

Supporting Information for:

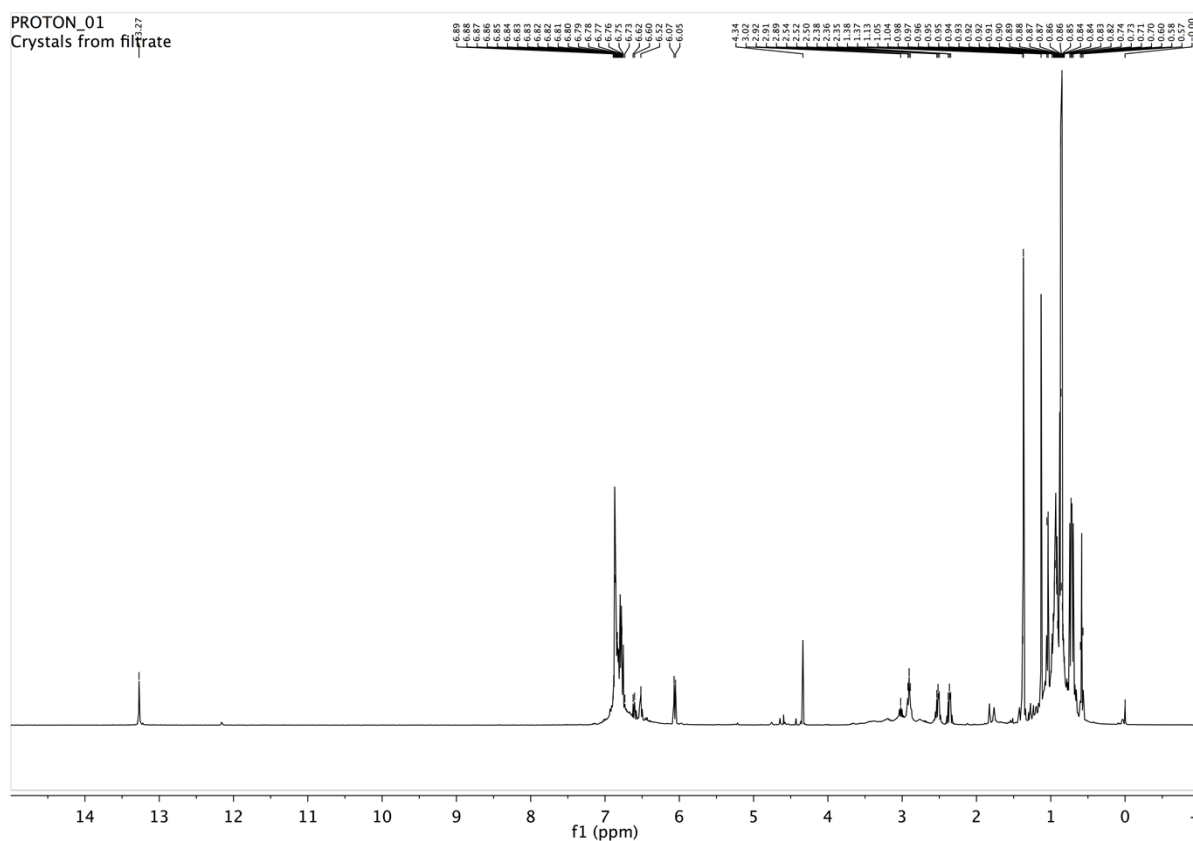
# Lead and tin $\beta$ -diketiminato amido/anilido complexes: competitive nucleophilic reactivity at the $\beta$ -diketiminato $\gamma$ -carbon

Lisa A.-M. Harris,<sup>a</sup> Eric C. Y. Tam,<sup>a</sup> Martyn P. Coles,<sup>b</sup> and J. Robin Fulton<sup>\* b</sup>

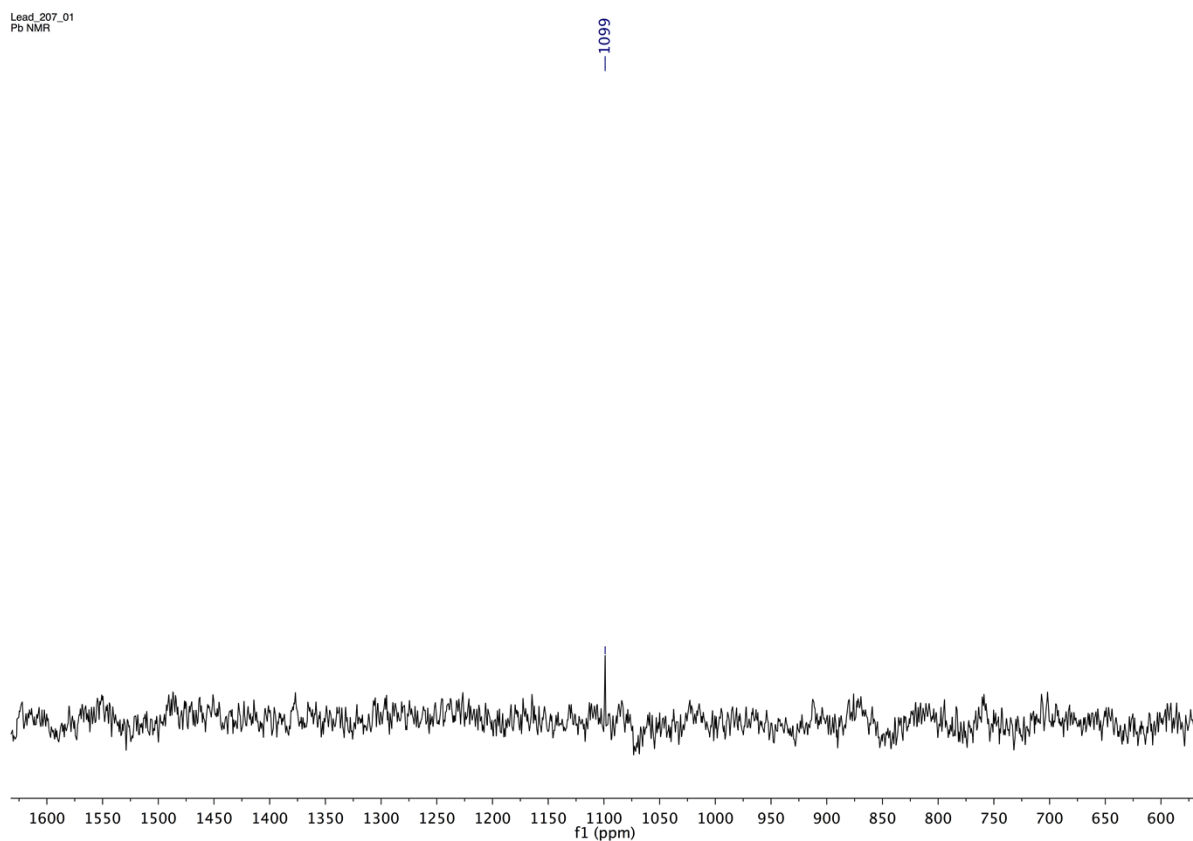
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|                        |                                                                                                                                                   |     |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|-----|
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**Figure S1.**  $^1\text{H}$  NMR spectrum of  $[(\text{BDI})\text{PbOC}(\text{NPh})(\text{C}\{\text{C}(\text{Me})\text{N}-2,6\text{-iPr}_2\text{C}_6\text{H}_3\}\{\text{C}(\text{Me})\text{N}(\text{H})-2,6\text{-iPr}_2\text{C}_6\text{H}_3\})]$  (**9**).



**Figure S2.**  $^{207}\text{Pb}$  NMR spectrum of  $[(\text{BDI})\text{PbOC}(\text{NPh})(\text{C}\{\text{C}(\text{Me})\text{N}-2,6\text{-iPr}_2\text{C}_6\text{H}_3\}\{\text{C}(\text{Me})\text{N}(\text{H})-2,6\text{-iPr}_2\text{C}_6\text{H}_3\})]$  (**9**).



**CARBON\_01**  
**C NMR**

Chemical shift (ppm): 172.32, 164.15, 163.81, 163.76, 161.10, 147.32, 146.29, 142.39, 142.21, 141.11, 140.37, 140.44, 131.92, 127.85, 127.66, 127.38, 125.44, 125.39, 125.29, 125.20, 123.17, 123.07, 121.93, 118.54, 106.10, 97.75, 93.90, 34.02, 28.37, 28.22, 28.14, 28.08, 27.98, 27.77, 27.72, 26.53, 26.46, 26.41, 26.19, 26.09, 25.94, 23.88, 23.74, 23.68, 23.52, 23.23, 23.07, 22.71, 22.18, 20.37, 19.54, 13.84.

Peak labels: 9, 9, 9+L, 9, 9, L, 9, 9, L, 9.

