Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radical-Coupling Reactions (Pn = N, P, As)

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Experimental

General considerations

All air and moisture-sensitive manipulations were carried out using standard Schlenk techniques or in a glovebox containing purified argon. Solvents were purified by distillation using the appropriate drying agents, degassed and stored over molecular sieves (4 Å) prior to use. Deuterated solvents used for NMR spectroscopy were dried, degassed and stored over molecular sieves (4 Å) under dry argon prior to use. Bis(4-trifluoromethylphenyl)amine,[1] $Bi(NMe_2)_3$ (**4**),[2] bis(4-trifluoromethylphenyl)phosphane,[3] bis(4-methoxyphenyl)phosphane,[4] bis(4-chlorophenyl)phosphane[4] and diphenylarsane[5] were synthesized according to the literature. $BiCl_3$ was sublimed prior to use.
All NMR spectra were acquired either on a Bruker Avance 400 spectrometer or on a Bruker Avance I 500 spectrometer. ^{1}H and ^{13}C chemical shifts are reported relative to $SiMe_4$ using the residual solvent peak of the solvent as secondary standard. ^{19}F chemical shifts are reported relative to $CFCl_3$ as an external standard. ^{15}N chemical shifts are reported relative to CH_3NO_2 (90% in $CDCl_3$) and were determined by two-dimensional ^{1}H-^{15}N correlation NMR spectroscopic experiments. Elemental analyses (C, H, N, S) were conducted on a Vario Micro Cube by Elementar Analysesysteme GmbH. Reproducibly satisfactory elemental analyses of **1-CF$_3$** and **1-OMe** proved to be difficult to obtain, which was ascribed to the air and temperature sensitivity of the compounds. In order to provide evidence for the efficacy of the synthesis of these compounds, the bismuth content of **1-CF$_3$** and **1-OMe** was determined by complexometric titrations according to previously reported procedures using a solution of the disodium salt of ethylenediaminetetraacetic acid as a titrant and Xylenol Orange as an indicator. For mass spectrometric analyses, an Exactive plus instrument (Thermo Scientific) was used.
Single-crystals suitable for X-ray diffraction analysis were coated with perfluorinated polyether oil in a glovebox, transferred to a nylon loop and then transferred to the goniometer of a diffractometer (Bruker D8 Quest or Bruker X8-Apex II) equipped with a molybdenum X-ray tube (λ = 0.71073 Å).
EPR measurements at X-band were carried out at ambient temperature using a Bruker ELEXSYS E580 CW/FT EPR spectrometer. The spectral simulations were performed using MATLAB 9.6 (2019a) and the EasySpin 5.2.25 toolbox.[6]

Discussion

In the original procedure, compound **1-H** was purified by re-crystallization from CH_2Cl_2 over a period of days, resulting in an isolated yield of 30% (the reported ^{13}C NMR spectrum showed signals of the hydrazine Ph_4N_2 (**3-H**), which were not identified as such).[7] Our procedure avoids the use of CH_2Cl_2 which was confirmed as one cause of decomposition. Keeping **1-H** in solution for extended periods of time was avoided because it also favors the decomposition of **1-H**. In combination, these modifications resulted in 88% yield of analytically pure material (route 1). Compounds **1-Me** and **1-OMe** were obtained in an analogous approach, albeit with somewhat lower yields of 79% and 51%, respectively. The reduced yields were ascribed to the high reactivity of compounds **1-Me** and **1-OMe** in solution (see main part). For other derivatives of **1-H**, different synthetic approaches were required. In the case of **1-Br** and **1-Ph** this is due to limited solubility of the amines. Also, route 1 does not give quantitative conversion of the *in situ* generated lithium amides to the bismuth compounds in these cases. As an alternative route, a salt elimination reaction of the potassium amides (generated in situ from KH and the respective amine) and BiI_3 was established (route 2). Due to the sufficiently poor solubility of KI in THF, the reaction can be carried out in THF and the by-product KI can be filtered off without changing to another solvent system. The products **1-Ph** and **1-Br** were obtained in 87% and 83% yield by precipitation through addition of pentane. The use of this method for **1-OMe** improved the yield from 51% to 78% which highlights the advantage of route 2. Routes 1 and 2 are not as easily feasible for **1-CF$_3$** due to the lability of the lithium or potassium amides at temperatures above –78 °C. Rapid decomposition of these species was observed. A mild transamination reaction of $Bi(NMe_2)_3$ (**4**) with the amine $HN(4\text{-}CF_3\text{-}C_6H_4)_2$ was successful in this case. This required extended reaction times, but was facilitated by the stability of **1-CF$_3$** in solution.

[Bi(NPh$_2$)$_3$] (1-H). The synthesis was conducted according to an optimized procedure based on the synthesis published by Clegg *et. al.*.[7] Diphenylamine (2.42 g, 14.3 mmol) was dissolved in THF (15 mL) and cooled to 0 °C. A solution of *n*-BuLi in hexanes (8.9 mL, 1.6 M, 14.3 mmol) was added dropwise. The reaction mixture turned yellow and was stirred at ambient temperature for 90 min. $BiCl_3$ (1.50 g, 4.80 mmol) was dissolved in THF (15 mL) and cooled to 0 °C. The yellow amide solution was slowly transferred to the $BiCl_3$ solution with an immediate color change to orange. After completion of the addition, the reaction mixture was warmed to ambient temperature and stirred for 30 min followed by removal of the solvent under reduced pressure. The orange residue was dissolved in benzene (5 mL) and filtered over celite. The solvent was removed under reduced pressure and the residue was washed with pentane (3 × 5 mL). The orange powder was dried *in vacuo* for 3 h.
Yield: 3.01 g (4.22 mmol, 88%)
^{1}H NMR: (298 K, 400 MHz, Benzene-d_6): δ = 6.66 – 6.77 (m, 18H, 2,4,6-C_6H_5), 7.04 – 7.09 (m, 12H, 3,5-C_6H_5) ppm.
^{13}C NMR: (298 K, 100 MHz, Benzene-d_6): δ = 122.5 (s, 4-C_6H_5), 124.5 (s, 2,6-C_6H_5), 129.6 (s, 3,5-C_6H_5), 151.3 (s, 1-C_6H_5) ppm.
^{1}H NMR: (298 K, 400 MHz, Methylenedichloride-d_2): δ = 6.60 (dd, 12H, $^{3}J_{HH}$ = 8.6 Hz, $^{4}J_{HH}$ = 0.93 Hz, 2,6-C_6H_5), 6.86 (t, 6H, $^{3}J_{HH}$ = 7.4 Hz, 5-C_6H_5) 7.18 (dd, 12 H, $^{3}J_{HH}$ = 7.4 Hz, $^{3}J_{HH}$ = 8.5 Hz, 3,5-C_6H_5) ppm.

^{13}C NMR: (298 K, 100 MHz, Methylenedichloride-d_2): δ = 122.7 (s, 4-C_6H_5), 124.5 (s, 2,6-C_6H_5), 129.7 (s, 3,5-C_6H_5), 151.3 (s, 1-C_6H_5) ppm.
Elemental analysis: Anal. calc. for $C_{36}H_{30}BiN_3$ (713.64 g · mol^{-1}): C, 60.59; H, 4.24; N, 5.89; found: C, 60.48; H, 4.38; N, 5.81.

[Bi[N(4-Me-C_6H_4)$_2$]$_3$] (1-Me). Di(*p*-tolyl)amine (3.75 g, 19.0 mmol) was dissolved in THF (9 mL). After cooling to 0 °C, a solution of *n*-BuLi in *n*-hexanes (7.60mL, 2.5 M, 19.0 mmol) was added dropwise. A yellow solution was obtained, which gradually changed its color to deep green while stirring for 1 h at 0 °C. $BiCl_3$ (2.00 g, 6.34 mmol) was dissolved in THF (9 mL) and cooled to 0 °C. The green amide solution was slowly added resulting in an immediate color change to orange. After completion of the addition, the reaction mixture was stirred for 30 min at 0 °C. All volatiles were removed under reduced pressure. Benzene (10 mL) was added to the residue and an orange suspension with a grey solid was formed. The mixture was filtrated over celite. After removing the solvent under reduced pressure from the filtrate and drying the resulting solid for one hour *in vacuo*, the residue was washed with pentane to give a red powder after drying for 3 h *in vacuo*.
Yield: 3.97 g (4.98 mmol, 79%)
^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 2.16 (s, 18H, C_6H_4*Me*), 6.76 (d, 12H, $^3J_{HH}$ = 8.3 Hz, 2,6-C_6H_4Me), 6.94 (d, 12H, $^3J_{HH}$ = 8.3 Hz, 3,5-C_6H_4Me,) ppm.
^{13}C NMR (298 K, 125 MHz, Benzene-d_6): δ = 20.6 (s, C_6H_4*Me*), 124.5 (s, 2,6-C_6H_4Me), 130.1 (s, 3,5-C_6H_4Me), 131.3 (s, 4-C_6H_4Me), 149.4 (s, 1-C_6H_4Me) ppm.
^{15}N NMR (298 K, 50 Hz, Benzene-d_6): δ = –217.1 (s) ppm.
Elemental analysis. Anal. calc. for $C_{42}H_{42}BiN_3$ (797.32 g · mol^{-1}): C, 63.23; H, 5.31; N, 5.27; found: C, 62.90; H, 5.44; N, 5.08.

[Bi[N(4-MeO-C_6H_6)$_2$]$_3$] (1-OMe). 4,4'-Dimethoxydipyhenylamine (400 mg, 1.75 mmol) was dissolved in THF (5 mL). After cooling to 0 °C, a solution of *n*-BuLi in *n*-hexanes (1.09 mL, 1.6 M, 1.75 mmol) was added dropwise. A yellow solution was obtained while stirring for 1 h at 0 °C. $BiCl_3$ (184 mg, 0.58 mmol) was dissolved in THF (5 mL) and cooled to 0 °C. The yellow amide solution was slowly added resulting in an immediate color change to orange. After completion of the addition, the reaction mixture was stirred for 20 min at 0 °C, and all volatiles were removed under reduced pressure. Benzene (5 mL) was added and the orange suspension was filtered over celite. After removing all volatiles from the filtrate under reduced pressure, the residue was washed with pentane to give a brown powder as product after drying for 3 h *in vacuo*.
Yield: 267 mg (0.30 mmol, 51%)

A solution of 4,4'-Dimethoxydipyhenylamine (875 mg, 3.82 mmol) in THF (8 mL) was cooled to 0 °C and a dispersion of potassium hydride (154 mg, 3.83 mmol) in THF (2 mL) was slowly added. An immediate gas evolution and a color change to dark green were observed. The solution was allowed to warm to ambient temperature while stirring for 4 h. BiI_3 (750 mg, 1.27 mmol) was dissolved in THF (8 mL) and cooled to –78 °C. The amide solution was slowly added with an immediate color change to red. While warming to around –20 °C a white solid precipitated. After stirring for 10 min, all solids were removed by filtration over celite. The solvent was removed from the filtrate under reduced pressure. The resulting solid was washed with pentane (6 × 5 mL) and dried *in vacuo* for 30 min.
Yield: 882 mg (0.99 mmol, 78%)
^{1}H NMR (298 K, 500 MHz, Benzene-d_6): δ = 3.33 (s, 18H, C_6H_4O*Me*), 6.77 – 6.82 (m, 24H, 2,3,5,6-C_6H_4OMe) ppm.
^{13}C NMR (298 K, 125 MHz, Benzene-d_6): δ = 55.2 (s, C_6H_4O*Me*), 115.0 (s, 2,6-C_6H_4OMe), 125.7 (s, 3,5-C_6H_4OMe), 145.6 (s,1-C_6H_4OMe), 155.8 (s, 4-C_6H_4OMe) ppm.
^{15}N NMR (298 K, 50 Hz, Benzene-d_6): δ = –221.1 (s) ppm.
Elemental analysis. Anal. calc. for $C_{42}H_{42}BiN_3O_6$ (893.79 g · mol^{-1}): Bi, 23.4; found: Bi, 23.7.

[Bi[N(4-Br-C_6H_4)$_2$]$_3$] (1-Br). A solution of bis(4-bromophenyl)amine (998 mg, 3.05 mmol) in THF (8 mL) was cooled to 0 °C and a dispersion of potassium hydride (123 mg, 3.06 mmol) in THF (2 mL) was slowly added. An immediate gas evolution and a color change to slightly yellow were observed. The solution was allowed to warm to ambient temperature while stirring for 2 h. BiI_3 (600 mg, 1.02 mmol) was dissolved in THF (9 mL) and cooled to 0 °C. The yellow amide solution was slowly added with an immediate color change to red. While warming to ambient temperature a white solid precipitated. After stirring for 45 min, all solids were removed by filtration over celite. The solvent was narrowed down to 3 mL under reduced pressure. Pentane (30 mL) was added while stirring leading to precipitation of an orange solid, which was isolated by filtration. The solid was washed with pentane (6 × 5 mL) and dried *in vacuo* for 5 min (exposure to vacuum for extended periods of time leads to decomposition). The product contains n equiv. THF (n needs to be evaluated individually for every batch and typically ranges from 0.3 to 1.0, values given here refer to n = 0.75).
Yield: 1.05 g (0.84 mmol, 83%)
^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 6.15 (d, 12 H, $^3J_{HH}$ = 7.9 Hz, 2,6-C_6H_4Br,), 7.13 (d, 12H, $^3J_{HH}$ = 7.9 Hz, 3,5-C_6H_4Br) ppm. Resonances due to THF were also detected.
^{13}C NMR (298 K, 126 MHz, Benzene-d_6): δ = 116.2 (s, 4-C_6H_4Br). 125.6 (s, 2,6-C_6H_4Br), 132.7 (s, 3,5-C_6H_4Br), 149.3 (s, 1-C_6H_4Br) ppm.
Elemental analysis. Anal. calc. for $C_{36}H_{32}BiN_3Br_3$ × 0.75 [C_4H_8O] (1187.01 g · mol^{-1}): C, 37.74; H, 2.44; N, 3.39; found: C, 37.38; H, 2.50; N, 3.43.

