3LYP-def2-qzvpp



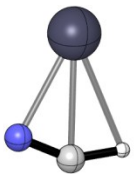
| | | | |
|---|---|---|---|
| H | 3.077158 | -0.756558 | 0.470569 |
| C | 1.861810 | 0.740756 | 0.019166 |
| N | 2.315264 | -0.389041 | -0.099943 |
| Pb | -0.371401 | -0.011765 | 0.001391 |

HCNPb_singlet_6_HCNPb_singlet_8-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | -1.925249 | 1.338598 | 0.674191 |
| C | 1.280819 | 1.649755 | -0.026615 |
| N | -1.789381 | 0.700123 | -0.117907 |
| Pb | 0.082512 | -0.196805 | 0.003791 |

HCNPb_singlet_7_HCNPb_singlet_11-B3LYP-def2-qzvpp



| | | | |
|---|---|---|---|
| H | 1.537284 | -1.799268 | 0.000000 |
| C | 0.514944 | -2.209560 | 0.000000 |
| N | -0.660992 | -2.012712 | 0.000000 |
| Pb | 0.000000 | 0.355434 | 0.000000 |

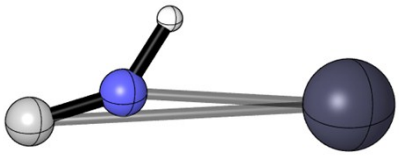
HCNPb_singlet_7_HCNPb_singlet_8-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -0.008913 | -3.094821 | 0.000000 |
| C | 0.673865 | -2.021243 | 0.000000 |

| | | | |
|---|---|---|---|
| N | -0.576325 | -2.027390 | 0.000000 |
| Pb | 0.000000 | 0.358707 | 0.000000 |

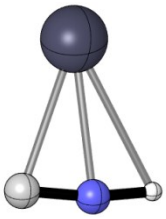
HCNPb_singlet_8_HCNPb_singlet_10-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | -1.699122 | 1.029270 | 0.000057 |
| C | -3.389919 | -0.209785 | 0.000015 |
| N | -2.260826 | 0.137685 | -0.000015 |
| Pb | 0.461761 | -0.008956 | -0.000001 |



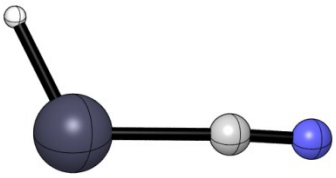
HCNPb_singlet_8_HCNPb_singlet_9-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 2.081406 | 1.438894 | 0.000002 |
| C | 2.190546 | -0.751485 | 0.000000 |
| N | 2.223006 | 0.441728 | 0.000000 |
| Pb | -0.375436 | -0.000269 | 0.000000 |



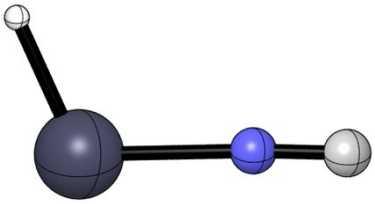
HCNPb_triplet_1-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.667981 | 1.147313 | 0.000000 |
| Pb | 0.000000 | 0.376877 | 0.000000 |
| C | -0.076397 | -1.844452 | 0.000000 |
| N | -0.172800 | -2.997791 | 0.000000 |



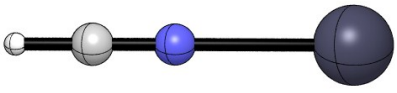
HCNPb_triplet_2-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 1.784491 | 0.977089 | 0.000000 |
| Pb | 0.000000 | 0.363156 | 0.000000 |
| C | -0.191699 | -2.995672 | 0.000000 |
| N | -0.090614 | -1.825981 | 0.000000 |



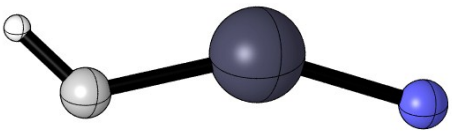
HCNPb_triplet_3-B3LYP-def2-qzvpp

| | | | |
|---|---|---|---|
| H | 0.010137 | -4.237795 | 0.000000 |
| C | 0.002504 | -3.172602 | 0.000000 |
| N | -0.003595 | -2.023850 | 0.000000 |
| Pb | 0.000000 | 0.456590 | 0.000000 |



HCNPb_triplet_4-B3LYP-def2-qzvpp

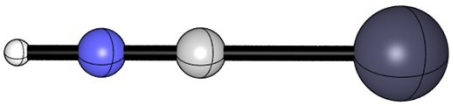
| | | | |
|---|---|---|---|
| H | 2.797969 | -0.163355 | 0.000000 |
| C | 1.876501 | -0.750331 | 0.000000 |
| Pb | 0.000000 | 0.067802 | 0.000000 |



N -2.008139 -0.127774 0.000000

HCNPb_triplet_5-B3LYP-def2-qzvpp

H 0.000000 0.000000 -4.069390
N 0.000000 0.000000 -3.074825
C 0.000000 0.000000 -1.905893
Pb 0.000000 0.000000 0.451567