CARBON\_01  
Crystals  
L.H.269  
15/2/10

165.49  
162.07  
147.76  
144.18  
142.95  
142.95  
142.55  
142.55  
129.34  
128.30  
128.30  
127.94  
127.06  
127.06  
125.84  
125.84  
124.62  
124.62  
123.73  
123.73  
122.98  
122.98  
102.24  
66.33  
28.82  
28.75  
28.75  
28.10  
28.10  
25.18  
25.18  
24.60  
24.60  
24.30  
24.30  
23.65  
23.65  
19.94  
19.94

f1 (ppm)

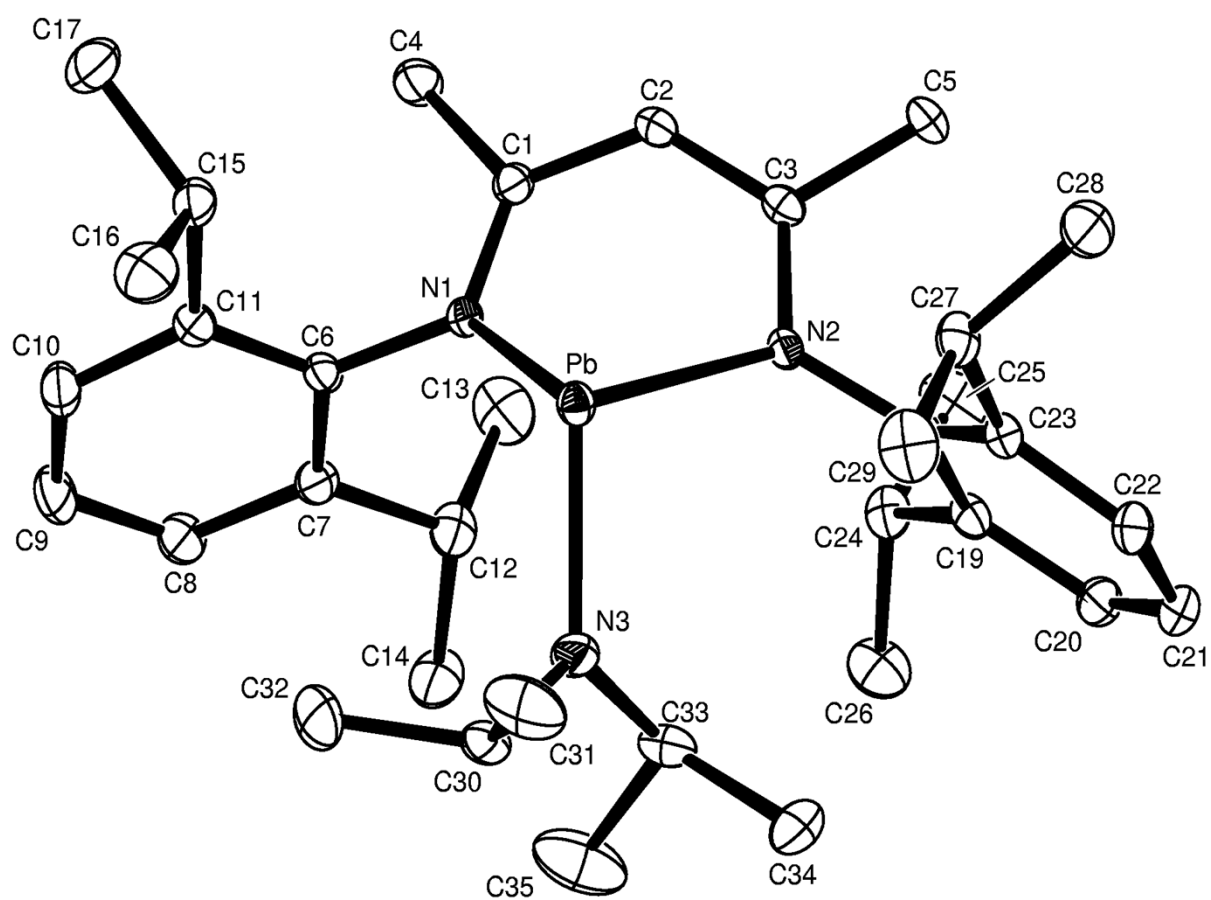
1H NMR spectrum of compound 10a in CDCl<sub>3</sub>. The x-axis represents the chemical shift in ppm, ranging from -1.0 to 14.0. The spectrum shows several peaks with corresponding integration values:

- ~13.5 ppm (NH, integration ~1.00)
- 6.5-7.5 ppm (aromatic protons, integration ~1.00)
- ~4.8 ppm (OH, integration ~1.00)
- 3.0-4.0 ppm (sugar protons, integration ~1.00)
- ~2.1 ppm (CH<sub>3</sub>, integration ~3.00)
- 0.5-2.0 ppm (sugar protons, integration ~1.00)

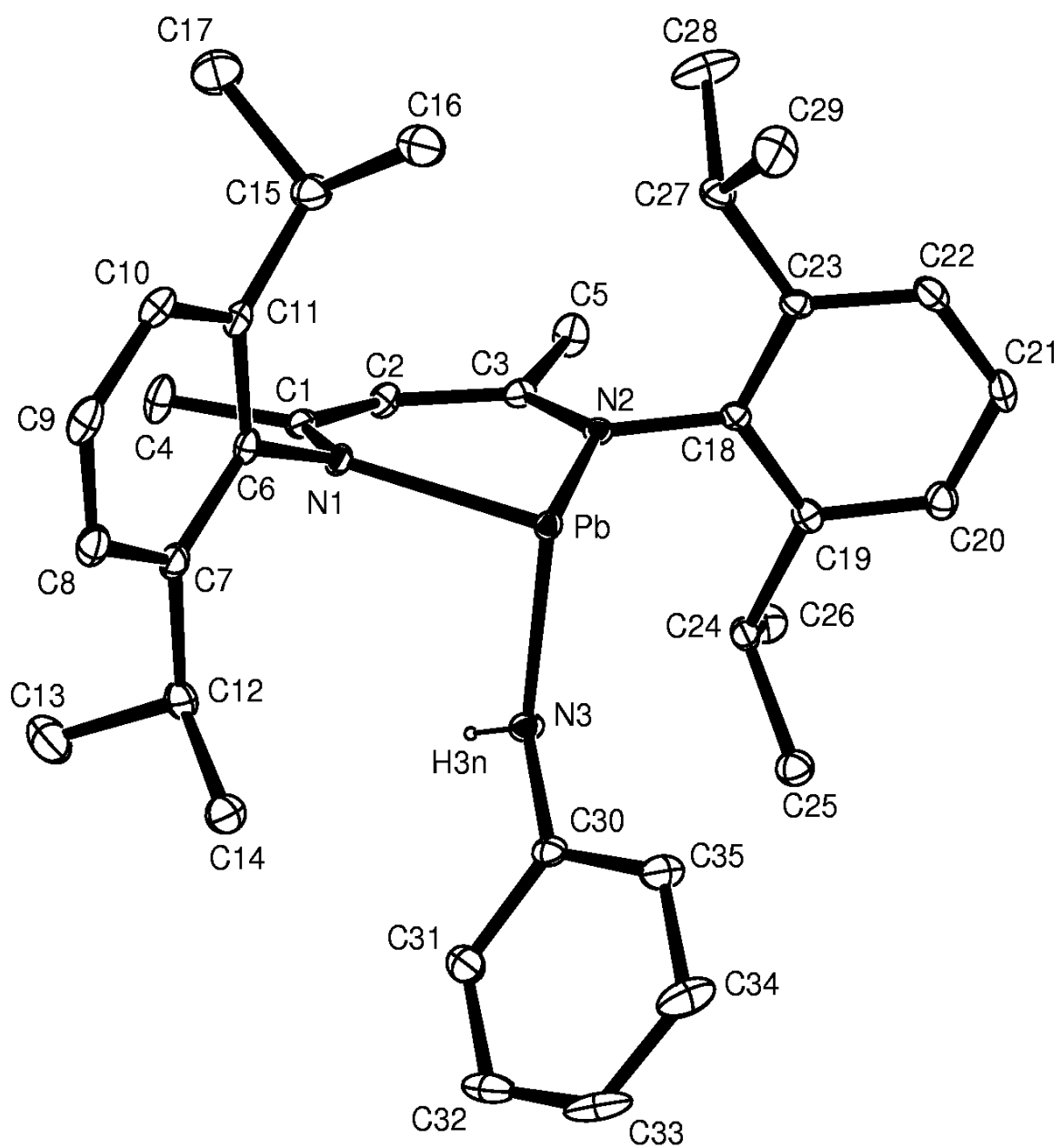
Tin119\_01  
119Sn signal of NMR sample

The figure displays a 119Sn NMR spectrum. The x-axis is labeled 'f1 (ppm)' and ranges from -300 to -500. A single, sharp, intense peak is observed at a chemical shift of -398 ppm, as indicated by the label '-398' above the peak. The baseline is relatively flat with some minor noise.