[Bi[N(*p*-biphenyl)$_2$]$_3$] (1-Ph). A solution of bis(4,4'-dipyhenyl)amine (999 mg, 3.11 mmol) in THF (20 mL) was cooled to 0 °C and a dispersion of potassium hydride (125 mg, 3.12 mmol) in THF (2 mL) was slowly added. An immediate gas evolution and a color change to orange were observed. The solution was allowed to warm to ambient temperature while stirring for 4 h. BiI_3 (611 mg, 1.04 mmol) was dissolved in THF (9 mL) and cooled to –78 °C. The amide solution was slowly added with an immediate color change to red. A white solid precipitated. After stirring for 10 min, all solids were removed by filtration over celite. The solvent was removed from the filtrate under reduced pressure. The resulting solid was washed with pentane (6 × 5 mL) and dried *in vacuo* for 5 min (exposure to vacuum for extended periods of time leads to decomposition).
The product contains n equiv. THF (n needs to be evaluated individually for every batch and typically ranges from 0.4 to 1.2, values given here refer to n = 1.0).
Yield: 1.12 g (0.90 mmol, 87%)
^{1}H NMR (298 K, 500 MHz, Benzene-d_6): δ = 6.99 (d, 12H, $^3J_{HH}$ = 8.0 Hz, 2,12-$C_{12}H_9$), 7.10 (t, 6H, $^3J_{HH}$ = 7.5 Hz, 8-$C_{12}H_9$), 7.20 (dd, 12 H, $^3J_{HH}$ = 7.5 Hz, $^3J_{HH}$ = 7.4 Hz, 7,9-$C_{12}H_9$,), 7.44 (d, 12H, $^3J_{HH}$ = 6.9 Hz, 6,10-$C_{12}H_9$) 7.48 (d, 12H, $^3J_{HH}$ = 8.4 Hz, 3,11-$C_{12}H_9$) ppm. Resonances due to THF were also detected.
^{13}C NMR (298 K, 126 MHz, Benzene-d_6): δ = 124.8 (s, 2,12-$C_{12}H_9$), 127.0 (s, 8-$C_{12}H_9$), 127.1 (s, 6,10-$C_{12}H_9$), 128.4 (s, 3,11-$C_{12}H_9$), 129.1 (s, 7,9-$C_{12}H_9$), 135.9 (s, 5-$C_{12}H_9$), 141.1 (s, 4-$C_{12}H_9$), 150.7 (s, 1-$C_{12}H_9$) ppm. Resonances due to THF were also detected.
^{15}N NMR (298 K, 50 Hz, Benzene-d_6): δ = –212.9 (s) ppm.
Elemental analysis. Anal. calc. for $C_{72}H_{54}BiN_3$ × 1.0 [C_4H_8O] (g · mol^{-1}): C: 73.48; H, 5.03; N, 3.38; found: C, 73.59; H, 4.78; N, 3.43.

[Bi[N(4-CF_3-C_6H_4)$_2$]$_3$] (1-CF_3). A solution of *bis*(4-trifluoromethyl)amine (268 mg, 0.88 mmol) in benzene (2 mL) was added to a solution of tris(dimethylamido)bismuth (**4**) (100 mg, 0.29 mmol) in benzene (2 mL). The reaction mixture was stirred for 5 d at room temperature resulting in a dark red solution. All volatiles were removed under reduced pressure. Washing with pentane (3 × 5 mL) and drying *in vacuo* for 45 min resulted in a violet powder.
Yield: 206 mg (0.18 mmol, 63%)
^{1}H NMR: (298 K, 400 MHz, Benzene-d_6): δ = 6.30 (d, 12H, $^3J_{HH}$ = 7.85 Hz, 2,6-$C_6H_4CF_3$), 7.27 (d, 12H, $^3J_{HH}$ = 7.85 Hz, 3,5-$C_6H_4CF_3$) ppm.
^{19}F NMR: (298 K, 377 MHz, Benzene-d_6): δ = –61.53 (s) ppm.
^{13}C NMR: (298 K, 101 MHz, Benzene-d_6): δ = 123.7 (s, 2,6-$C_6H_4CF_3$), 124.7 (q, $^1J_{CF}$ = 271.5 Hz, CF_3), 127.2 (q, $^3J_{CF}$ = 3.6 Hz, 3,5-$C_6H_4CF_3$), 128.6 (s, 4-$C_6H_4CF_3$), 152.7 (s, 1-$C_6H_4CF_3$) ppm.
Elemental analysis. Anal. calc. for $C_{42}H_{24}BiF_{18}N_3$ (1121.63 g · mol^{-1}): Bi: 18.6; found: Bi: 18.2.

Single Crystal X-ray Analysis

Deposition Numbers 2044877-2044880 contain the supplementary crystallographic information for this work. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service under www.ccdc.cam.ac.uk/structures.

[Bi(NPh_2)$_3$] (1-H). Analogously to the literature,[7] **1-H** crystallizes in the triclinic space group $P\bar{1}$ with Z = 4 as a twin with two components in a ratio of 68:32 that are related by a 180° rotation about the reciprocal [001] axis (Figure S1). The asymmetric unit contains two chemically identical but crystallographically independent molecules. The bismuth atom is coordinated by three diphenylamido ligands with an angular sum of 294° around Bi1, resulting in a slightly distorted trigonal pyramidal coordination geometry. The angular sums around the nitrogen atoms are close to 360°, indicating a trigonal planar coordination geometry. In comparison to previously reported data for **1-H**, the margin of error was slightly improved (Bi1–N1: 2.17(2) Å to 2.167(6) Å), however the bonding parameters are in the same order of magnitude.[7] Weak interactions between the bismuth atom and the phenyl group of a neighboring molecule are present based on distance criteria.

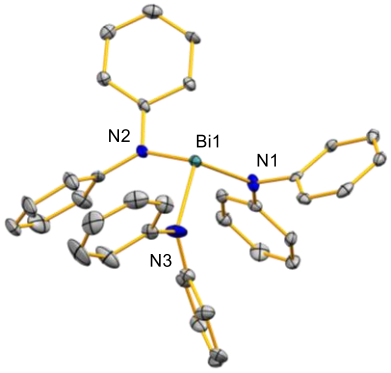


Figure S1. Molecular Structure of **1-H** in the solid state. The elemental cell contains two crystallographically independent, but chemically identical molecules of the bismuth amide. Only one of them is depicted since the bonding parameters are highly similar. Ellipsoids are shown at the 50% probability level; hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles[°]: Bi1–N1, 2.167(6); Bi1–N2, 2.184(7); Bi1–N3, 2.148(7); N1–Bi1–N2, 96.8(2); N1–Bi1–N3, 97.0(3); N2–Bi1–N3, 100.3(3); Σ(Bi1) 294, Σ(N1) 360, Σ(N2) 352, Σ(N3) 360.

[Bi[N(4-Me-C$_6$H$_4$)$_2$]$_3$] (1-Me). 1-Me crystallizes in the triclinic space group $P\bar{1}$ with Z = 2 (Figure S2a). The bismuth atom is coordinated by three di(*p*-tolyl)amide ligands. The bond angles around Bi1 are 100.68(8)° (N1–Bi1–N2), 97.92(8)° (N1–Bi1–N3), and 95.03° (N2–Bi1–N3) with an angular sum of 294° around bismuth. This results in a distorted trigonal pyramidal geometry. The two *p*-tolyl substituents of each amide are twisted relatively to each other. The idealized planes defined by the *p*-tolyl groups of each amide ligand form angles of 86.16° (N1), 79.82° (N2), and 59.02° (N3). The distances between Bi1 and the three nitrogen atoms vary between 2.158(2) Å (Bi1–N2) and 2.185(2) Å (Bi1–N3) which is in accordance with the only literature-known bismuth arylamide **1-H** with distances between 2.149(7) Å and 2.183(7) Å. The N–Bi–N bond angles are also in the same range as previously reported for **1-H** with angles between 96.7(3)° and 100.3(3)°. The angular sums of the nitrogen atoms are 357° (N1), 359° (N2), and 354° (N3) resulting in a near trigonal planar geometry. The distance between bismuth atoms of neighboring molecules of **1-Me** amounts to 3.79 Å, suggesting Bi···Bi interactions in the solid state (Figure S2b).

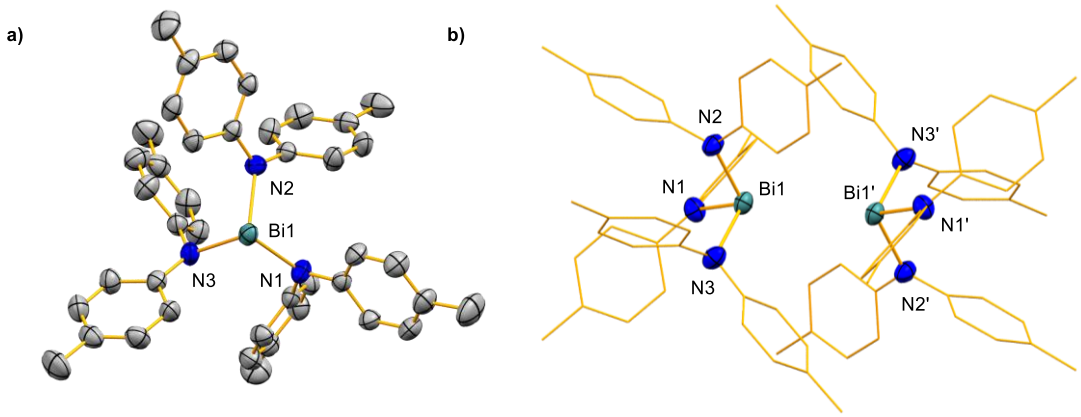


Figure S2. Molecular structure of **1-Me** in the solid state (a: one formula unit; b: two formula unit with potential Bi···Bi interactions). Ellipsoids are set at 50% probability; hydrogen atoms are omitted and carbon atoms in (b) are shown as wireframe for clarity. Selected bond lengths [Å] and angles [°]: Bi1–N1, 2.1598(19); Bi1–N2, 2.158(2); Bi1–N3, 2.185(2); N1–Bi1–N2, 100.68(8); N1–Bi1–N3, 97.92(8); N2–Bi1–N3, 95.03(8); Σ(Bi1) 294, Σ(N1) 357, Σ(N2) 359, Σ(N3) 354.

[Bi[N(4-Br-C$_6$H$_4$)$_2$]$_3$] (1-Br). 1-Br crystallizes in the triclinic space group $P\bar{1}$ with Z = 1 (Figure S3). The bismuth atom Bi1 is coordinated by three bis(*p*-bromophenyl) amide ligands with bond angles of N1–Bi1–N2 94.18(12)°, N1–Bi1–N3 95.03(11)° and N2–Bi1–N3 95.87(11)°. In comparison to **1-H** and **1-Me**, the three bond angles show less variance with a difference of only 1.69° between the smallest and largest angle (**1-H**: 3.6°; **1-Me**: 5.7°).[7] Also, the angular sum of 285° around the bismuth is 9° smaller than observed for the two previously described examples. Nevertheless, this results in a slightly distorted trigonal pyramidal geometry, as well. The two 4-bromophenyl substituents of each amide are twisted relatively to each other. The idealized planes defined by the 4-bromophenyl groups of each amide ligand form angles of 86.03° (N1), 78.39° (N2), and 85.97° (N3). The distances between Bi1 and the three nitrogen atoms vary between 2.157(3) Å (Bi1–N2) and 2.172(3) Å (Bi1–N1), which is in accordance with Bi(NPh$_2$)$_3$ with distances between 2.149(7) Å and 2.183(7) Å.[7] The average Bi–N bond lengths (2.1666 Å) are as long as in **1-Me** (2.1676 Å). The angular sums of the nitrogen atoms are 359°(N1) and 360° (N2, N3), resulting in a trigonal planar geometry. Weak interactions between the bismuth atom and the bromine atom of a neighboring molecule are present based on distance criteria.

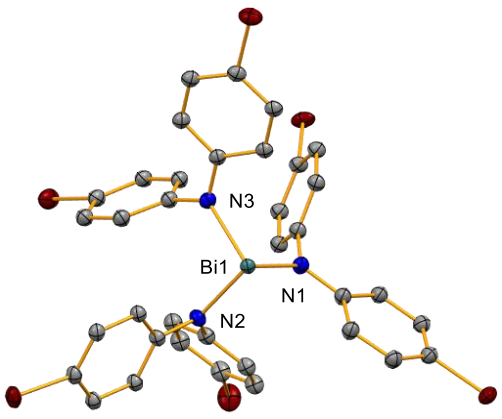


Figure S3. Molecular structure of **1-Br** in the solid state. Ellipsoids are shown at the 50% probability level; hydrogen atoms and two lattice-bound toluene molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]: Bi1–N1 2.172(3), Bi1–N2 2.157(3); Bi1–N3 2.171(3); N1–Bi1–N2 94.18(12), N1–Bi1–N3 95.03(11), N2–Bi1–N3 95.87(11); Σ(Bi1) 285, Σ(N1) 359, Σ(N2) 360, Σ(N3) 360.

[Bi[N(4-biphenyl)$_2$]$_3$] (1-Ph). 1-Ph crystallizes in the triclinic space group $P\bar{1}$ with Z = 2 as a two-component twin (the two domains are related by a rotation around direct lattice direction [100]; Figure S4). The asymmetric unit contains two chemically identical but crystallographically independent molecules, only one of which is discussed due to their similarity. The angular sum around Bi1_1 amounts to 303°, resulting in a distorted trigonal pyramidal geometry. The angular sum around the central atom is somewhat larger than that in Bi(NPh$_2$)$_3$ (**1-H**) (294°). The bismuth atom in **1-Ph** is coordinated by three *bis*(4-biphenyl) amide ligands with bond angles between 96.7(2)° (N1_1–Bi1_1–N3_1) and 107.5(3)° (N2_1–Bi1_1–N3_1). The N–Bi–N angles in **1-Ph** span a wider range than those in **1-H** (96.2(3)°-100.3(3)).[7] The greater variance of the bond angles can arise due to π-interactions between the phenyl ring attached to N1_1 and the phenyl ring attached to N2_1 (3.670 Å). In the ring-slipped π-stacking, the smallest distance of the centroid of one aryl ring to a carbon atom of the other aryl ring (and vice versa) amounts to 3.32 Å (and to 3.59 Å), suggesting a significant interaction.[8] The high steric demand of the *bis*(4-biphenyl) amide substituents may also contribute to the N–Bi–N bond angles differing from those in **1-H**, **1-Me**, and **1-Br**. In addition, the Bi–N bonds in **1-Ph** (2.16-2.23 Å) are slightly elongated compared to those in **1-H** (2.15-2.18 Å), **1-Me** (2.16-2.19 Å), and **1-Br** (2.16-2.17 Å). Weak interactions between the bismuth atom and the phenyl group of a neighboring molecule are present based on distance criteria.