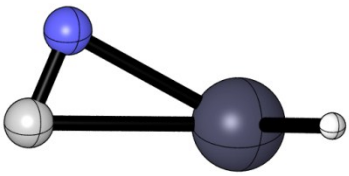


HCNPb_triplet_6-B3LYP-def2-qzvpp

H -2.377522 -0.941089 0.000000
N -1.424460 -1.310627 0.000000
Pb 0.000000 0.062983 0.000000
C 2.058123 0.825141 0.000000

HCNPb_triplet_7-B3LYP-def2-qzvpp

C -2.144743 -0.575213 0.184528
N -1.962673 0.564926 -0.089407
Pb 0.310532 -0.013684 -0.024838
H 1.143578 0.618841 1.555405

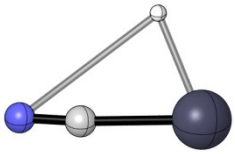


HCNPb_triplet_8-def2-qzvpp-B3LYP

H -0.429329 1.821515 0.000000
Pb 0.000000 0.095655 0.000000
N -1.745259 -1.049241 0.000000
C 2.107691 -0.386757 0.000000

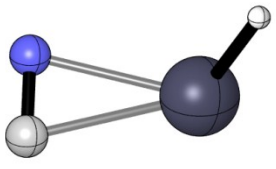
HCNPb_triplet_1_HCNPb_triplet_3-B3LYP-def2-qzvpp

C 1.890065 -0.077518 0.000051
N 3.050972 -0.025928 0.000079
H 0.454114 1.973720 -0.000050
Pb -0.404284 -0.016184 -0.000010



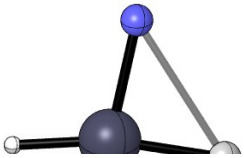
HCNPb_triplet_1_HCNPb_triplet_7-B3LYP-def2-qzvpp

H 1.118882 1.092269 1.313978
C -2.096154 -0.569116 0.252911
N -2.053641 0.549522 -0.156970
Pb 0.315043 -0.018588 -0.021130



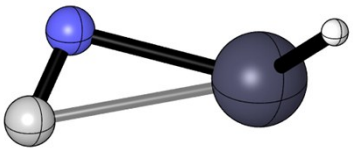
HCNPb_triplet_1_HCNPb_triplet_8-B3LYP-def2-qzvpp

H 0.956218 -1.638893 -0.000280
C -0.338453 1.930477 0.000237
N -1.990749 -0.480239 0.000227



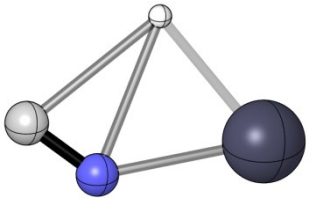
Pb 0.183046 -0.080272 -0.000033

HCNPb_triplet_2_HCNPb_triplet_7-B3LYP-def2-qzvpp



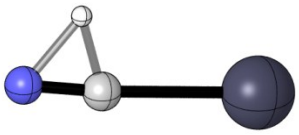
H 1.168616 0.527173 1.586469
C -2.358016 -0.503448 0.171359
N -1.887617 0.552478 -0.090982
Pb 0.319424 -0.016754 -0.024119

HCNPb_triplet_3_HCNPb_triplet_5-B3LYP-def2-qzvpp*



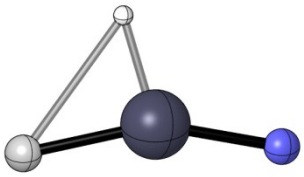
H -1.016473 1.681311 0.000029
C -2.812589 0.245262 -0.000003
N -1.861974 -0.448966 -0.000022
Pb 0.377144 -0.000123 0.000002

HCNPb_triplet_3_HCNPb_triplet_5-B3LYP-def2-qzvpp



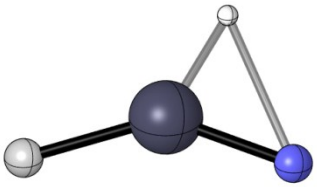
H 2.337958 1.043336 0.000025
N 3.147272 -0.060088 0.000007
C 1.946221 -0.097048 0.000003
Pb -0.439588 -0.000493 -0.000001

HCNPb_triplet_4_HCNPb_triplet_8-B3LYP-def2-qzvpp



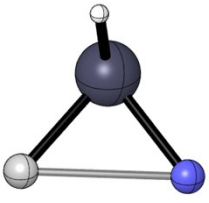
H -0.522904 1.779575 0.000039
C -2.118404 -0.424604 0.000013
N 2.006293 -0.315927 0.000013
Pb -0.009887 0.036336 -0.000003

HCNPb_triplet_6_HCNPb_triplet_8-B3LYP-def2-qzvpp



H 0.877439 -1.657046 -0.000124
N 1.939398 0.633642 -0.000018
C -2.167003 0.558118 -0.000028
Pb -0.017698 -0.074721 0.000005

HCNPb_triplet_7_HCNPb_triplet_8-B3LYP-def2-qzvpp



H 0.802504 -0.061646 1.717110
C -1.161210 1.740769 0.033950
N -1.833450 -1.008822 0.048174
Pb 0.231694 -0.040503 -0.027537