**Figure S7.** Thermal ellipsoid plot of  $[(\text{BDI})\text{Pb}(\text{N}\{i\text{Pr}\}_2)_2]$  (**2**).



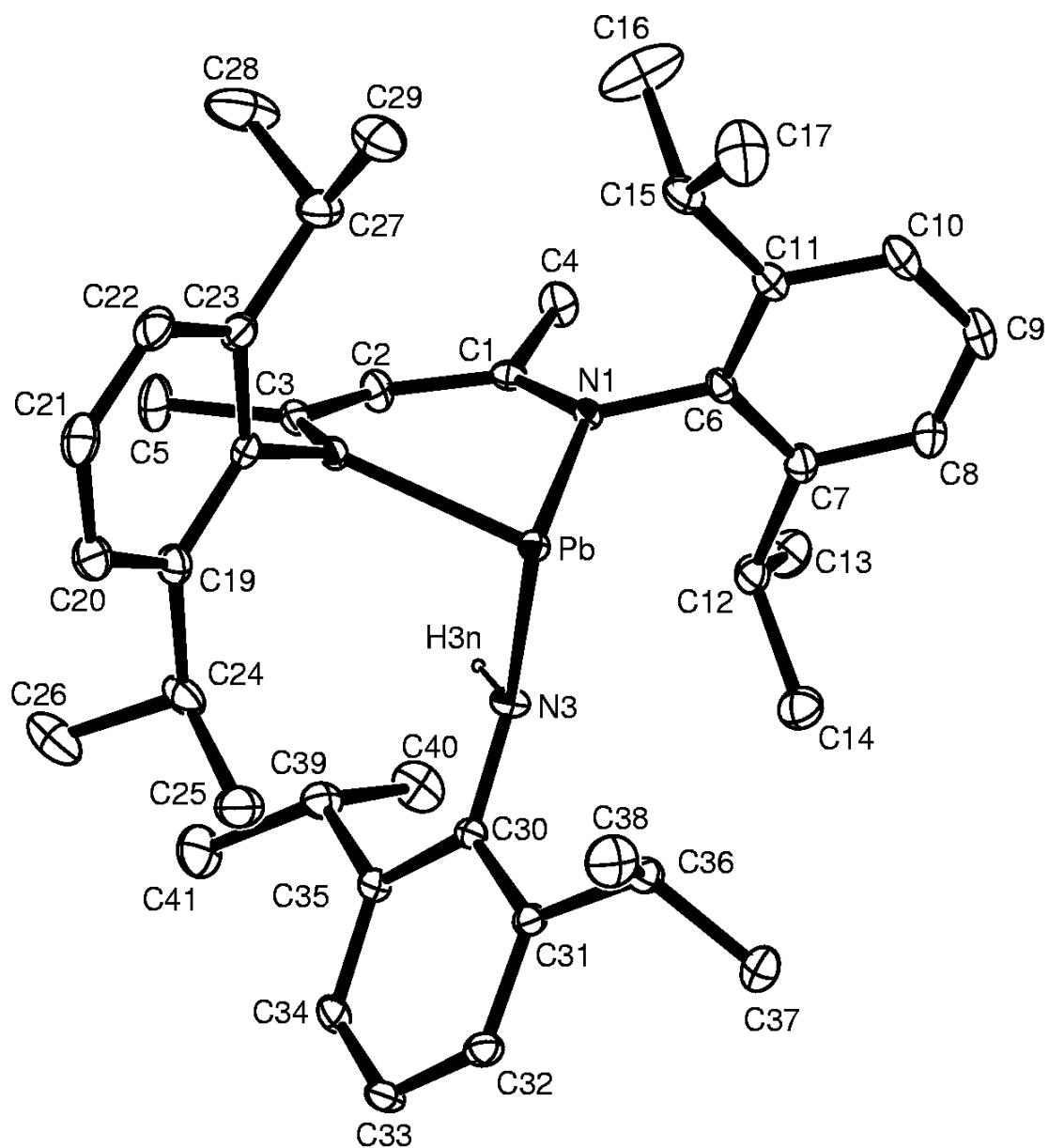
**Figure S8.** Thermal ellipsoid plot of [(BDI)Pb(NHPh)] (3).



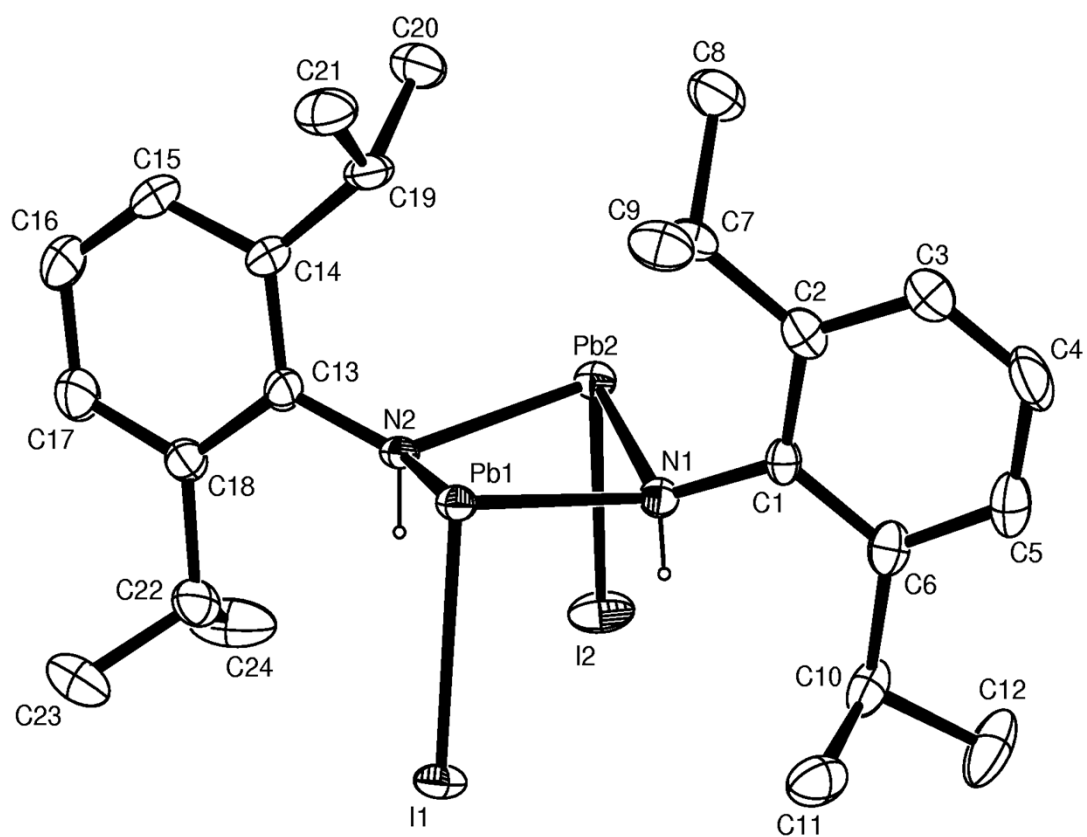




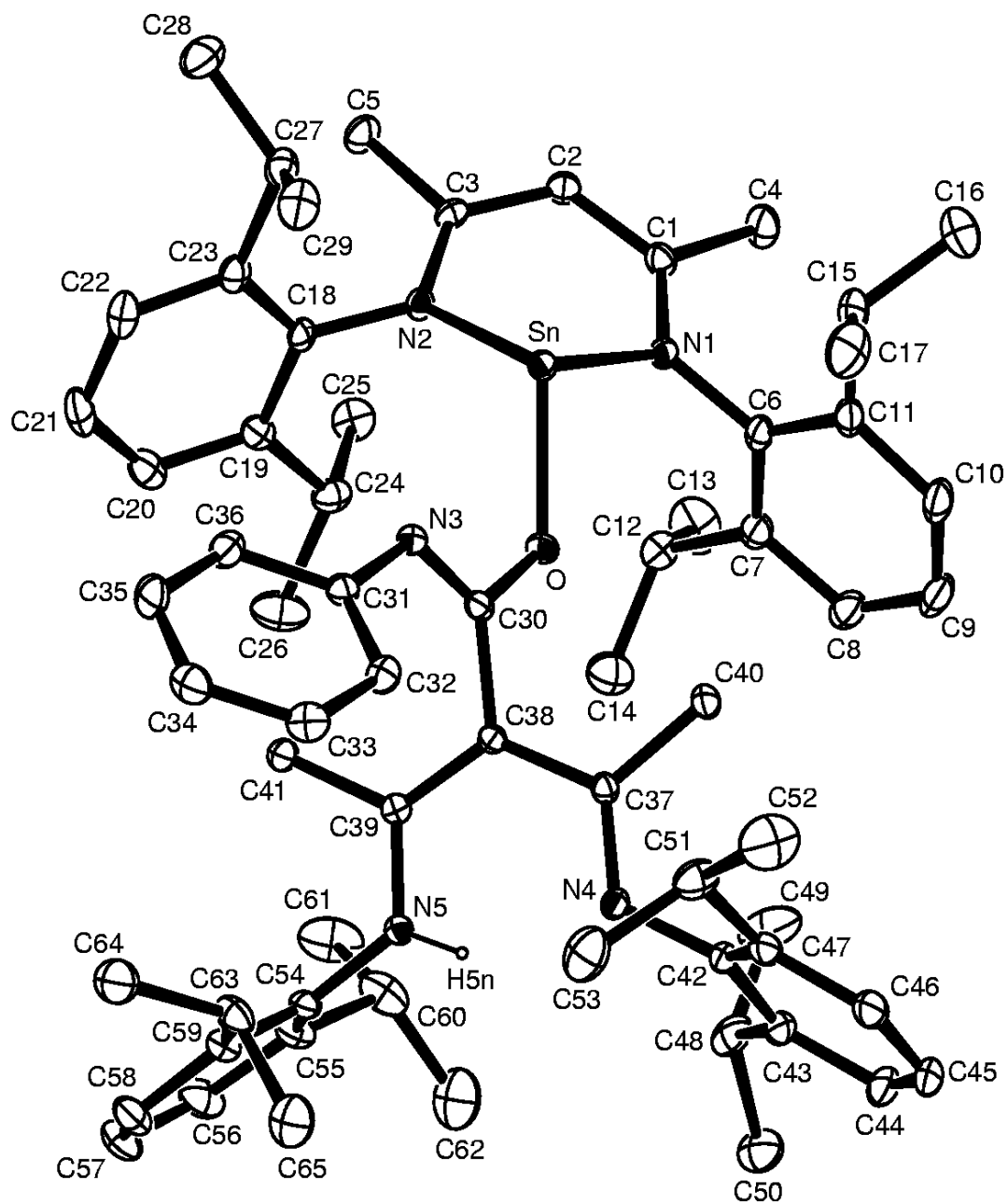
**Figure S10.** Thermal ellipsoid plot of [(BDI)Pb(NH{2,6-*i*Pr<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>})] (**5**).