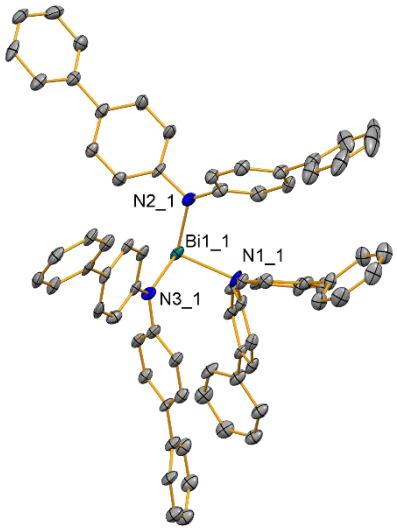


Figure S4. Molecular structure of **1-Ph** in the solid state. The elemental cell contains two crystallographically independent, but chemically identical molecules of the bismuth amide. Only one of them is depicted since the bonding parameters are highly similar. Ellipsoids are shown at the 50% probability level; hydrogen atoms and one lattice-bound THF molecule are omitted for clarity. Selected bond lengths [Å] and angles [°]: Bi1_1–N1_1 2.197(6), Bi1_1–N2_1 2.162(7), Bi1_1–N3_1 2.230(6); N1_1–Bi1_1–N2_1 98.4(3), N2_1–Bi1_1–N3_1 107.5(2), N1_1–Bi1_1–N3_1 96.7(2),; Σ(Bi1_1) 303, Σ(N1_1) 360, Σ(N2_1) 360, Σ(N3_1) 359.

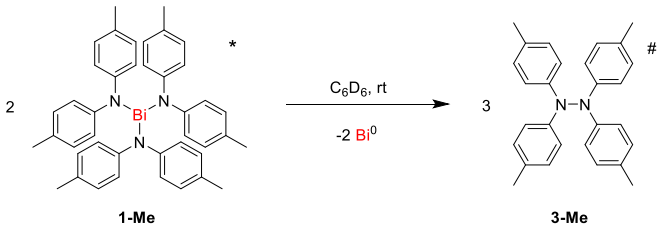
Literature-Known Bismuth Amides and Related Species

A small group of bismuth compounds with amide ligands that contain one aryl group, (NArR)$^-$, has been reported (R = H, Si(alkyl)$_3$). These include mono-, di-, and trinuclear complexes of type [Bi(NArR)$_3$], [BiZ$_2$(NArR)], [Bi$_2$(NAr)$_2$(NHAr)$_2$], and [Bi$_3$(NAr)$_4$(NHAr)] (Z = halide, weakly coordinating anion).[9]
Unforeseen reactions such as CH activation,[9a, 9f] dearomatization,[9f] N–Si bond cleavage,[10] Bi–N/B–Li metathesis,[9d] methyl migration (from Si to Bi),[9g] and transamination/aggregation sequences[9j] have been documented for these species, but have not mechanistically been rationalized in many cases.

As outlined in the main part, homolytic Bi-O bond cleavage has previously been discussed in the context of the SOHIO process.[11] Different mechanistic scenarios have also been discussed in the SOHIO process and have recently been suggested to be more likely based on kinetic investigations.[12]

Reaction Monitoring: Formation of Compounds 3-X from 1-X

General procedure: a sample of the bismuth compound (**1-H**, **1-Me**, **1-OMe**, **1-Br**, or **1-Ph**, respectively; n = 1.25 · 10^{-5} mmol in each case) was dissolved in C_6D_6 (0.5 mL) at room temperature and the progress of the reaction was monitored by ^{1}H NMR spectroscopy. Examples of the reaction equation and selected NMR spectra are shown in Scheme S1 and Figure S5 for compound **1-Me**. Half-life periods were determined (Table S1).



Scheme S1. Formation of **3-Me** from **1-Me** in an N–N bond formation reaction.

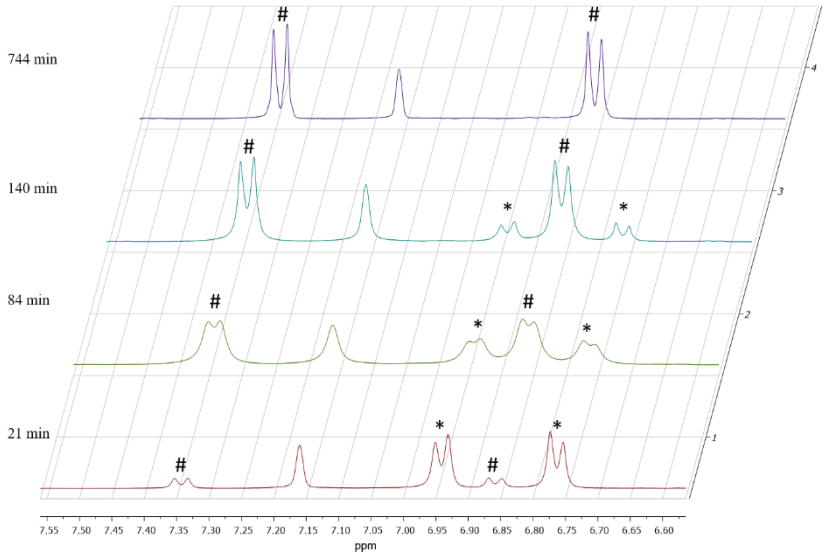


Figure S5. Aromatic region of the ^{1}H NMR spectra of **1-Me** over time. The intensity of the doublets of the bismuth amide at 6.77 (*) and 6.95 (*) ppm decreases whereas the intensity of the doublets of the hydrazine derivative **3-Me** at 6.87 (#) and 7.35 (#) ppm increases over time.

Table S1. Half-life periods of the bismuth amides **1-X** in their selective N–N bond formation reactions in benzene at 23 °C.

Compound	$t_{1/2}$ [h]	Compound	$t_{1/2}$ [h]
1-H	63	**1-Me**	1.4
1-OMe	1.2	**1-Br**	84
1-Ph	74	**1-CF_3**	stable

Kinetic Investigations of Formation of 3-Me from 1-Me

General procedure: 5 mg ($6.2\cdot10^{-3}$ mmol), 10 mg ($1.3\cdot10^{-2}$ mmol), 15 mg ($1.9\cdot10^{-2}$ mmol), 30 mg ($3.7\cdot10^{-2}$ mmol), or 45 mg ($5.6\cdot10^{-2}$ mmol) of **1-Me** were dissolved in C_6D_6 (0.5 mL) and the progress of the formation of **3-Me** was monitored by ^{1}H NMR spectroscopy at 23 °C and determined by the integration intensity of the ^{1}H NMR spectroscopic resonances of the methyl groups of **1-Me** and **3-Me**. The related time-conversion plot is shown in Figure S6. It is apparent that higher initial concentrations of **1-Me** decrease the rate at which **3-Me** is formed. In agreement with this, the aggregation of two equivalents **1-Me** to give the dinuclear species **(1-Me)$_2$** was found to be exothermic (ΔH = –29.6 kcal·mol^{-1}) and exergonic (ΔG = –6.6 kcal·mol^{-1}) according to DFT calculations. Analyses of kinetic parameters of the reaction are hampered by the fact that at least three (and probably more) elementary steps are involved in the reaction and that no intermediates could be detected or isolated (in agreement with the energies of potential intermediates investigated by DFT calculations). Visual kinetic analyses[13] suggest that the *apparent* order of the reaction in **1-Me** amounts to 0.5 at low initial concentrations of **1-Me** ($c_{low} \leq 25$ mmol·L^{-1} (up to 10 mg of **1-Me** under our conditions)), but deviates from this value at higher initial concentrations (Figure S7). Thus, the kinetic analyses confirm the complexity and suggest a concentration-dependency of the reaction mechanism.

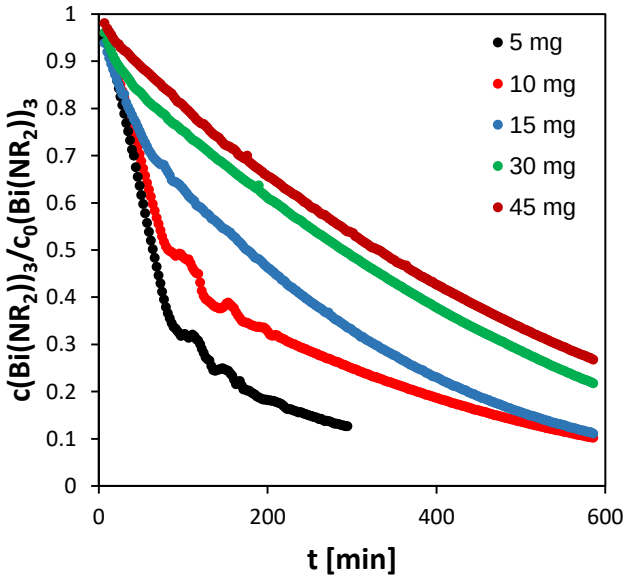


Figure S6. Concentration-dependency of the formation of **3-Me** from **1-Me**.

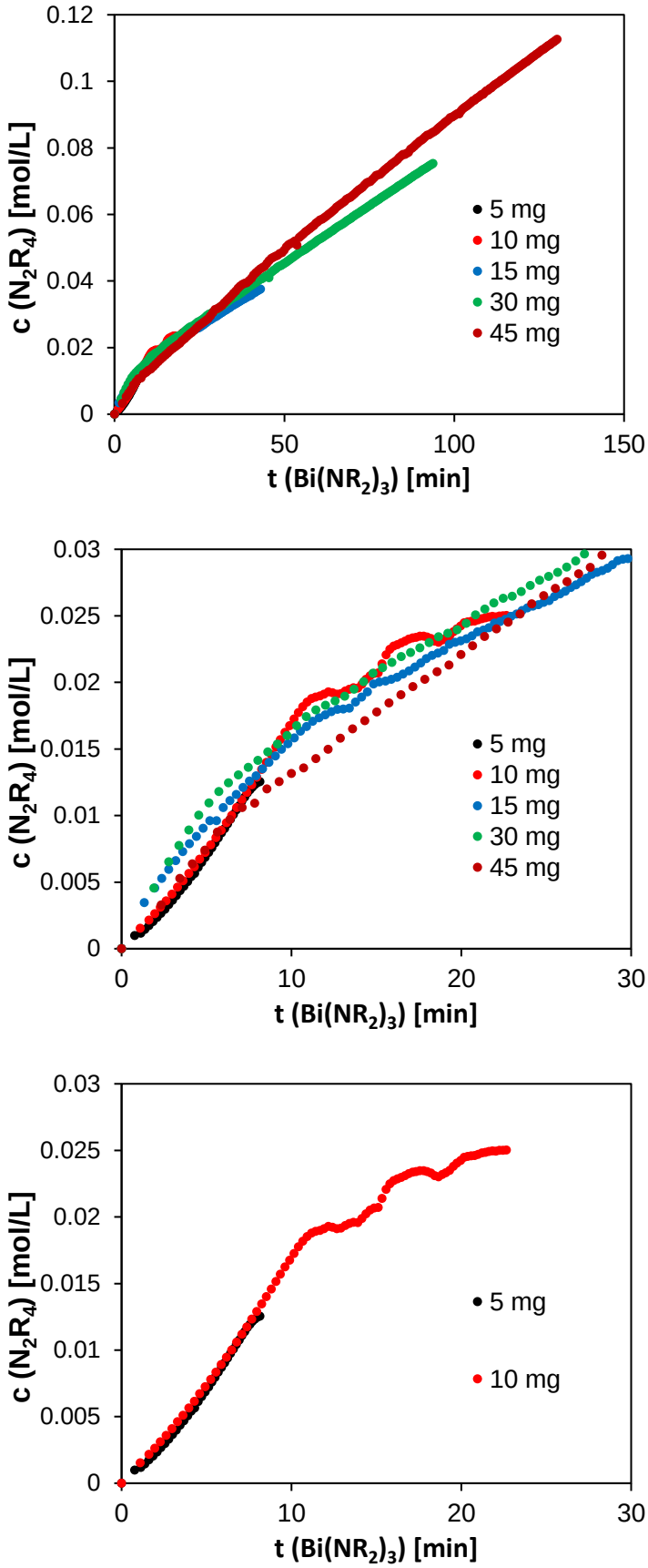


Figure S7. Plots according to Variable Time Normalisation Analysis (VTNA) for **1-Me** (i.e. R = 4-Me-C_6H_4).[13] Plots show the result obtained for a reaction order of 0.5. Variation of this parameter did not result in a better fit of all data. The graphs show plots of all initial concentrations (top), all initial concentrations in a selected region (middle), and the lowest concentrations (bottom).

NMR Spectroscopic data of the hydrazine derivatives 3-X

Reaction of **1-H** yielding **3-H**:

^{1}H NMR: (298 K, 400 MHz, Benzene-d_6): δ = 6.71 (t, 4H, $^3J_{HH}$ = 7.2 Hz, 4-C_6H_5), 6.99 (dd, 8H, $^3J_{HH}$ = 7.8 Hz, 3,5-C_6H_5), 7.32 (d, 8H, $^3J_{HH}$ = 7.9 Hz, 2,6-C_6H_5) ppm.
^{1}H NMR: (298 K, 400 MHz, Chloroform-d_1): δ = 6.90 (t, 4H, 4-C_6H_5), 7.21 (dd, 8H, 3,5-C_6H_5), 7.32 (d, 8H, 2,6-C_6H_5) ppm.[14]
^{13}C NMR: (298 K, 125 MHz, Methylenechloride-d_2): δ = 118.6 (s, 2,6-C_6H_5), 122.7 (s, 4-C_6H_5), 129.9 (s, 3,5-C_6H_5), 143.0 (s, 1-C_6H_5) ppm.

The ^{13}C NMR spectroscopic data of **3-H** furthermore provides an explanation of the reported ^{13}C NMR spectroscopic data of **1-H** (*vide supra*). Closer investigation of the literature known compound **1-H** showed the expected four signals in the aromatic region of the ^{13}C NMR spectrum for the phenyl groups (**1-H**: 122.5, 124.5, 129.6, 151.3 ppm (in C_6D_6)). This is in contrast to the NMR spectroscopic data reported, which shows seven resonances in the aromatic region, however in dichloromethane (DCM).[7] We found that four of these signals can be assigned to **1-H** and the other three to Ph_4N_4 (**3-H**). The resonance at 122.7 ppm (in DCM) represents two overlapping signals (4-C_6H_5 of **1-H** and 4-C_6H_5 of **3-H**).

Reaction of **1-Me** yielding **3-Me**:

^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 2.01 (s, 12H, C_6H_4*Me*), 6.86 (d, 8H,$^3J_{HH}$ = 8.3 Hz, 2,6-C_6H_4Me), 7.34 (d, 8H, $^3J_{HH}$ = 8.4 Hz, 3,5-C_6H_4Me) ppm.
^{1}H NMR (298 K, 400 MHz, Chloroform-d_1): δ = 2.23 (s, 12H, C_6H_4*Me*), 6.98 (d, 8H, $^3J_{HH}$ = 8.4 Hz, 2,6-C_6H_4Me), 7.17 (d, 8H, $^3J_{HH}$ = 8.6 Hz, 3,5-C_6H_4Me) ppm.[14]
^{13}C NMR (298 K, 125 MHz, Benzene-d_6): δ = 20.6 (s, C_6H_4*Me*), 118.5 (s, 2,6-C_6H_4Me), 130.1 (s, 3,5-C_6H_4Me), 131.2 (s, 4-C_6H_4Me), 142.0 (s, 1-C_6H_4Me) ppm.

Reaction of **1-OMe** yielding **3-OMe**:

^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 3.27 (s, 12H, C_6H_4O*Me*), 6.70 (d, 8H, $^3J_{HH}$ = 9.0 Hz, 2,6-C_6H_4OMe), 7.31 (d, 8H, $^3J_{HH}$ = 9.0 Hz, 3,5-C_6H_4OMe) ppm.
Identification also by EPR spectroscopy (*vide supra*).

Reaction of **1-Br** yielding in **3-Br**:

^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 6.63 (d, 8H, $^3J_{HH}$ = 9.0 Hz, 2,6-C_6H_4Br), 7.07 (d, 8H, $^3J_{HH}$ = 9.0 Hz, 3,5-C_6H_4Br) ppm.
^{1}H NMR (298 K, 400 MHz, Chloroform-d_1): δ = 7.34 (d, J = 8.8 Hz, 8H), 7.10 (d, J = 8.8 Hz, 8H) [14]

Reaction of **1-Ph** yielding in **3-Ph**:

^{1}H NMR (298 K, 400 MHz, Benzene-d_6): δ = 7.10 (t, 4H, 8-$C_{12}H_9$, $^3J_{HH}$ = 7.5 Hz), 7.19 (dd, 8H, $^3J_{HH}$ = 7.7 Hz, 7,9-$C_{12}H_9$), 7.42 (m, 16H, 2,6,10,12-$C_{12}H_9$), 7.51 (d, 8H, $^3J_{HH}$ = 8.5 Hz, 3,11-$C_{12}H_9$) ppm.

Reaction of 1-Me and 1-Br in C_6D_6

Mixing of **1-Me** and **1-Br** in a 1:1 ratio in C_6D_6 resulted in the formation of **3-Me**, **3-Br** and the hetero-coupled product, (4-Me-C_6H_4)$_2$N–N(4-Br-C_6H_4)$_2$, in a statistically expected ratio of 1:1:2 after 5 days. This suggests rapid ligand exchange between **1-Me** and **1-Br**, which was verified by instantaneous NMR-spectroscopic analysis of the above-mentioned reaction mixture.

1-Br (15.5 mg, $1.25\cdot10^{-2}$ mmol) and **1-Me** (10.0 mg, $1.25\cdot10^{-2}$ mmol) were dissolved in C_6D_6 (0.5 mL) and the reaction monitored by ^{1}H NMR spectroscopy. In the first spectrum, measured after 10 min, neither **1-Br** nor **1-Me** were identified indicating rapid ligand exchange. A black solid precipitated. After 7 days, a colorless solution had formed and ^{1}H NMR spectroscopy allowed the identification of **3-Me**, **3-Br** and **3-Br/Me** (cross-coupled hydrazine derivative) by comparison to previous recorded spectra in a statistical distribution of 1:1:2. The products were confirmed by mass spectrometry.

HR-ASAP-MS, positive mode, found: m/z = 648.8120; calculated for $C_{24}H_{17}Br_4N_2^+$: m/z = 648.8125; m/z = 521.0223; calculated for $C_{26}H_{23}Br_2N_2^+$: m/z = 521.0228; m/z = 393.2236; calculated for $C_{28}H_{29}N_2^+$: m/z = 393.2331.

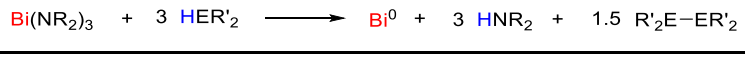
Reactivity of secondary pnictogens towards bismuth amides

A defined amount of the required bismuth amide (typically 0.1-0.3 mmol) was dissolved in C_6D_6 at room temperature in a silanized J. Young-type NMR tube, and the required amount of a secondary pnictogen was added (typically 0.1-0.3 mmol). The ratios (n[(Bi(NR$_2$)$_3$)]/m(HER'$_2$) (E = N, P, As) are given in Table S2. However, as initial ratio 1:3 was chosen. If required, further equivalents of the bismuth amide were added resulting in the ratios described in Table S2. If this was required, the reactions were repeated with the final ratios with same results. The reaction mixture was kept at the desired temperature (23 °C or 60 °C, see Table S2). The formation of a side product was obtained in some cases (entries 3, 5, 6, 9), which was identified as product of the P–N bond formation in the case of entry 2[15]. In order to obtain the correct spectroscopic yield, traces of PCy_3 were added as internal standard to each reaction (one spectrum of the phosphane with PCy_3 was recorded and then the required amount of the bismuth amide was added and additional spectra were recorded). The experiments were also performed in the absence of PCy_3 and no relevant difference was observed. Furthermore, quantitative ^{31}P NMR spectra of selected reactions were recorded to exclude integration errors.

Entries 18-21 show that no reactions were observed between bulky dialkylphosphanes and **1-Me**, while 4 reacted with these phosphanes. This highlights the different reactivity of aryl-substituted amides in comparison to alkyl-substituted amides. However, for $HAsPh_2$ as a substrate, no difference in reactivity between **4** and **1-Me** was observed, and the same yields of the coupled product were obtained (see entries 22 and 23).

Analytical data for P_2Xyl_4. Compound P_2Xyl_4 (*cf*. Table S2, entries 11,12) has previously been synthesized,[16] but analytical data were not reported in detail. From reactions performed under the conditions described in Table S2 (entry 12), the following analytical data were obtained for P_2Xyl_4: ^{1}H NMR (298 K, 400 MHz, benzene-d_6): δ = 1.99 (s, 24H, $C_6H_3\mathit{Me}_2$), 6.69 (s, 4H, *4*-$C_6\mathit{H}_3Me_2$), 7.40 (s, 8H, *2,6*-$C_6\mathit{H}_3Me_2$) ppm; for ^{31}P NMR data see Table S2; HR-LIFDI-MS, positive mode, found: m/z = 482.2280; calculated for $[P_2Xyl_4]^{\bullet+}$: m/z = 482.2287; m/z = 241.1136; calculated for $[PXyl_2]^+$: m/z = 241.1141.

Table S2. Summary of reaction conditions and yields of the dehydrocoupling reaction.



#	Reagent	Substrate	Conditions	Ratio (n(Reagent)/n(Substrate))	Yield[a] [%]	^{31}P NMR C_6D_6 (ppm)	^{31}P NMR $CDCl_3$ (ppm)	^{31}P NMR CD_2Cl_2 (ppm)
1	**4**	HN(*p*tol)$_2$	rt, 3 d	1:3	85	/	/	/
2	**4**	$HPPh_2$	rt, t < 7 min	1:3	80[b]	–14.8[4]	/	/
3	**1-Me**	$HPPh_2$	rt, t < 7 min	1:3	Quant.	–14.8[4]	/	/
4	**4**	HP(4-Cl-Ph)$_2$	rt, t < 7 min	2:3	78[b]	–17.3	/	–17.7[4]
5	**1-Me**	HP(4-Cl-Ph)$_2$	rt, t < 3 h	1.2:3	97	–17.3	/	–17.7[4]
6	**4**	HP(4-OMe-Ph)$_2$	rt, t < 7 min	1:3	65[b]	–18.9	/	–20.1[4]
7	**1-Me**	HP(4-OMe-Ph)$_2$	rt, t < 2 h	1.5:3	92[b]	–18.9	/	–20.1[4]
8	**4**	HP(4-CF_3-Ph)$_2$	rt, t < 15 min	2:3	77[b]	–14.3[3]	/	/
9	**1-Me**	HP(4-CF_3-Ph)$_2$	rt, t < 3 h	2:3	Quant.	–14.3[3]	/	/
10	**4**	$HPMes_2$	rt, 16 h	2:3	Quant.	–30.4	–30.0[16]	/
11	**4**	HP(Xyl)$_2$[c]	rt, 15 min	2:3	80[b]	–15.6	/	/
12	**1-Me**	HP(Xyl)$_2$[c]	rt, 3 h	2:3	90[b]	–15.6	–14.8	/
13	**4**	HP*i*Pr$_2$	rt, t < 3.5 h	1.2:3	96[b]	–12.1[17]	/	/
14	**1-Me**	HP*i*Pr$_2$	rt, t < 6 h	1.2:3	99[b]	–12.1[17]	/	/
15	**4**	HP(C_5H_9)$_2$[d]	rt, t < 3h	2:3	94[b]	–10.8[18]	/	/
16	**1-Me**	$HPCy_2$	rt, 1.5 h	1:3	Quant.	–21.7[19]	–21.4	/
17	**4**	$HPCy_2$	rt, 6 h	1:3	85[b]	–21.7[19]	–21.4	/
18	**4**	HP*t*Bu$_2$	60 °C, 1 d	2:3	Quant.	–39.8[20]	–41.3[21]	/
19	**1-Me**	HP*t*Bu$_2$	rt, 6 d	1:3	n.d.			
20	**4**	HPAd$_2$[e]	60 °C, 2 d	2:1	Quant.	33.2	34.3[22]	/
21	**1-Me**	HPAd$_2$[e]	60 °C, 4 h	1:3	n.d.	/	/	/
22	**4**	$HAsPh_2$	–78 °C, t < 7 min	1:3	80[b][f]	/	/	/
23	**1-Me**	$HAsPh_2$	rt, t < 7 min	1:3	80[b][f]	/	/	/

[a] determined by ^{1}H and/or ^{31}P NMR spectroscopy. [b] lower yield due to E–N bond formation. [c] Xyl = 3,5-Me_2-C_6H_3. [d] = cyclopentyl. [e] Ad = adamantyl. [f] identification by comparison of ^{1}H NMR spectroscopic data;[23] quant. = quantitative; n.d. = not detected.

SUPPORTING INFORMATION

Reactions of bismuth amides such as **1-Me** and **4** with phosphanes to give diphosphanes involve at least two types of elementary reactions. These are i) the formation of a species with a Bi–P bond and ii) the homolysis of Bi–P bonds to release phosphorus-centered radicals as discussed in the main text and shown through EPR-spectroscopic experiments.

The following observations are helpful for a discussion of the first step of these reactions (Bi–P bond formation): Reactions of **1-Me**, **1-H**, and **4** with 3 equiv. $HPPh_2$ all gave **5-Ph** as the main product in instantaneous reactions. Reactions of **4** with $HPAd_2$ gave **5-Ad**, while reaction of **1-Me** with $HPAd_2$ mainly gave **3-Me** (and unreacted $HPAd_2$). These observations demonstrate that the formation of the P–P coupling products does not correlate with the ability of the bismuth amide precursors to form aminyl radicals. We thus propose that the initiating step of the reaction (the reaction of a Bi–NR_2 functional group with HPR'_2 to give a Bi–PR_2 functional group and HNR_2) may well proceed in a polar fashion.

Work-up protocol for the isolation of diphosphanes. Work-up protocols for the isolation of diphosphanes are presented, using the coupling reaction of *t*Bu_2PH with **4** and $(4\text{-Cl-Ph})_2PH$ with **1-Me** as examples. These protocols were optimized for simplicity of the work-up procedure rather than maximized isolated yield.