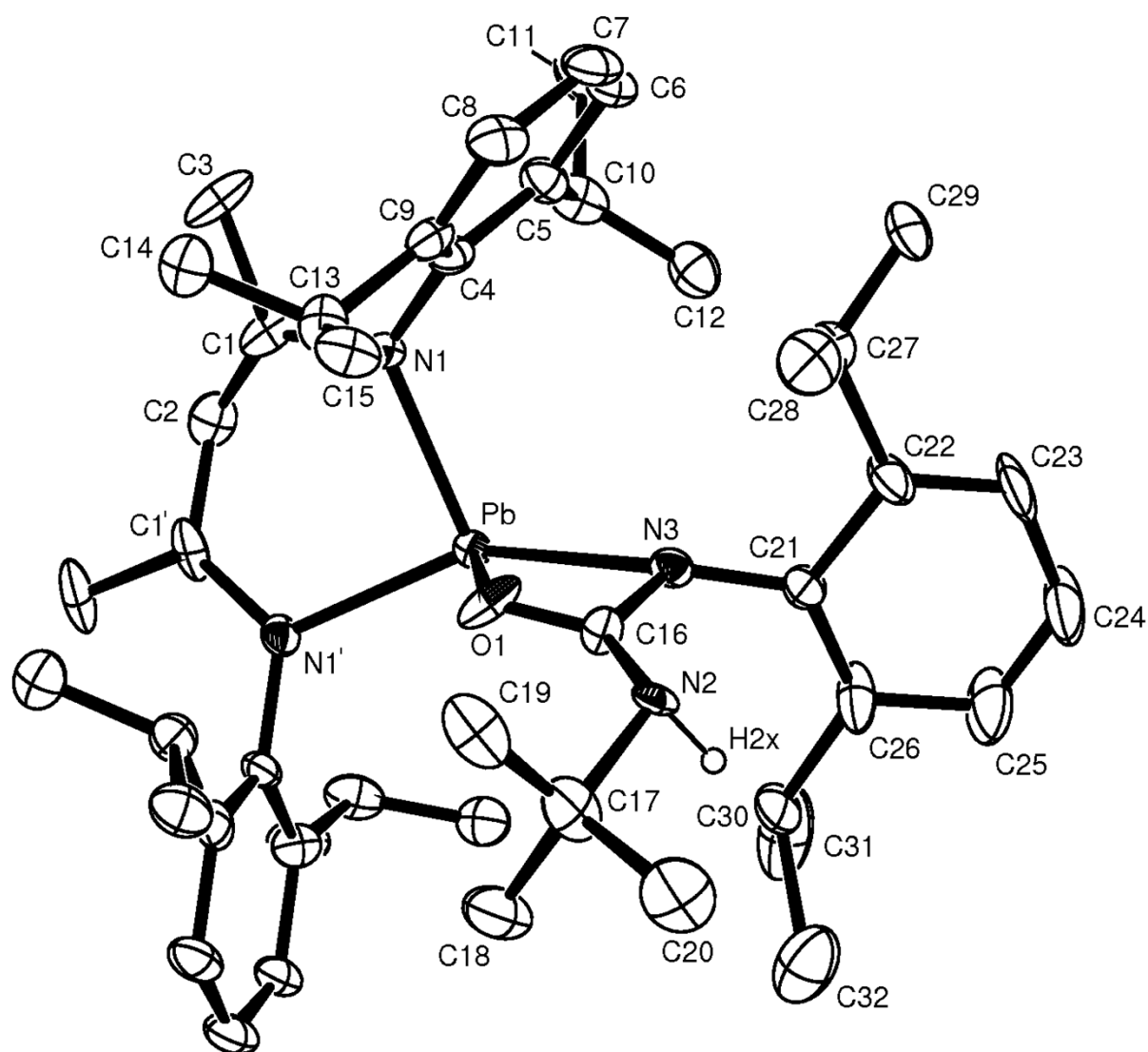
**Figure S11.** Thermal ellipsoid plot of  $[\text{IPb}(\mu\text{-NH}(2,6\text{-}i\text{Pr}_2\text{C}_6\text{H}_3))_2]$  (**8**).



**Figure S12.** Thermal ellipsoid plot of  $[(\text{BDI})\text{SnOC}(\text{NPh})(\text{C}\{\text{C}(\text{Me})\text{N}-2,6\text{-iPr}_2\text{C}_6\text{H}_3\}\{\text{C}(\text{Me})\text{N}(\text{H})\{2,6\text{-iPr}_2\text{C}_6\text{H}_3\})])]$  (**12**).



**Figure S13.** Thermal ellipsoid plot of  $[(\text{BDI})\text{Pb}(\text{OC}\{\text{=N}t\text{Bu}\}\{\text{NH}(2,6\text{-}i\text{Pr}_2\text{-C}_6\text{H}_3)\})]$  (**14**).



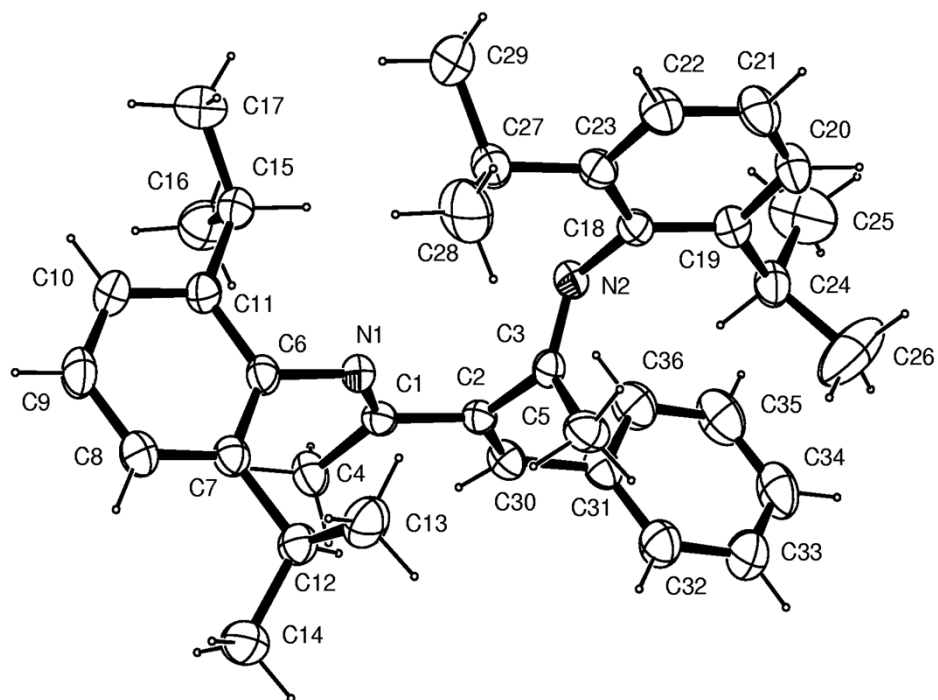
**Table S1.** Data collection parameters for [(BDI)Pb(OC{=N*t*Bu}{NH(2,6-*i*Pr<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>))}] (**14**).

|                                   |                                                              |                       |
|-----------------------------------|--------------------------------------------------------------|-----------------------|
| Identification code               | mpc_lh602                                                    |                       |
| Empirical formula                 | C <sub>46</sub> H <sub>68</sub> N <sub>4</sub> O Pb          |                       |
| Formula weight                    | 900.23                                                       |                       |
| Temperature                       | 173(2) K                                                     |                       |
| Wavelength                        | 0.71073 Å                                                    |                       |
| Crystal system                    | Orthorhombic                                                 |                       |
| Space group                       | <i>P c m n</i> (No.62)                                       |                       |
| Unit cell dimensions              | <i>a</i> = 9.3058(1) Å                                       | $\alpha = 90^\circ$ . |
|                                   | <i>b</i> = 19.5694(3) Å                                      | $\beta = 90^\circ$ .  |
|                                   | <i>c</i> = 27.4022(4) Å                                      | $\gamma = 90^\circ$ . |
| Volume                            | 4990.19(12) Å <sup>3</sup>                                   |                       |
| Z                                 | 4                                                            |                       |
| Density (calculated)              | 1.20 Mg/m <sup>3</sup>                                       |                       |
| Absorption coefficient            | 3.413 mm <sup>-1</sup>                                       |                       |
| F(000)                            | 1848                                                         |                       |
| Crystal size                      | 0.12 x 0.06 x 0.06 mm <sup>3</sup>                           |                       |
| Theta range for data collection   | 1.49 to 27.50°.                                              |                       |
| Index ranges                      | -12 ≤ <i>h</i> ≤ 8, -25 ≤ <i>k</i> ≤ 25, -35 ≤ <i>l</i> ≤ 35 |                       |
| Reflections collected             | 64880                                                        |                       |
| Independent reflections           | 5878 [R(int) = 0.069]                                        |                       |
| Completeness to theta = 27.50°    | 99.7 %                                                       |                       |
| Absorption correction             | Semi-empirical from equivalents                              |                       |
| Max. and min. transmission        | 0.8214 and 0.6848                                            |                       |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                  |                       |
| Data / restraints / parameters    | 5878 / 67 / 381                                              |                       |
| Goodness-of-fit on F <sup>2</sup> | 1.338                                                        |                       |
| Final R indices [I > 2σ(I)]       | R1 = 0.059, wR2 = 0.195                                      |                       |
| R indices (all data)              | R1 = 0.075, wR2 = 0.212                                      |                       |
| Largest diff. peak and hole       | 2.08 and -1.76 e.Å <sup>-3</sup>                             |                       |

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN  
Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

The molecule lies on a mirror plane. The BDI ligand is disordered and was modelled over two positions with each being constrained to be equal. The hydrogen atom was located on N2; the N-H distance was restrained to be 0.91 Å. Due to the severe disorder, discussion of bond lengths and angles should be treated with care.

**Figure S14.** Thermal ellipsoid plot of  $[\text{C}_6\text{H}_5\text{CH}=\text{C}\{(\text{Me})\text{CN-2,6-iPr}_2\text{C}_6\text{H}_3\}_2]$  (**15**).



**Table S2.** Cartesian coordinates of optimized structure of [(BDI)Pb(N*i*Pr<sub>2</sub>)] (**2**) at B3LYP/LANL2DZ/6-31G\* level.<sup>1</sup>

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -1.490366               | 0.296002  | -1.035057 |
| 2                | 7                | 0              | 1.603712                | 0.500616  | -0.938251 |
| 3                | 7                | 0              | -0.270365               | -1.015186 | 1.950161  |
| 4                | 6                | 0              | -1.199424               | 0.669352  | -2.295479 |
| 5                | 6                | 0              | 0.093982                | 0.795023  | -2.824986 |
| 6                | 1                | 0              | 0.123933                | 1.050304  | -3.878597 |
| 7                | 6                | 0              | 1.364546                | 0.871185  | -2.184964 |
| 8                | 6                | 0              | -2.337708               | 0.949586  | -3.267601 |
| 9                | 1                | 0              | -2.838351               | 0.010058  | -3.532094 |
| 10               | 1                | 0              | -1.970174               | 1.411274  | -4.186518 |
| 11               | 1                | 0              | -3.100284               | 1.597715  | -2.830829 |
| 12               | 6                | 0              | 2.469699                | 1.420759  | -3.079901 |
| 13               | 1                | 0              | 3.392300                | 1.618030  | -2.534145 |
| 14               | 1                | 0              | 2.142827                | 2.342664  | -3.570804 |
| 15               | 1                | 0              | 2.686583                | 0.694646  | -3.873349 |
| 16               | 6                | 0              | -2.817542               | 0.509440  | -0.530642 |
| 17               | 6                | 0              | -3.149530               | 1.777314  | 0.022024  |
| 18               | 6                | 0              | -4.442357               | 1.975610  | 0.521103  |
| 19               | 1                | 0              | -4.709353               | 2.943630  | 0.935943  |
| 20               | 6                | 0              | -5.393290               | 0.959159  | 0.503887  |
| 21               | 1                | 0              | -6.389128               | 1.133154  | 0.902916  |
| 22               | 6                | 0              | -5.056846               | -0.280694 | -0.027769 |
| 23               | 1                | 0              | -5.800892               | -1.073037 | -0.042848 |
| 24               | 6                | 0              | -3.783293               | -0.527914 | -0.557677 |
| 25               | 6                | 0              | -2.146452               | 2.931470  | 0.068573  |
| 26               | 1                | 0              | -1.152378               | 2.505523  | -0.097718 |
| 27               | 6                | 0              | -2.402184               | 3.964649  | -1.049643 |
| 28               | 1                | 0              | -3.405719               | 4.398561  | -0.959240 |
| 29               | 1                | 0              | -2.315478               | 3.522292  | -2.046057 |
| 30               | 1                | 0              | -1.675482               | 4.783816  | -0.985202 |
| 31               | 6                | 0              | -2.125876               | 3.650919  | 1.431825  |
| 32               | 1                | 0              | -3.050818               | 4.211005  | 1.613073  |
| 33               | 1                | 0              | -1.301399               | 4.373502  | 1.460294  |
| 34               | 1                | 0              | -1.991654               | 2.950010  | 2.261228  |
| 35               | 6                | 0              | -3.495017               | -1.905537 | -1.150966 |
| 36               | 1                | 0              | -2.490783               | -1.877569 | -1.587748 |
| 37               | 6                | 0              | -4.471341               | -2.271852 | -2.286834 |
| 38               | 1                | 0              | -4.185367               | -3.228135 | -2.740863 |
| 39               | 1                | 0              | -4.480404               | -1.510492 | -3.074206 |
| 40               | 1                | 0              | -5.497702               | -2.376552 | -1.916507 |
| 41               | 6                | 0              | -3.504391               | -3.001786 | -0.066779 |
| 42               | 1                | 0              | -4.499628               | -3.104574 | 0.381936  |
| 43               | 1                | 0              | -2.801060               | -2.770464 | 0.739878  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 44 | 1  | 0 | -3.229319 | -3.973349 | -0.495613 |
| 45 | 6  | 0 | 2.896580  | 0.641356  | -0.342237 |
| 46 | 6  | 0 | 3.893259  | -0.347158 | -0.546101 |
| 47 | 6  | 0 | 5.121965  | -0.208469 | 0.114276  |
| 48 | 1  | 0 | 5.892537  | -0.959885 | -0.038211 |
| 49 | 6  | 0 | 5.377479  | 0.869207  | 0.952917  |
| 50 | 1  | 0 | 6.337480  | 0.958902  | 1.454422  |
| 51 | 6  | 0 | 4.392224  | 1.835026  | 1.146504  |
| 52 | 1  | 0 | 4.598432  | 2.674037  | 1.803188  |
| 53 | 6  | 0 | 3.145137  | 1.743554  | 0.519118  |
| 54 | 6  | 0 | 3.696937  | -1.547688 | -1.473031 |
| 55 | 1  | 0 | 2.693316  | -1.485076 | -1.904579 |
| 56 | 6  | 0 | 4.702004  | -1.539801 | -2.643979 |
| 57 | 1  | 0 | 4.652395  | -0.606613 | -3.213852 |
| 58 | 1  | 0 | 4.494770  | -2.369751 | -3.330316 |
| 59 | 1  | 0 | 5.731993  | -1.655312 | -2.286638 |
| 60 | 6  | 0 | 3.787588  | -2.887352 | -0.715457 |
| 61 | 1  | 0 | 4.780808  | -3.031750 | -0.274466 |
| 62 | 1  | 0 | 3.599786  | -3.726213 | -1.396642 |
| 63 | 1  | 0 | 3.056027  | -2.942897 | 0.097652  |
| 64 | 6  | 0 | 2.089660  | 2.827118  | 0.736196  |
| 65 | 1  | 0 | 1.112596  | 2.330050  | 0.707542  |
| 66 | 6  | 0 | 2.213170  | 3.550684  | 2.088997  |
| 67 | 1  | 0 | 3.081551  | 4.220259  | 2.114378  |
| 68 | 1  | 0 | 2.302638  | 2.851314  | 2.925685  |
| 69 | 1  | 0 | 1.325204  | 4.169673  | 2.260585  |
| 70 | 6  | 0 | 2.106737  | 3.875802  | -0.396765 |
| 71 | 1  | 0 | 3.084043  | 4.371476  | -0.449429 |
| 72 | 1  | 0 | 1.347954  | 4.647380  | -0.215521 |
| 73 | 1  | 0 | 1.900685  | 3.430140  | -1.372505 |
| 74 | 6  | 0 | -0.917223 | 0.137990  | 2.593399  |
| 75 | 1  | 0 | -1.113893 | 0.856206  | 1.790788  |
| 76 | 6  | 0 | -2.284571 | -0.220028 | 3.212750  |
| 77 | 1  | 0 | -2.948534 | -0.648745 | 2.456585  |
| 78 | 1  | 0 | -2.771960 | 0.671497  | 3.627754  |
| 79 | 1  | 0 | -2.179447 | -0.944872 | 4.029713  |
| 80 | 6  | 0 | -0.036012 | 0.862623  | 3.631140  |
| 81 | 1  | 0 | 0.150388  | 0.240319  | 4.514460  |
| 82 | 1  | 0 | -0.526727 | 1.780182  | 3.979506  |
| 83 | 1  | 0 | 0.930287  | 1.134275  | 3.197238  |
| 84 | 6  | 0 | 0.245956  | -2.049669 | 2.866429  |
| 85 | 1  | 0 | -0.217393 | -1.884487 | 3.849141  |
| 86 | 6  | 0 | 1.773095  | -1.972554 | 3.075485  |
| 87 | 1  | 0 | 2.307080  | -2.183691 | 2.140080  |
| 88 | 1  | 0 | 2.110991  | -2.702918 | 3.823161  |
| 89 | 1  | 0 | 2.078467  | -0.976476 | 3.406368  |
| 90 | 6  | 0 | -0.155187 | -3.476566 | 2.445378  |
| 91 | 1  | 0 | -1.241614 | -3.563081 | 2.342857  |
| 92 | 1  | 0 | 0.180858  | -4.210469 | 3.188588  |
| 93 | 1  | 0 | 0.300040  | -3.763315 | 1.487986  |
| 94 | 82 | 0 | 0.057042  | -1.247156 | -0.163800 |