In a silanized J. Young-type NMR tube, *t*Bu_2PH (13 mg, 0.089 mmol) was dissolved in 0.5 mL C_6D_6. **4** (20 mg, 0.059 mmol) was added and the reaction mixture was kept at 60 °C for one day. After completion of the reaction, the black precipitate was removed by filtration, and all volatiles (solvent and the by-product dimethylamine) were removed under reduced pressure. The product was isolated as white powder.
Yield: 10.4 mg (0.036 mmol, 81%).
This simple work up procedure should be suitable for the alkyl substituted diphosphanes.
^{1}H NMR (298 K, 400 MHz, Chloroform-*d*$_1$): δ = 1.38 (t, 36H, $^3J_{PH}$ = 6.2 Hz, CH_3) ppm.[21]
^{31}P NMR (298 K, 162 MHz, Chloroform-*d*$_1$): δ = –41.3 (s) ppm.[21]

In a silanized flask, $(4\text{-Cl-Ph})_2PH$ (60 mg, 0.235 mmol) was dissolved in benzene (3 mL) and a solution of **1-Me** (75 mg, 0.094 mmol) in benzene (2 mL) was added. The reaction mixture was stirred at room temperature for 16 h until a slightly yellow color of the liquid phase and a black precipitate were observed. The black solid was removed by filtration, and all volatiles were removed under reduced pressure. The white residue was washed with pentane (5 × 2 mL). The product was isolated as white powder.
Yield: 45 mg (0.089 mmol, 76%)
^{1}H NMR (298 K, 400 MHz, Methylenechloride-*d*$_2$): δ = 7.22 – 7.25 (m, 8H, 3,5-C_6H_4Cl), 7.28 – 7.31 (m, 8H, 2,6-C_6H_4Cl) ppm.
^{31}P NMR (298 K, 162 MHz, Methylenechloride-*d*$_2$): δ = –17.7 (s) ppm.[4]

Comparison with literature protocols. In the main part, the results on phosphane dehydrocoupling presented in this work have been compared to literature-known protocols that are based on main group species in some detail. A more detailed comparison with protocols that are based on transition metal compounds is presented here. It has to be noted that catalytic reactions are possible with transition metal species based on elements such as titanium, zirconium, iron, and rhodium.[3, 18, 24] However, long reaction times from ca. 8 hours and up to 12 days were required, even for substrates such as $HPPh_2$.[3, 18, 24c, 24d, 24f] In addition, elevated temperatures (typically 70-140°C) were applied for efficient conversion of the same substrate.[3, 18, 24c, 24d, 24f] In comparison, the stoichiometric reaction of **1-Me** with $HPPh_2$ proceeds at room temperature (or below) to give $Ph_2P–PPh_2$ in quantitative amounts in less than 10 minutes. Most importantly, the substrate scope includes dialkylphosphanes with moderate steric bulk (e.g. $HP(cyclohexyl)_2$) as well as very bulky dialkyl and diraylphosphanes such as $HP(adamantyl)_2$ and $HP(mesityl)_2$, when bismuth species are applied. In contrast, the conversion of bulky dialkyl or diaryl phosphanes was generally more problematic in the case of transition metal catalysis[3, 18, 24] (for instance: $HPtBu_2$ showed no conversion with a rhodium catalyst),[18] in some cases dialkylphosphanes with moderate ($HP(cyclohexyl)_2$)[18] or low steric profiles ($HPEt_2$)[24c] showed low conversions, and in some cases of transition metal catalysis only the conversion of primary phosphanes has been reported.[24e]

EPR Spectroscopic Measurements

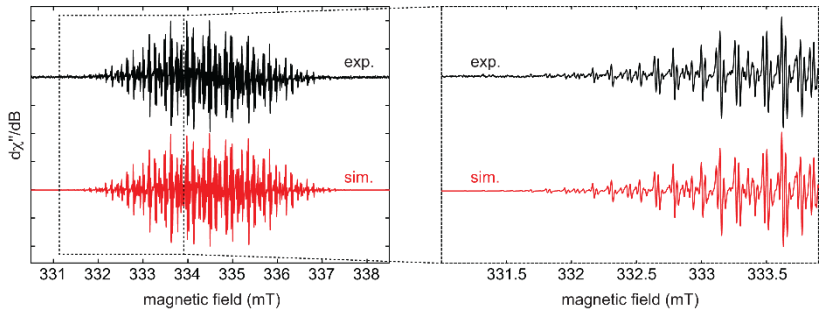


Figure S8. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of the degradation of **1-Me** in benzene. The spectra are in accordance with reported data of the di(*p*-tolyl)aminyl radical.[25] The observed resonance shows coupling constants of $a(^{14}N)$ = 24.3 MHz (8.7 G), $a(^{1}H)$ = 13.3, 10.1, 4.0 MHz (4.8, 3.6, 1.4 G) and a g_{iso} value of 2.0036. Spectrometer settings: microwave frequency = 9.38 GHz, 0.1 G modulation amplitude at 100 kHz, power = 0.2 mW, number of accumulated scans = 29, conversion time = 40 ms.

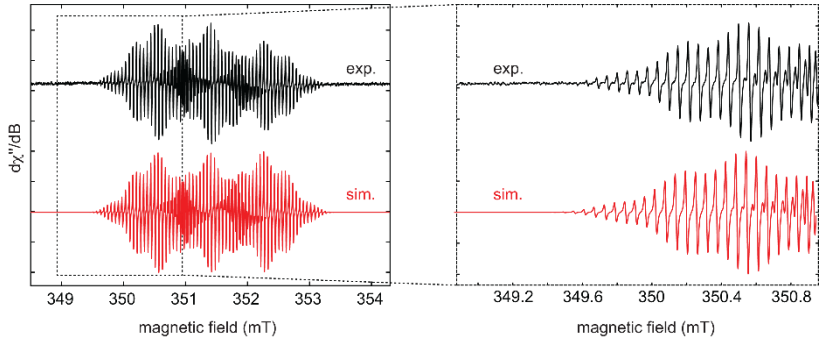


Figure S9. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of the degradation **1-OMe** in benzene. The spectra are in accordance with reported data of the di(*p*-methoxyphenyl)aminyl radical.[25] The observed resonance shows coupling constants of $a(^{14}N)$ = 23.9 MHz (8.7 G), $a(^{1}H)$ = 9.8, 3.3, 1.7 MHz (3.5, 1.2, 0.6 G) and a g_{iso} value of 2.0037. Spectrometer settings: microwave frequency = 9.86 GHz, 0.1 G modulation amplitude at 100 kHz, power = 0.2 mW, number of accumulated scans = 19, conversion time = 40 ms.

The observed spectrum has its origin in the homolytic Bi–N bond cleavage (as observed for **1-Me**) and the dissociation of **3-OMe**.[25]

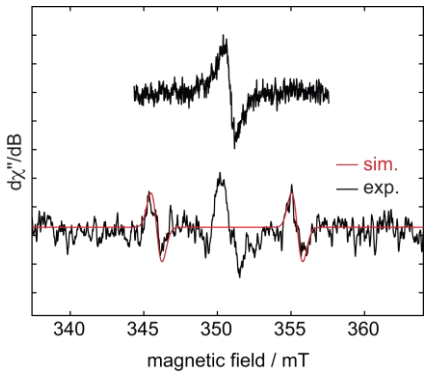


Figure S10. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of **4** (top) and of the reaction of **4** with Mes_2PH (bottom) in benzene. The observed doublet has an isotropic coupling constant of $a(^{31}P)$ = 270 MHz (96 G) and a g_{iso} value of 2.007. Spectrometer settings: microwave frequency = 9.85 GHz, 1 G modulation amplitude at 100 kHz, power = 4 mW, number of accumulated scans = 48, conversion time = 20 ms. The resonance detected in solutions of **4** could not be removed by sublimation of the bismuth amide.

NMR Spectra of Isolated Compounds

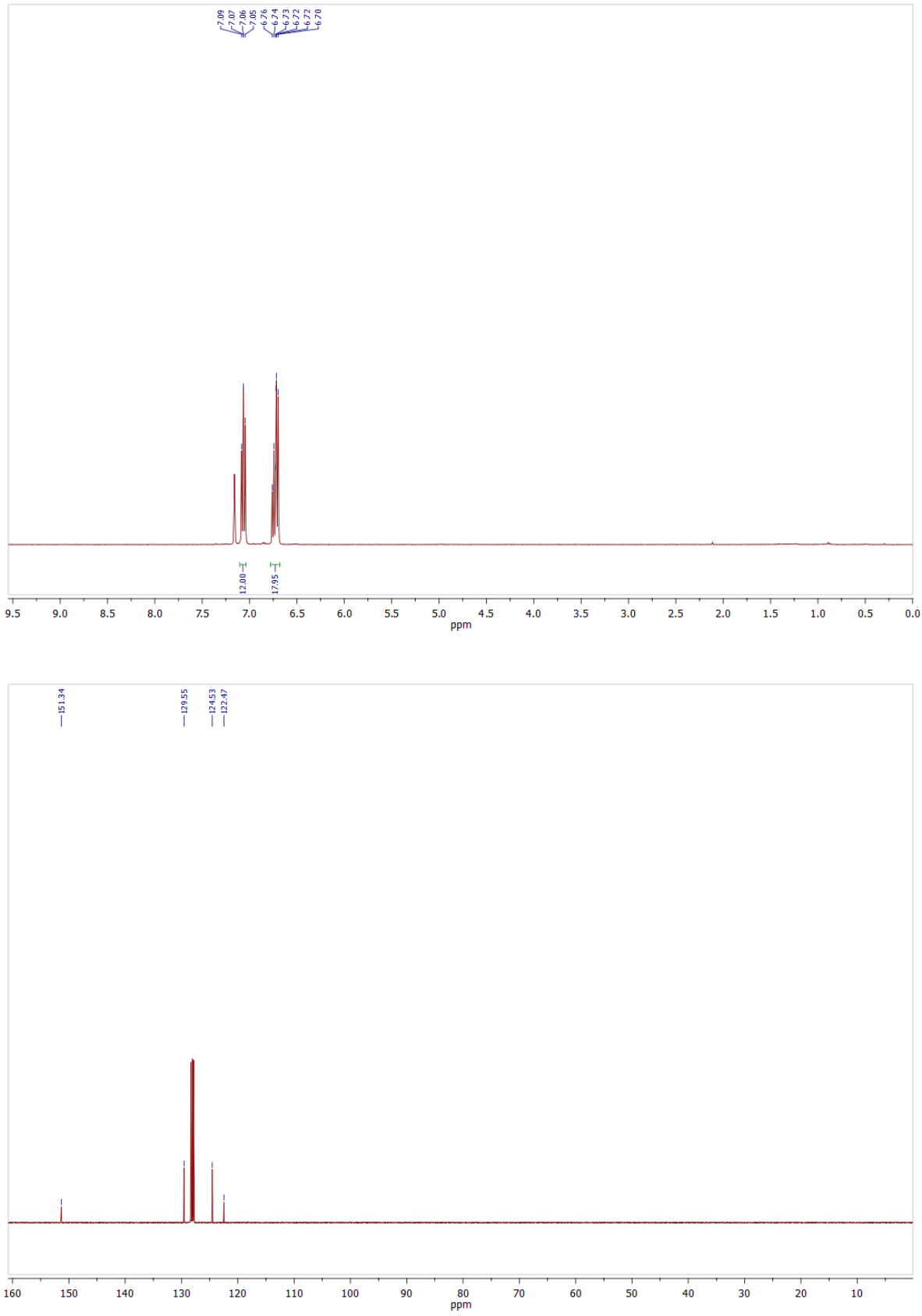


Figure S11. ^{1}H and ^{13}C spectra of $[Bi(NPh_2)_3]$ (**1-H**) in Benzene-d_6.

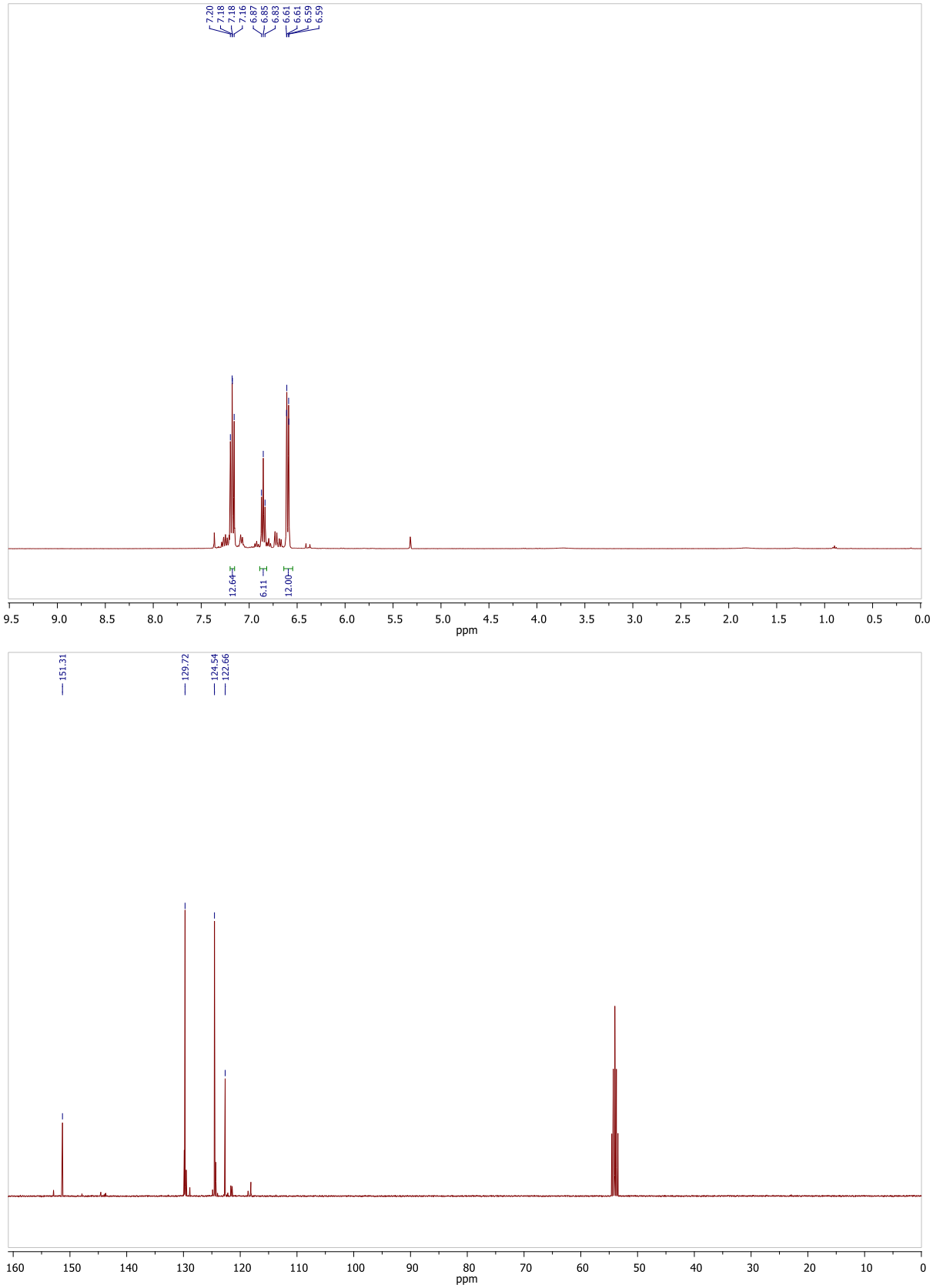


Figure S12. ^{1}H and ^{13}C spectra of $[Bi(NPh_2)_3]$ (**1-H**) in Methylenedichloride-d_2. Decomposition due to the choice of solvent can be observed in both spectra.