**Table S3.** Cartesian coordinates of optimized structure of [(BDI)Pb(NH{2,6-*i*Pr<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>})] (**5**) at B3LYP/LANL2DZ/6-31G\* level.<sup>1</sup>

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 82               | 0              | -0.255077               | 0.055220  | -0.825669 |
| 2                | 7                | 0              | -1.787141               | -0.679097 | 0.757389  |
| 3                | 7                | 0              | 0.056920                | 1.828135  | 0.681856  |
| 4                | 7                | 0              | 1.188349                | -1.290770 | 0.136704  |
| 5                | 1                | 0              | 1.024908                | -1.235246 | 1.136012  |
| 6                | 6                | 0              | -1.762404               | -0.311505 | 2.040279  |
| 7                | 6                | 0              | -0.913391               | 0.671681  | 2.596051  |
| 8                | 1                | 0              | -0.976826               | 0.749375  | 3.674419  |
| 9                | 6                | 0              | -0.174063               | 1.711583  | 1.989854  |
| 10               | 6                | 0              | -2.745481               | -0.946760 | 3.011045  |
| 11               | 1                | 0              | -2.560898               | -0.610730 | 4.033171  |
| 12               | 1                | 0              | -2.695647               | -2.037389 | 2.984256  |
| 13               | 1                | 0              | -3.771704               | -0.673122 | 2.740526  |
| 14               | 6                | 0              | 0.316258                | 2.795567  | 2.937701  |
| 15               | 1                | 0              | 1.313310                | 3.147882  | 2.665183  |
| 16               | 1                | 0              | 0.335901                | 2.430039  | 3.967175  |
| 17               | 1                | 0              | -0.349408               | 3.665465  | 2.903578  |
| 18               | 6                | 0              | -2.790303               | -1.602125 | 0.282620  |
| 19               | 6                | 0              | -2.586721               | -3.004969 | 0.370651  |
| 20               | 6                | 0              | -3.579829               | -3.857608 | -0.128769 |
| 21               | 1                | 0              | -3.432259               | -4.932117 | -0.062885 |
| 22               | 6                | 0              | -4.744724               | -3.365184 | -0.706226 |
| 23               | 1                | 0              | -5.502621               | -4.047612 | -1.081757 |
| 24               | 6                | 0              | -4.925608               | -1.990516 | -0.805276 |
| 25               | 1                | 0              | -5.832130               | -1.604083 | -1.263142 |
| 26               | 6                | 0              | -3.964153               | -1.090795 | -0.327924 |
| 27               | 6                | 0              | -1.329325               | -3.635746 | 0.965617  |
| 28               | 1                | 0              | -0.689756               | -2.832394 | 1.336635  |
| 29               | 6                | 0              | -1.640857               | -4.584183 | 2.141803  |
| 30               | 1                | 0              | -0.708035               | -4.953870 | 2.583647  |
| 31               | 1                | 0              | -2.217575               | -5.456917 | 1.813652  |
| 32               | 1                | 0              | -2.214127               | -4.091437 | 2.934757  |
| 33               | 6                | 0              | -0.525344               | -4.388832 | -0.112831 |
| 34               | 1                | 0              | 0.407535                | -4.778897 | 0.310405  |
| 35               | 1                | 0              | -0.261568               | -3.727240 | -0.941475 |
| 36               | 1                | 0              | -1.094480               | -5.235855 | -0.514862 |
| 37               | 6                | 0              | -4.228066               | 0.405022  | -0.486415 |
| 38               | 1                | 0              | -3.345082               | 0.942963  | -0.128289 |
| 39               | 6                | 0              | -5.423808               | 0.869537  | 0.369283  |
| 40               | 1                | 0              | -5.567931               | 1.952574  | 0.273573  |
| 41               | 1                | 0              | -5.271328               | 0.642779  | 1.430250  |
| 42               | 1                | 0              | -6.353388               | 0.380337  | 0.055104  |
| 43               | 6                | 0              | -4.441051               | 0.785095  | -1.965446 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 44 | 1 | 0 | -4.579061 | 1.866723  | -2.069407 |
| 45 | 1 | 0 | -5.328758 | 0.296784  | -2.383442 |
| 46 | 1 | 0 | -3.582602 | 0.491580  | -2.580237 |
| 47 | 6 | 0 | 0.567186  | 3.063558  | 0.144775  |
| 48 | 6 | 0 | 1.949464  | 3.216596  | -0.134058 |
| 49 | 6 | 0 | 2.392735  | 4.426219  | -0.686188 |
| 50 | 1 | 0 | 3.451768  | 4.553950  | -0.892667 |
| 51 | 6 | 0 | 1.513621  | 5.464230  | -0.971757 |
| 52 | 1 | 0 | 1.881284  | 6.393853  | -1.398152 |
| 53 | 6 | 0 | 0.157574  | 5.298782  | -0.710267 |
| 54 | 1 | 0 | -0.531354 | 6.107421  | -0.940408 |
| 55 | 6 | 0 | -0.340575 | 4.112850  | -0.157732 |
| 56 | 6 | 0 | 2.983666  | 2.130972  | 0.156018  |
| 57 | 1 | 0 | 2.455679  | 1.238672  | 0.502991  |
| 58 | 6 | 0 | 3.772912  | 1.739883  | -1.109452 |
| 59 | 1 | 0 | 4.416713  | 0.878552  | -0.905312 |
| 60 | 1 | 0 | 4.407537  | 2.564024  | -1.457226 |
| 61 | 1 | 0 | 3.103973  | 1.471623  | -1.933738 |
| 62 | 6 | 0 | 3.962218  | 2.557852  | 1.269124  |
| 63 | 1 | 0 | 4.692398  | 1.761943  | 1.454201  |
| 64 | 1 | 0 | 3.445716  | 2.767206  | 2.212311  |
| 65 | 1 | 0 | 4.516718  | 3.460886  | 0.986688  |
| 66 | 6 | 0 | -1.845879 | 3.996984  | 0.075846  |
| 67 | 1 | 0 | -2.044782 | 3.025437  | 0.536992  |
| 68 | 6 | 0 | -2.376722 | 5.080756  | 1.035701  |
| 69 | 1 | 0 | -3.445945 | 4.929913  | 1.227049  |
| 70 | 1 | 0 | -2.254568 | 6.085958  | 0.615685  |
| 71 | 1 | 0 | -1.856422 | 5.060788  | 1.999351  |
| 72 | 6 | 0 | -2.617137 | 4.045608  | -1.258056 |
| 73 | 1 | 0 | -3.693292 | 3.924230  | -1.085130 |
| 74 | 1 | 0 | -2.289565 | 3.253053  | -1.939602 |
| 75 | 1 | 0 | -2.469533 | 5.003939  | -1.769534 |
| 76 | 6 | 0 | 2.515289  | -1.640464 | -0.127274 |
| 77 | 6 | 0 | 2.930148  | -2.007591 | -1.441897 |
| 78 | 6 | 0 | 4.277656  | -2.295647 | -1.682758 |
| 79 | 1 | 0 | 4.585726  | -2.555865 | -2.692939 |
| 80 | 6 | 0 | 5.230349  | -2.273309 | -0.669901 |
| 81 | 1 | 0 | 6.272130  | -2.497881 | -0.881453 |
| 82 | 6 | 0 | 4.815452  | -1.985209 | 0.629924  |
| 83 | 1 | 0 | 5.550045  | -1.999388 | 1.429440  |
| 84 | 6 | 0 | 3.487517  | -1.673298 | 0.928910  |
| 85 | 6 | 0 | 1.942975  | -2.148354 | -2.599343 |
| 86 | 1 | 0 | 0.932604  | -2.047809 | -2.188810 |
| 87 | 6 | 0 | 2.001615  | -3.549673 | -3.241639 |
| 88 | 1 | 0 | 1.224310  | -3.653361 | -4.009131 |
| 89 | 1 | 0 | 1.849338  | -4.332638 | -2.491445 |
| 90 | 1 | 0 | 2.967853  | -3.733904 | -3.725141 |
| 91 | 6 | 0 | 2.125971  | -1.061494 | -3.676412 |
| 92 | 1 | 0 | 1.380168  | -1.169696 | -4.474291 |
| 93 | 1 | 0 | 3.119906  | -1.127873 | -4.134689 |
| 94 | 1 | 0 | 2.028108  | -0.052853 | -3.258897 |
| 95 | 6 | 0 | 3.063834  | -1.434690 | 2.379118  |

|     |   |   |          |           |          |
|-----|---|---|----------|-----------|----------|
| 96  | 1 | 0 | 2.320299 | -0.624142 | 2.391919 |
| 97  | 6 | 0 | 2.389756 | -2.696357 | 2.966500 |
| 98  | 1 | 0 | 2.000144 | -2.503601 | 3.974246 |
| 99  | 1 | 0 | 3.117455 | -3.513983 | 3.033479 |
| 100 | 1 | 0 | 1.561660 | -3.045832 | 2.341002 |
| 101 | 6 | 0 | 4.196625 | -0.980722 | 3.314504 |
| 102 | 1 | 0 | 3.783941 | -0.710194 | 4.293584 |
| 103 | 1 | 0 | 4.726604 | -0.108605 | 2.917636 |
| 104 | 1 | 0 | 4.932079 | -1.775820 | 3.484152 |