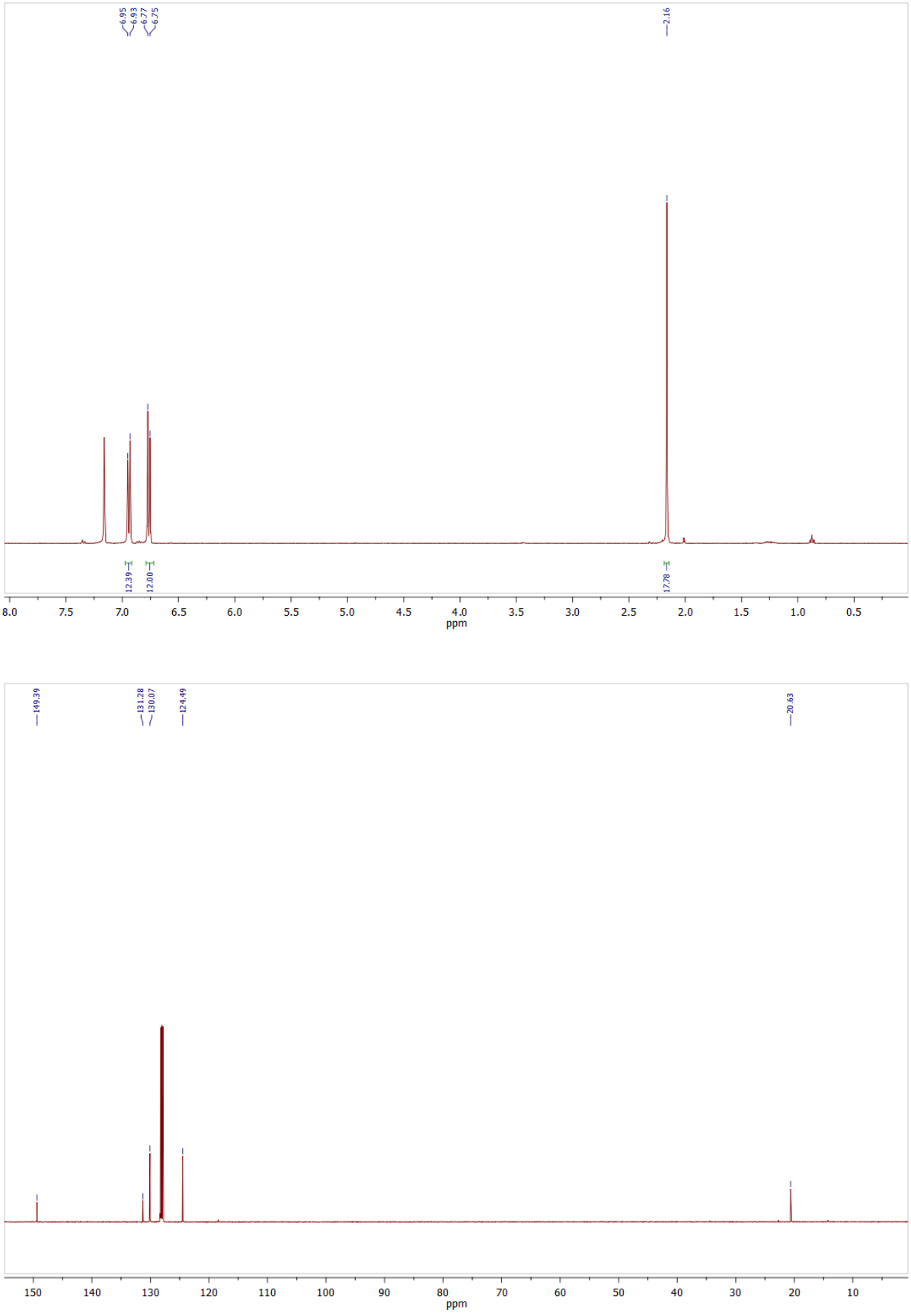


Figure S13. ^{1}H and ^{13}C spectra of compound **1-Me** in Benzene-d_6.

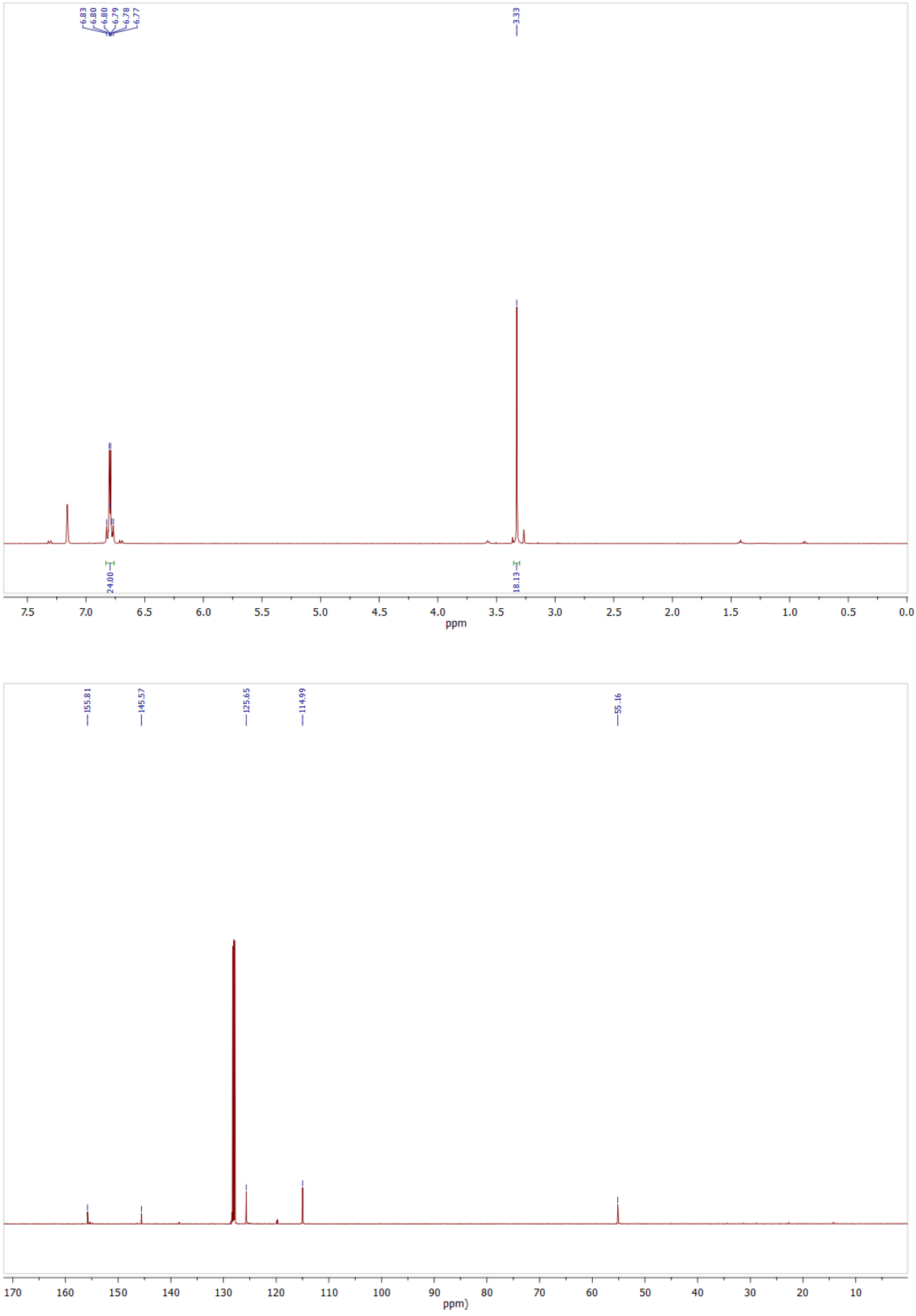


Figure S14. ^{1}H and ^{13}C spectra of compound **1-OMe** in Benzene-d_6.

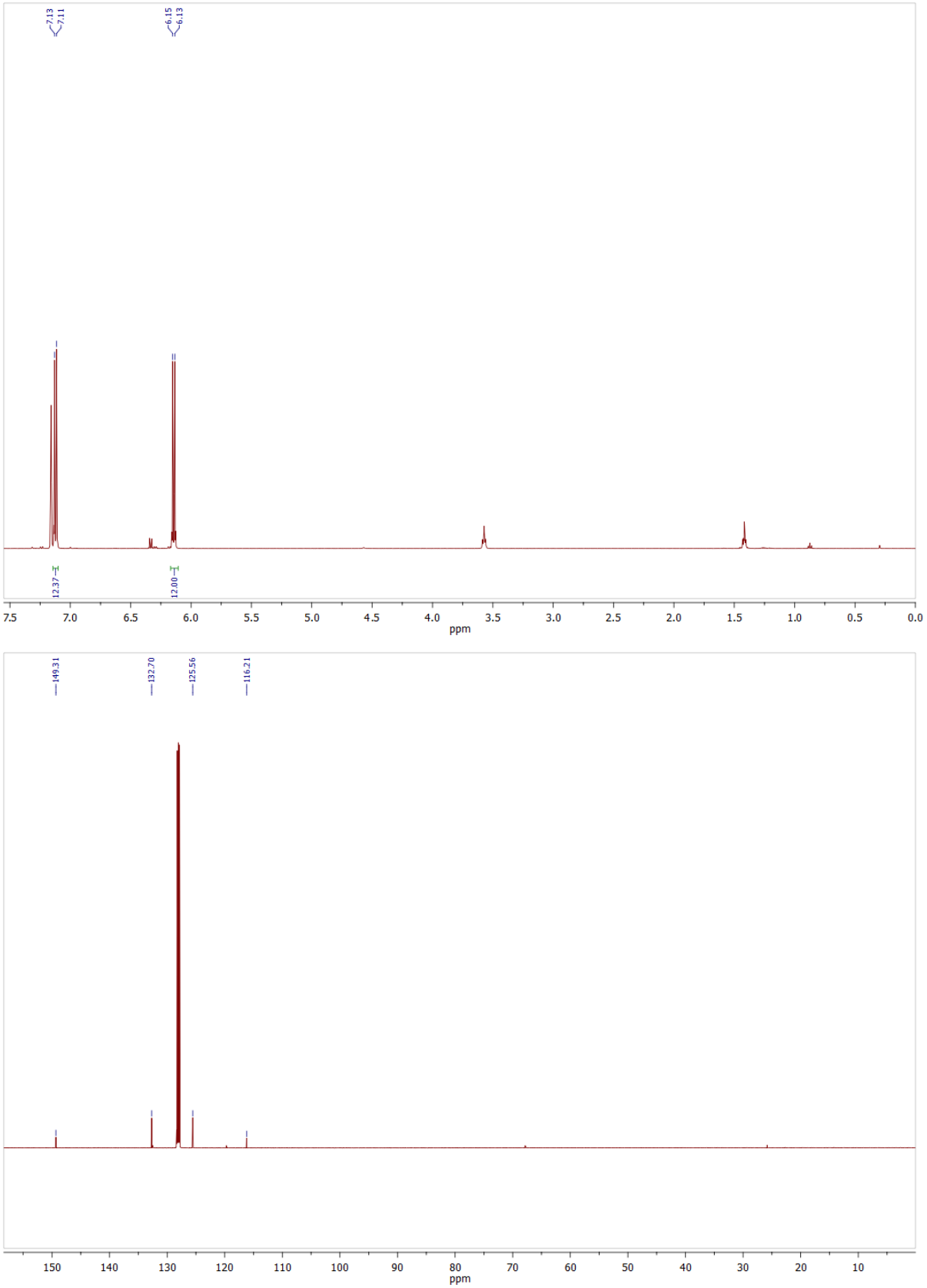


Figure S15. ^{1}H and ^{13}C spectra of compound **1-Br** in Benzene-d_6.