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**Table S4.** Cartesian coordinates of optimized structure of [(BDI)Pb(N*i*Pr<sub>2</sub>)] (**10**) at B3LYP/LANL2DZ/6-31G\* level.<sup>1</sup>

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 50               | 0              | 0.053293                | -1.329605 | -0.161074 |
| 2                | 7                | 0              | -1.469145               | 0.114174  | -1.014148 |
| 3                | 7                | 0              | 1.555940                | 0.317307  | -0.943817 |
| 4                | 7                | 0              | -0.194761               | -1.018293 | 1.867492  |
| 5                | 6                | 0              | -1.212500               | 0.449240  | -2.295398 |
| 6                | 6                | 0              | 0.070260                | 0.555699  | -2.848014 |
| 7                | 1                | 0              | 0.094389                | 0.773885  | -3.909818 |
| 8                | 6                | 0              | 1.335575                | 0.653640  | -2.205954 |
| 9                | 6                | 0              | -2.368662               | 0.695939  | -3.251826 |
| 10               | 1                | 0              | -2.866108               | -0.254498 | -3.479288 |
| 11               | 1                | 0              | -2.017957               | 1.131230  | -4.189959 |
| 12               | 1                | 0              | -3.128120               | 1.352276  | -2.822867 |
| 13               | 6                | 0              | 2.448218                | 1.172511  | -3.105591 |
| 14               | 1                | 0              | 3.364433                | 1.393250  | -2.558678 |
| 15               | 1                | 0              | 2.123747                | 2.073455  | -3.635212 |
| 16               | 1                | 0              | 2.674165                | 0.416324  | -3.867644 |
| 17               | 6                | 0              | -2.792076               | 0.349779  | -0.495132 |
| 18               | 6                | 0              | -3.117013               | 1.642052  | 0.002253  |
| 19               | 6                | 0              | -4.404450               | 1.863426  | 0.505745  |
| 20               | 1                | 0              | -4.666514               | 2.849076  | 0.880065  |
| 21               | 6                | 0              | -5.356687               | 0.848902  | 0.541142  |
| 22               | 1                | 0              | -6.348064               | 1.041278  | 0.942849  |
| 23               | 6                | 0              | -5.028845               | -0.411279 | 0.054794  |
| 24               | 1                | 0              | -5.775408               | -1.200940 | 0.074929  |
| 25               | 6                | 0              | -3.761129               | -0.684080 | -0.477511 |
| 26               | 6                | 0              | -2.121302               | 2.803939  | -0.021226 |
| 27               | 1                | 0              | -1.127658               | 2.381110  | -0.196841 |
| 28               | 6                | 0              | -2.415252               | 3.790633  | -1.171916 |
| 29               | 1                | 0              | -3.420301               | 4.218811  | -1.072781 |
| 30               | 1                | 0              | -2.349635               | 3.311020  | -2.152491 |
| 31               | 1                | 0              | -1.695385               | 4.618189  | -1.158030 |
| 32               | 6                | 0              | -2.074158               | 3.578624  | 1.310962  |
| 33               | 1                | 0              | -3.000352               | 4.136596  | 1.491746  |
| 34               | 1                | 0              | -1.257213               | 4.309839  | 1.288972  |
| 35               | 1                | 0              | -1.912654               | 2.914646  | 2.165273  |
| 36               | 6                | 0              | -3.494434               | -2.081862 | -1.033937 |
| 37               | 1                | 0              | -2.483884               | -2.091032 | -1.455939 |
| 38               | 6                | 0              | -4.468851               | -2.452511 | -2.170709 |
| 39               | 1                | 0              | -4.198417               | -3.424509 | -2.599971 |
| 40               | 1                | 0              | -4.457276               | -1.710495 | -2.976116 |
| 41               | 1                | 0              | -5.500154               | -2.527628 | -1.806593 |
| 42               | 6                | 0              | -3.543491               | -3.152810 | 0.073125  |
| 43               | 1                | 0              | -4.546896               | -3.227365 | 0.509409  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 44 | 1 | 0 | -2.844833 | -2.919128 | 0.881723  |
| 45 | 1 | 0 | -3.280456 | -4.137405 | -0.331977 |
| 46 | 6 | 0 | 2.851004  | 0.476125  | -0.344043 |
| 47 | 6 | 0 | 3.845568  | -0.520078 | -0.517995 |
| 48 | 6 | 0 | 5.067866  | -0.368486 | 0.152197  |
| 49 | 1 | 0 | 5.836741  | -1.126387 | 0.027076  |
| 50 | 6 | 0 | 5.320565  | 0.730444  | 0.962889  |
| 51 | 1 | 0 | 6.275090  | 0.827928  | 1.473369  |
| 52 | 6 | 0 | 4.343367  | 1.712168  | 1.111436  |
| 53 | 1 | 0 | 4.552279  | 2.572499  | 1.738661  |
| 54 | 6 | 0 | 3.101786  | 1.610611  | 0.473996  |
| 55 | 6 | 0 | 3.671304  | -1.728621 | -1.440698 |
| 56 | 1 | 0 | 2.668463  | -1.687002 | -1.875680 |
| 57 | 6 | 0 | 4.687470  | -1.702447 | -2.603004 |
| 58 | 1 | 0 | 4.637815  | -0.766515 | -3.168037 |
| 59 | 1 | 0 | 4.493235  | -2.529709 | -3.296256 |
| 60 | 1 | 0 | 5.714868  | -1.812634 | -2.236382 |
| 61 | 6 | 0 | 3.781644  | -3.068451 | -0.687742 |
| 62 | 1 | 0 | 4.764780  | -3.186752 | -0.217129 |
| 63 | 1 | 0 | 3.640631  | -3.905815 | -1.381620 |
| 64 | 1 | 0 | 3.022547  | -3.152934 | 0.095371  |
| 65 | 6 | 0 | 2.064899  | 2.724189  | 0.629698  |
| 66 | 1 | 0 | 1.079448  | 2.243985  | 0.644617  |
| 67 | 6 | 0 | 2.216517  | 3.540401  | 1.926255  |
| 68 | 1 | 0 | 3.092169  | 4.199783  | 1.888413  |
| 69 | 1 | 0 | 2.310222  | 2.905348  | 2.811564  |
| 70 | 1 | 0 | 1.338253  | 4.181428  | 2.063341  |
| 71 | 6 | 0 | 2.085251  | 3.698750  | -0.568025 |
| 72 | 1 | 0 | 3.074203  | 4.161950  | -0.671861 |
| 73 | 1 | 0 | 1.352871  | 4.501642  | -0.417162 |
| 74 | 1 | 0 | 1.842753  | 3.202341  | -1.509537 |
| 75 | 6 | 0 | -0.758243 | 0.187317  | 2.497699  |
| 76 | 1 | 0 | -0.928286 | 0.897936  | 1.683040  |
| 77 | 6 | 0 | -2.125885 | -0.075420 | 3.161017  |
| 78 | 1 | 0 | -2.838510 | -0.475139 | 2.434270  |
| 79 | 1 | 0 | -2.544099 | 0.850489  | 3.576127  |
| 80 | 1 | 0 | -2.038421 | -0.791742 | 3.987271  |
| 81 | 6 | 0 | 0.195413  | 0.873865  | 3.496317  |
| 82 | 1 | 0 | 0.329161  | 0.280891  | 4.408735  |
| 83 | 1 | 0 | -0.203927 | 1.849309  | 3.800886  |
| 84 | 1 | 0 | 1.179558  | 1.028597  | 3.046642  |
| 85 | 6 | 0 | 0.269980  | -2.055041 | 2.817976  |
| 86 | 1 | 0 | -0.112077 | -1.777003 | 3.808302  |
| 87 | 6 | 0 | 1.805130  | -2.115507 | 2.938612  |
| 88 | 1 | 0 | 2.258093  | -2.455931 | 1.999935  |
| 89 | 1 | 0 | 2.113989  | -2.813720 | 3.728144  |
| 90 | 1 | 0 | 2.222516  | -1.130778 | 3.165971  |
| 91 | 6 | 0 | -0.300424 | -3.455581 | 2.528889  |
| 92 | 1 | 0 | -1.394719 | -3.435635 | 2.522060  |
| 93 | 1 | 0 | 0.024324  | -4.168343 | 3.297661  |
| 94 | 1 | 0 | 0.037213  | -3.844619 | 1.560747  |

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**Table S5.** Cartesian coordinates of optimized structure of [(BDI)Sn(NH{2,6-*i*Pr<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>})] (**11**) at B3LYP/LANL2DZ/6-31G\* level.<sup>1</sup>

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 50               | 0              | -0.278020               | 0.100466  | -0.818487 |
| 2                | 7                | 0              | -1.786312               | -0.574041 | 0.692828  |
| 3                | 7                | 0              | 0.130912                | 1.789550  | 0.617073  |
| 4                | 7                | 0              | 1.069114                | -1.245263 | 0.084338  |
| 5                | 1                | 0              | 0.929524                | -1.218484 | 1.087914  |
| 6                | 6                | 0              | -1.768199               | -0.220083 | 1.980759  |
| 7                | 6                | 0              | -0.874282               | 0.712829  | 2.550207  |
| 8                | 1                | 0              | -0.934859               | 0.791695  | 3.628400  |
| 9                | 6                | 0              | -0.076875               | 1.697920  | 1.934639  |
| 10               | 6                | 0              | -2.787486               | -0.820322 | 2.933477  |
| 11               | 1                | 0              | -3.802822               | -0.672687 | 2.551861  |
| 12               | 1                | 0              | -2.716602               | -0.361280 | 3.921340  |
| 13               | 1                | 0              | -2.646103               | -1.899033 | 3.041083  |
| 14               | 6                | 0              | 0.517998                | 2.743667  | 2.861838  |
| 15               | 1                | 0              | 1.578425                | 2.901180  | 2.648518  |
| 16               | 1                | 0              | 0.407026                | 2.446515  | 3.907025  |
| 17               | 1                | 0              | 0.023827                | 3.711408  | 2.727757  |
| 18               | 6                | 0              | -2.818538               | -1.463965 | 0.202727  |
| 19               | 6                | 0              | -2.690847               | -2.870609 | 0.345114  |
| 20               | 6                | 0              | -3.706096               | -3.687856 | -0.168935 |
| 21               | 1                | 0              | -3.616899               | -4.765792 | -0.066555 |
| 22               | 6                | 0              | -4.820202               | -3.155803 | -0.807654 |
| 23               | 1                | 0              | -5.596541               | -3.810959 | -1.193881 |
| 24               | 6                | 0              | -4.927814               | -1.777800 | -0.952756 |
| 25               | 1                | 0              | -5.796877               | -1.361766 | -1.454598 |
| 26               | 6                | 0              | -3.940696               | -0.911928 | -0.465082 |
| 27               | 6                | 0              | -1.492013               | -3.547360 | 1.007026  |
| 28               | 1                | 0              | -0.845503               | -2.768470 | 1.417059  |
| 29               | 6                | 0              | -1.899289               | -4.488326 | 2.159872  |
| 30               | 1                | 0              | -1.004802               | -4.872669 | 2.663851  |
| 31               | 1                | 0              | -2.464384               | -5.352827 | 1.793082  |
| 32               | 1                | 0              | -2.519778               | -3.987413 | 2.911243  |
| 33               | 6                | 0              | -0.658937               | -4.325177 | -0.030675 |
| 34               | 1                | 0              | 0.227910                | -4.764008 | 0.441554  |
| 35               | 1                | 0              | -0.317472               | -3.665414 | -0.830948 |
| 36               | 1                | 0              | -1.242619               | -5.139714 | -0.476425 |
| 37               | 6                | 0              | -4.132837               | 0.590024  | -0.663150 |
| 38               | 1                | 0              | -3.226219               | 1.096389  | -0.319080 |
| 39               | 6                | 0              | -4.326216               | 0.946910  | -2.150145 |
| 40               | 1                | 0              | -4.404011               | 2.032211  | -2.275640 |
| 41               | 1                | 0              | -5.240533               | 0.501683  | -2.558955 |
| 42               | 1                | 0              | -3.483198               | 0.593860  | -2.753930 |
| 43               | 6                | 0              | -5.304019               | 1.126480  | 0.184795  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 44 | 1 | 0 | -5.404743 | 2.211431  | 0.059438  |
| 45 | 1 | 0 | -5.155170 | 0.923062  | 1.251289  |
| 46 | 1 | 0 | -6.253925 | 0.666479  | -0.112225 |
| 47 | 6 | 0 | 0.680154  | 3.010693  | 0.070996  |
| 48 | 6 | 0 | 2.061326  | 3.118319  | -0.226670 |
| 49 | 6 | 0 | 2.538177  | 4.320687  | -0.767179 |
| 50 | 1 | 0 | 3.597259  | 4.413606  | -0.991119 |
| 51 | 6 | 0 | 1.692083  | 5.393371  | -1.020894 |
| 52 | 1 | 0 | 2.085690  | 6.316743  | -1.437614 |
| 53 | 6 | 0 | 0.334815  | 5.270216  | -0.743356 |
| 54 | 1 | 0 | -0.329495 | 6.104718  | -0.952032 |
| 55 | 6 | 0 | -0.196608 | 4.092514  | -0.204508 |
| 56 | 6 | 0 | 3.060960  | 1.990429  | 0.016530  |
| 57 | 1 | 0 | 2.513774  | 1.121914  | 0.392002  |
| 58 | 6 | 0 | 3.761201  | 1.565403  | -1.289845 |
| 59 | 1 | 0 | 4.379327  | 0.678076  | -1.120009 |
| 60 | 1 | 0 | 4.407839  | 2.363348  | -1.674928 |
| 61 | 1 | 0 | 3.034863  | 1.324781  | -2.072601 |
| 62 | 6 | 0 | 4.116050  | 2.373671  | 1.073871  |
| 63 | 1 | 0 | 4.811484  | 1.541297  | 1.229591  |
| 64 | 1 | 0 | 3.661071  | 2.617986  | 2.040287  |
| 65 | 1 | 0 | 4.703454  | 3.243370  | 0.755825  |
| 66 | 6 | 0 | -1.703088 | 4.024813  | 0.041813  |
| 67 | 1 | 0 | -1.937030 | 3.041481  | 0.459244  |
| 68 | 6 | 0 | -2.484678 | 4.166101  | -1.279670 |
| 69 | 1 | 0 | -3.562127 | 4.066943  | -1.100334 |
| 70 | 1 | 0 | -2.185665 | 3.400960  | -2.003733 |
| 71 | 1 | 0 | -2.315371 | 5.145684  | -1.741966 |
| 72 | 6 | 0 | -2.180278 | 5.082616  | 1.057443  |
| 73 | 1 | 0 | -3.255690 | 4.974524  | 1.243042  |
| 74 | 1 | 0 | -2.008538 | 6.100294  | 0.687862  |
| 75 | 1 | 0 | -1.663381 | 4.988225  | 2.018533  |
| 76 | 6 | 0 | 2.357745  | -1.708623 | -0.219143 |
| 77 | 6 | 0 | 2.707471  | -2.123590 | -1.537215 |
| 78 | 6 | 0 | 4.024065  | -2.517311 | -1.803936 |
| 79 | 1 | 0 | 4.285811  | -2.813436 | -2.817133 |
| 80 | 6 | 0 | 4.999854  | -2.557466 | -0.814914 |
| 81 | 1 | 0 | 6.015549  | -2.864883 | -1.048169 |
| 82 | 6 | 0 | 4.641327  | -2.222176 | 0.489710  |
| 83 | 1 | 0 | 5.391808  | -2.283493 | 1.271753  |
| 84 | 6 | 0 | 3.349187  | -1.802975 | 0.813954  |
| 85 | 6 | 0 | 1.692116  | -2.212447 | -2.675989 |
| 86 | 1 | 0 | 0.699661  | -2.005842 | -2.262039 |
| 87 | 6 | 0 | 1.622190  | -3.634162 | -3.271689 |
| 88 | 1 | 0 | 0.822598  | -3.695869 | -4.020356 |
| 89 | 1 | 0 | 1.422699  | -4.379510 | -2.494728 |
| 90 | 1 | 0 | 2.559436  | -3.912603 | -3.767150 |
| 91 | 6 | 0 | 1.951764  | -1.181359 | -3.790777 |
| 92 | 1 | 0 | 1.191318  | -1.260095 | -4.577708 |
| 93 | 1 | 0 | 2.933114  | -1.340799 | -4.253660 |
| 94 | 1 | 0 | 1.930221  | -0.155750 | -3.407211 |
| 95 | 6 | 0 | 2.987270  | -1.508204 | 2.271392  |

|     |   |   |          |           |          |
|-----|---|---|----------|-----------|----------|
| 96  | 1 | 0 | 2.303139 | -0.647407 | 2.288492 |
| 97  | 6 | 0 | 2.247048 | -2.708263 | 2.906665 |
| 98  | 1 | 0 | 1.907739 | -2.470046 | 3.922819 |
| 99  | 1 | 0 | 2.917668 | -3.573819 | 2.966105 |
| 100 | 1 | 0 | 1.374810 | -3.012027 | 2.318217 |
| 101 | 6 | 0 | 4.177613 | -1.118110 | 3.163698 |
| 102 | 1 | 0 | 3.814916 | -0.799047 | 4.147946 |
| 103 | 1 | 0 | 4.756759 | -0.295094 | 2.732552 |
| 104 | 1 | 0 | 4.858180 | -1.961171 | 3.329641 |

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#### Complete reference 49:

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