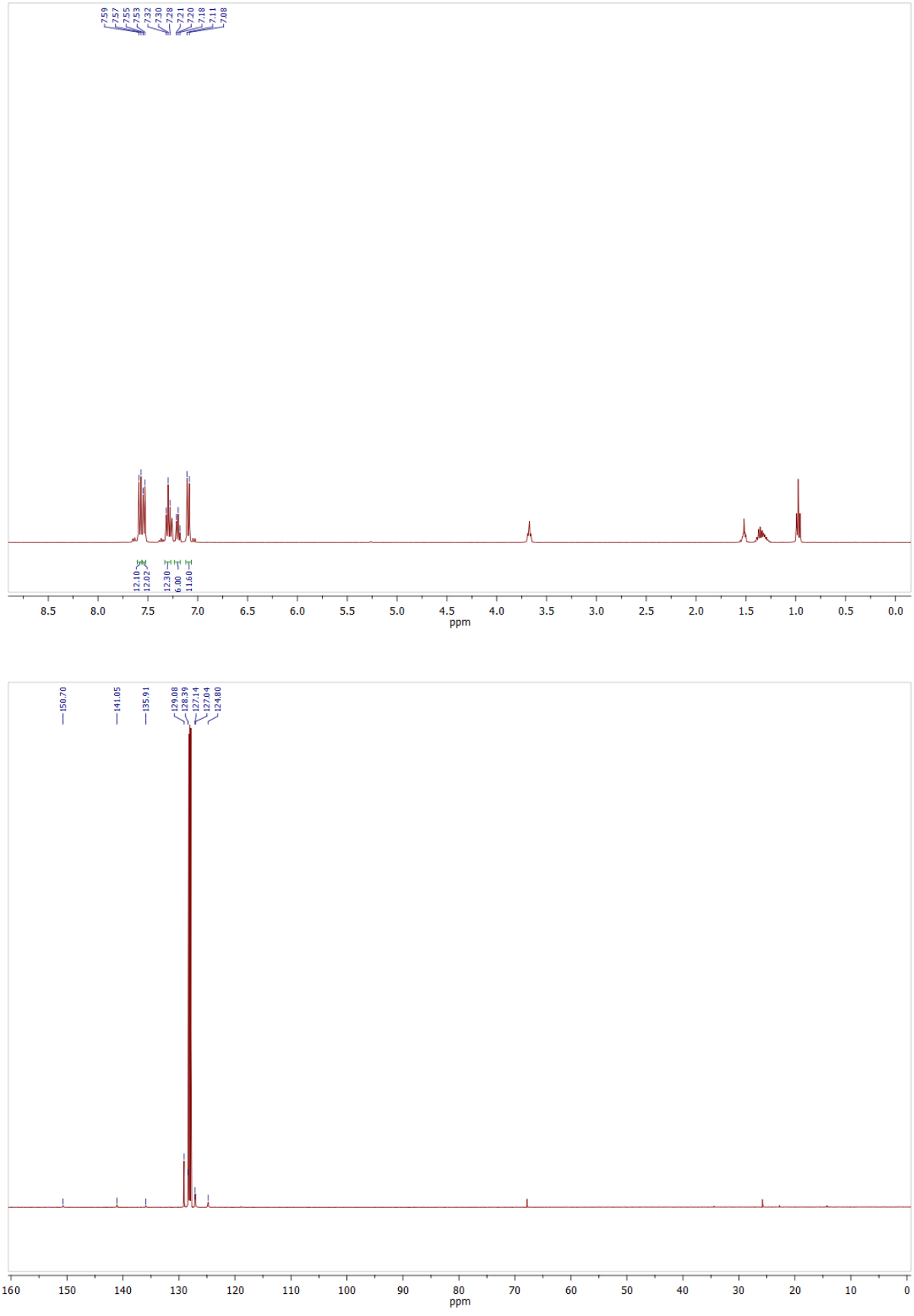
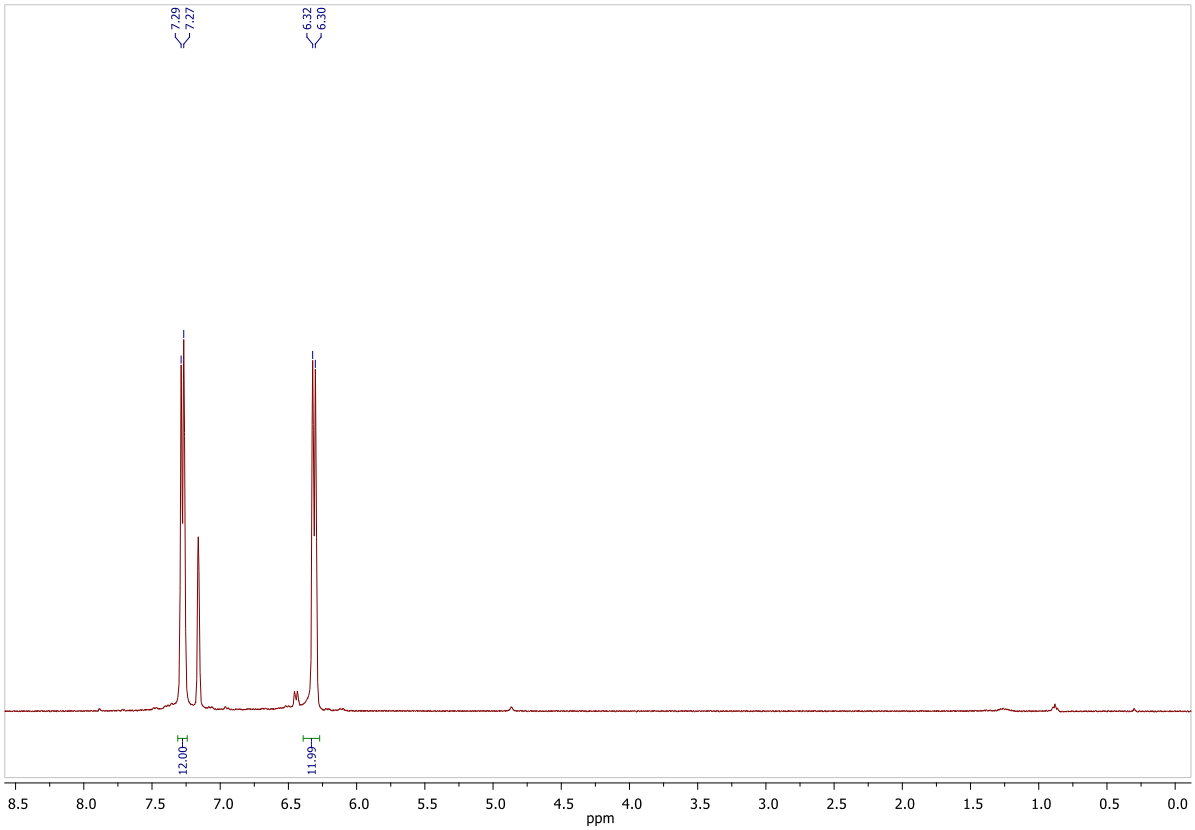


Figure S16. ^{1}H and ^{13}C spectra of compound **1-Ph** in Benzene-d_6.



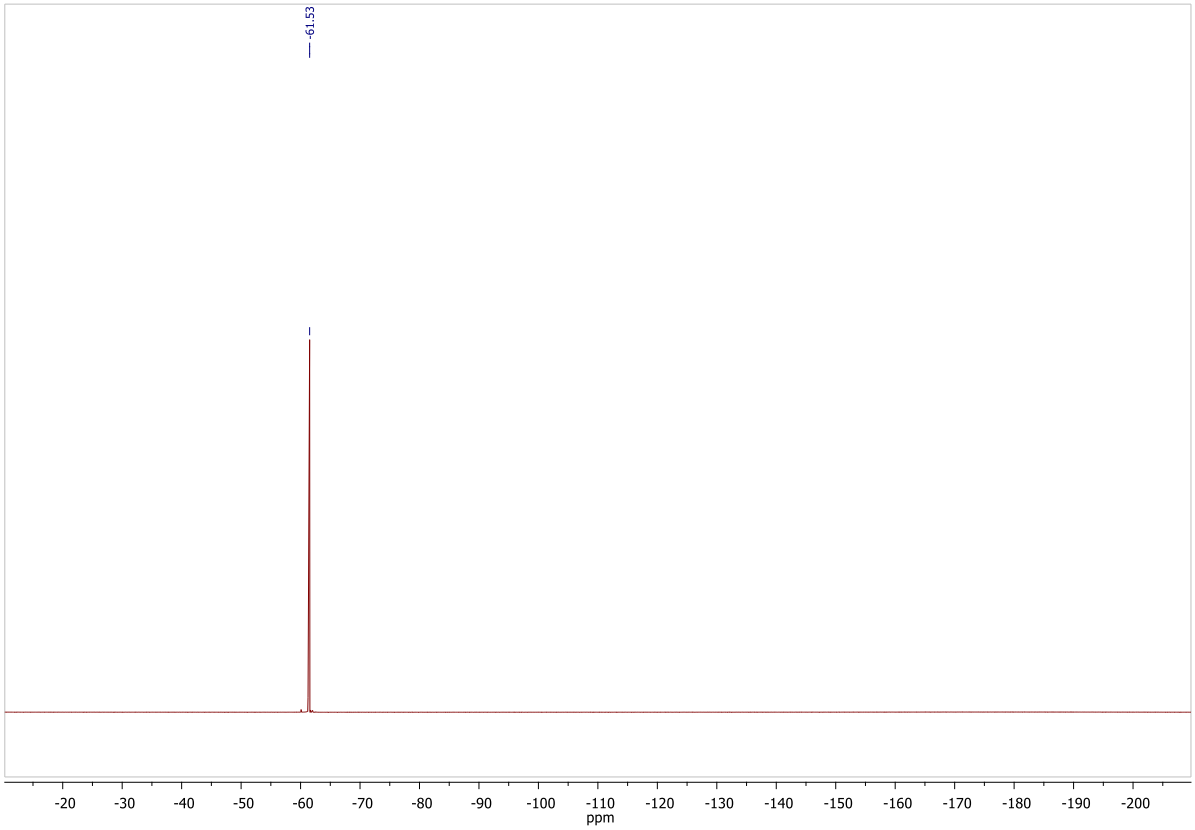


Figure S17. ^{1}H and ^{19}F spectra of compound **1-CF$_3$** in Benzene-d_6.

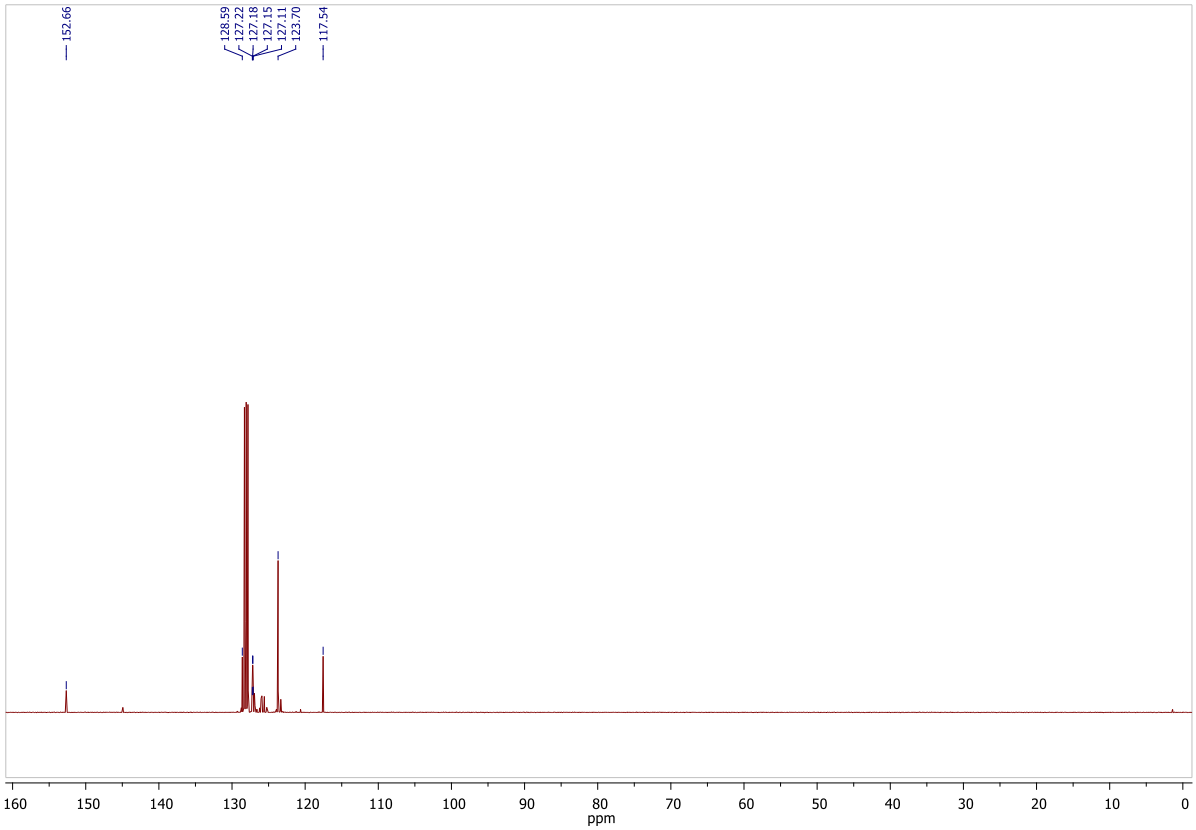


Figure S18. ^{13}C spectrum of compound **1-CF$_3$** in Benzene-d_6.

Quantum Chemical Analyses

All DFT calculations were performed with the Amsterdam Density Functional (ADF) program[26] using relativistic, dispersion-corrected density functional theory (DFT) at the ZORA-BLYP-D3BJ/TZ2P level of theory for geometry optimizations and energy calculations, with the full electron model for all atoms (no frozen core).[27],[28] Solvation in benzene was simulated by using the conductor-like screening model (COSMO).[29] Bismuth(0) has been calculated as a bulk by means of periodic DFT with the same ADF package (BAND) and at the same ZORA-BLYP(D3BJ)/TZ2P level of theory. All stationary points were verified to be minima on the potential energy surface through vibrational analysis.

The bonding mode in **2-X**, with special emphasis on Bi–NR_2 interactions, was analyzed within the framework of quantitative Kohn-Sham molecular orbital theory[30] in combination with a quantitative energy decomposition analysis (EDA)[30] in the gas phase. The electronic bond energy ΔE can be decomposed into the strain energy ΔE_{strain} associated with deforming two fragments (in triplet state) from their equilibrium structure to the geometry they adopt in **2-X** plus the interaction energy ΔE_{int} between these deformed fragments. The latter is further decomposed into the classical electrostatic attraction ΔV_{elstat}, Pauli repulsion ΔE_{Pauli} between occupied orbitals, stabilizing orbital interactions ΔE_{oi}, and dispersion interactions ΔE_{disp}.[30]

Table S3. Homolytic and heterolytic bond dissociation energies (in kcal mol^{-1}) of bismuth amides in benzene and in the gas phase.[a]

	benzene				gas			
	homolytic		heterolytic		homolytic		heterolytic	
System	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**
1-H	42.6	28.0	77.8	63.8	43.5	27.4	130.7	115.5
1-Me	39.4	25.4	76.3	62.2	40.2	25.0	120.8	105.1
1-OMe	36.1	18.7	74.5	55.2	37.0	19.7	116.1	97.1
1-Ph	47.1	31.9	75.3	59.8	47.6	28.0	113.5	94.6
1-Br	40.1	20.6	77.0	56.0	40.2	19.4	120.1	99.0
1-CF_3	44.5	24.5	78.2	59.9	44.9	26.2	122.6	104.2

[a] Computed at the ZORA-BLYP-D3BJ/TZ2P level of theory. Homolytic $Bi[N(C_6H_4X)_2]_3 \rightarrow Bi[N(C_6H_4X)_2]_2^{\bullet} + N(C_6H_4X)_2^{\bullet}$ vs. heterolytic $Bi[N(C_6H_4X)_2]_3 \rightarrow Bi[N(C_6H_4X)_2]_2^{+} + N(C_6H_4X)_2^{-}$ reactions have been computed.

Table S4. Comparison between homolytic and heterolytic bond dissociation energies (in kcal mol^{-1}) of **1-H** and **1-Me** and their protonated forms in benzene and in the gas phase.[a]

	benzene				gas			
	homolytic		heterolytic		homolytic		heterolytic	
System	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**
1-H	42.6	28.0	77.8	63.8	43.5	27.4	130.7	115.5
1-HH	45.1	29.2	15.5	0.4	55.4	38.8	28.8	13.1
1-Me	39.4	25.4	76.3	62.2	40.2	25.0	120.8	105.1
1-MeH	44.6	28.7	18.8	4.6	51.0	40.4	22.4	11.7

[a] Computed at the ZORA-BLYP-D3BJ/TZ2P level of theory. Homolytic $[Bi(N(C_6H_4X)_2)_2(HN(C_6H_4X)_2)]^{+} \rightarrow [Bi(N(C_6H_4X)_2)_2]^{\bullet} + [HN(C_6H_4X)_2]^{\bullet+}$ vs. heterolytic $[Bi(N(C_6H_4X)_2)_2(HN(C_6H_4X)_2)]^{+} \rightarrow [Bi(N(C_6H_4X)_2)_2]^{+} + HN(C_6H_4X)_2$ have been computed

Table S5. Energy decomposition analysis (in kcal mol^{-1}) in the gas phase of the homolytic Bi–N bond energy ΔE for bismuth amides optimized in benzene with COSMO.

System	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{int}	ΔE_{strain}	ΔE
1-OMe	256.5	-144.4	-136.0	-28.0	-51.9	15.0	-36.9
1-Me	251.5	-140.7	-135.8	-28.4	-53.3	13.2	-40.1
1-H	249.5	-138.6	-137.7	-29.3	-56.1	12.7	-43.4
1-Ph	261.7	-143.4	-131.4	-49.6	-62.7	15.1	-47.6
1-Br	245.7	-136.4	-134.4	-29.3	-54.4	14.3	-40.2
1-CF_3	240.0	-130.8	-135.4	-29.6	-55.7	11.1	-44.7

[a] Computed at ZORA-BLYP-D3BJ/TZ2P//COSMO(benzene)-ZORA-BLYP-D3BJ/TZ2P.

Table S6. Thermodynamics (in kcal mol^{-1}) of the elimination of **3-Me** from **1-Me** with formation of different types of bismuthinidenes (triplet (^{3}[Bi(NR$_2$)]) vs. singlet (^{1}[Bi(NR$_2$)]) and benzene adducts of the triplet bismuthinidene (^{3}[Bi(NR$_2$)(benzene)] and ^{3}[Bi(NR$_2$)(benzene)$_2$])) computed at ZORA-BLYP(D3BJ)/TZ2P level of theory in benzene.

System	Δ*H*	Δ*G*
1-Me → ^{3}[Bi(NR$_2$)] + **3-Me**	57.4	46.3
1-Me → ^{1}[Bi(NR$_2$)]^a + **3-Me**	67.2	54.3
1-Me + benzene → ^{3}[Bi(NR$_2$)](benzene) + **3-Me**	52.1	50.6
1-Me + 2 benzene → ^{3}[Bi(NR$_2$)](benzene)$_2$ + **3-Me**	44.8	53.3

^{a} The singlet **^{1}[Bi(NR$_2$)]** was computed as a single point on the geometry of **^{3}[Bi(NR$_2$)]** due to non-convergency.

[Bi(NR$_2$)] is more stable at its triplet state than its singlet state by about 7 kcal mol^{-1} (when referring to *ΔG*). This difference is kept when one benzene molecule is included as a discrete model of solvation, but it is decreased when two benzene molecules are included to become almost isoenergetic (data not included in Table S6). In any case, the high energies corresponding to the formation of this bismuthinidene in the reaction **1-Me** → **3-Me** + [Bi(NR$_2$)] make this reaction pathway highly unlikely to contribute to the experimentally observed formation **3-Me** from **1-Me**.

Rationale of radical catalysis. As outlined in the main part of this work, we suggest that the single steps proposed for the formation of **3-Me** from **1-Me** (and related reactions) may well proceed through catalysis by radicals such as (NR$_2$)$^\bullet$. Scheme S2 provides a rationale for this suggestion for the reaction of [Bi(NR$_2$)$_3$] to give [Bi$_2$(NR$_2$)$_4$]. Homolytic Bi–N bond dissociation of **1-Me** (*ΔG* = 25.4 kcal·mol^{-1}) or [Bi$_2$(NR$_2$)$_4$] (*ΔG* = 28.9 kcal·mol^{-1}) would readily provide sufficient concentrations of such radical species. These results suggest that multiple sources of radicals (NR$_2$)$^\bullet$ are possible. EPR spectroscopic experiments showed that these radicals are present in the reaction mixture and do not originate from N–N bond hemolysis of **3-Me**.

$$[Bi(NR_2)_3] \xrightarrow[-\,(NR_2)_2]{+\,[NR_2]^\bullet} [Bi(NR_2)_2]^\bullet \xrightarrow[-\,[NR_2]^\bullet]{+\,[Bi(NR_2)_3]} [Bi_2(NR_2)_4]$$

Scheme S2. Rationale of radical catalysis in reactions of [Bi(NR$_2$)$_3$] to give (NR$_2$)$_2$.

Table S7. Cartesian coordinates and ADF total electronic and Gibbs energies (in parentheses and in kcal mol^{-1}) of compounds **1-X** under analysis computed at the ZORA-BLYP(D3BJ)/TZ2P level of theory in benzene.

1-H (-10208.8, -9911.1)

1.Bi	1.019609	8.973795	9.961489
2.N	-0.463314	7.907714	11.278511
3.C	0.736260	5.853365	11.844803
4.H	1.622053	6.440790	12.063102
5.C	-1.072224	8.374801	7.475434
6.C	-2.836600	10.733697	11.831957
7.H	-3.147562	11.642585	11.321908
8.C	-1.111382	8.109546	6.089636
9.H	-0.356500	8.545756	5.443639
10.C	-2.039557	7.767754	8.298527
11.H	-2.030239	7.961839	9.362046
12.C	1.556497	12.480594	5.877772
13.H	1.969052	13.336182	5.349572
14.C	0.574356	5.609835	8.183993
15.H	0.076500	5.473836	9.136296
16.C	0.772164	5.100972	5.822717
17.H	0.417161	4.574589	4.940345
18.C	-0.371903	11.204397	6.627334
19.H	-1.448211	11.071114	6.692095
20.C	-0.450383	6.505774	11.472613
21.C	-1.469561	8.704265	11.850164
22.C	-2.996396	9.201142	13.687863
23.H	-3.423121	8.920946	14.648615
24.N	2.141334	7.202104	9.240859
25.C	-2.046794	8.369564	13.098860
26.H	-1.733803	7.457921	13.598861
27.C	-3.394202	10.395184	13.067532
28.H	-4.132723	11.040544	13.535515
29.C	0.166382	12.291279	5.942963
30.H	-0.500971	13.007950	5.469241
31.C	1.868499	10.441936	7.154903
32.H	2.535630	9.683633	7.559545
33.C	2.401937	11.552873	6.489719
34.H	3.481191	11.673001	6.430184
35.C	-2.999868	6.912446	7.757434
36.H	-3.729453	6.448128	8.417295
37.C	-1.602781	5.730330	11.229109
38.H	-2.527592	6.224862	10.948963
39.C	2.305459	6.664420	6.858640
40.H	3.148482	7.347322	6.796074
41.C	1.666556	6.483836	8.094380
42.C	-3.037077	6.659025	6.382623
43.H	-3.788303	5.995008	5.962819
44.C	-2.086763	7.270599	5.555496
45.H	-2.087716	7.072034	4.485889
46.C	-1.901948	9.893762	11.218947
47.H	-1.543689	10.144871	10.222558
48.C	0.129819	4.924127	7.051121
49.H	-0.729186	4.263308	7.128159
50.C	-1.551337	4.340487	11.327870
51.H	-2.446332	3.756062	11.126587
52.C	0.790073	4.459996	11.918562
53.H	1.727407	3.976654	12.181228
54.N	-0.063203	9.197915	8.017155
55.C	0.473196	10.260752	7.253193
56.C	3.233497	6.698323	9.959154
57.C	4.950308	6.985067	11.681366
58.H	5.437291	7.627586	12.411568
59.C	3.903124	7.497546	10.915866
60.H	3.616361	8.539062	11.056070
61.C	1.861402	5.974528	5.728298
62.H	2.358887	6.126745	4.773232
63.C	3.690897	5.371952	9.779954
64.H	3.196493	4.733007	9.056420
65.C	-0.351468	3.695330	11.658637
66.H	-0.310987	2.610618	11.716285
67.C	4.750926	4.874700	10.538778
68.H	5.074867	3.847991	10.380579
69.C	5.386863	5.666767	11.502188
70.H	6.207816	5.270556	12.093595

SUPPORTING INFORMATION

1-Me (-12418.9, -12027.3)

1.Bi	3.238724	9.309538	4.995706
2.N	2.868870	7.284791	5.831294
3.N	4.749996	8.643833	3.509799
4.N	1.528204	9.258797	3.577625
5.C	3.578396	6.868259	6.965237
6.C	4.726562	7.560703	7.414350
7.H	5.119280	8.403452	6.847440
8.C	5.410305	7.167741	8.565763
9.H	6.290905	7.731036	8.870317
10.C	5.007994	6.053728	9.316934
11.C	3.880481	5.351712	8.859794
12.H	3.538589	4.475549	9.409500
13.C	3.175251	5.741597	7.721943
14.H	2.305438	5.173928	7.408593
15.C	5.742935	5.633592	10.571737
16.H	5.839537	4.542888	10.632429
17.H	5.211336	5.962468	11.475883
18.H	6.748893	6.066090	10.606279
19.C	1.886866	6.416468	5.260586
20.C	2.283626	5.300246	4.507213
21.H	3.340113	5.107839	4.367590
22.C	1.331065	4.457104	3.938991
23.H	1.660886	3.607297	3.343891
24.C	-0.044596	4.699182	4.097369
25.C	-0.431480	5.815394	4.853693
26.H	-1.489123	6.035762	4.984163
27.C	0.519117	6.660006	5.434475
28.H	0.198393	7.522051	6.010164
29.C	-1.070967	3.778389	3.474919
30.H	-2.054021	4.257168	3.420106
31.H	-1.181780	2.857292	4.063326
32.H	-0.775525	3.481272	2.461881
33.C	5.480808	9.597856	2.789571
34.C	5.103151	10.960497	2.773407
35.H	4.199382	11.288694	3.284748
36.C	5.851397	11.915625	2.085087
37.H	5.520936	12.952971	2.103032
38.C	6.998591	11.567318	1.356572
39.C	7.369679	10.213033	1.363523
40.H	8.257359	9.900376	0.814862
41.C	6.642393	9.248415	2.060282
42.H	6.972147	8.214938	2.047905
43.C	7.777934	12.595913	0.565770
44.H	8.850810	12.370522	0.567679
45.H	7.640392	13.602176	0.976852
46.H	7.453592	12.623220	-0.484461
47.C	5.006191	7.254304	3.293395
48.C	4.557378	6.626329	2.121373
49.H	4.021022	7.209907	1.383281
50.C	4.797130	5.269448	1.911199
51.H	4.430298	4.799625	1.000338
52.C	5.483313	4.494284	2.861373
53.C	5.937087	5.133068	4.025530
54.H	6.472307	4.559128	4.779602
55.C	5.707710	6.495084	4.238383
56.H	6.064486	6.969785	5.146654
57.C	5.685739	3.009329	2.655113
58.H	6.552826	2.643348	3.214993
59.H	5.830974	2.769446	1.595968
60.H	4.808935	2.444126	3.000755
61.C	0.285915	9.772237	3.972295
62.C	0.013974	10.094060	5.322030
63.H	0.753671	9.897325	6.096555
64.C	-1.212756	10.633511	5.710044
65.H	-1.375812	10.861009	6.762307
66.C	-2.242490	10.861051	4.785484
67.C	-1.980399	10.526223	3.446994
68.H	-2.755040	10.680606	2.696805
69.C	-0.754029	10.002473	3.039813
70.H	-0.593804	9.763149	1.993911
71.C	-3.569602	11.455249	5.205376
72.H	-4.406165	10.972028	4.686524
73.H	-3.619744	12.528222	4.971699
74.H	-3.729786	11.346118	6.283641
75.C	1.680062	8.720951	2.261601
76.C	2.374911	9.427587	1.271938
77.H	2.801969	10.396813	1.508044
78.C	2.532599	8.887866	-0.007395
79.H	3.088292	9.448367	-0.756769
80.C	1.991328	7.636108	-0.338407
81.C	1.280731	6.943552	0.656625
82.H	0.852692	5.968708	0.429685
83.C	1.129177	7.471340	1.937842
84.H	0.584255	6.922263	2.695841
85.C	2.202135	7.030943	-1.708833
86.H	1.338867	6.430980	-2.017382
87.H	3.078770	6.368194	-1.712561
88.H	2.373339	7.804729	-2.464584

1-OMe (-13234.3, -12829.2)

1.Bi	3.234008	9.380741	4.886531
2.N	2.942999	7.377953	5.803014
3.N	4.638375	8.692621	3.313439
4.N	1.426144	9.282786	3.600585
5.C	3.731766	6.995090	6.900145
6.C	4.906053	7.707202	7.248388
7.H	5.247822	8.540417	6.636915
8.C	5.675341	7.357982	8.353638
9.H	6.572995	7.920427	8.597962
10.C	5.319741	6.259397	9.150154
11.C	4.174498	5.525938	8.816366
12.H	3.868410	4.667614	9.405113
13.C	3.393605	5.893116	7.713867
14.H	2.506379	5.313238	7.482861
15.H	5.819794	3.921223	10.464175
16.H	-5.348861	11.895895	5.431486
17.C	0.885233	7.434617	2.069915
18.H	0.388836	6.928176	2.888353
19.C	1.936933	6.482420	5.323861
20.C	2.288533	5.378882	4.537127
21.H	3.331470	5.213790	4.298635
22.C	1.321454	4.493273	4.055022
23.H	1.632444	3.659754	3.435381
24.C	-0.031353	4.712571	4.356068
25.C	-0.396220	5.812863	5.149824
26.H	-1.446995	5.978102	5.372342
27.C	0.580763	6.680488	5.631104
28.H	0.289795	7.530495	6.239224
29.H	-1.688258	2.329051	2.813133
30.H	3.365055	7.583776	-2.307341
31.C	1.473259	8.692285	2.301220
32.C	2.102185	9.339575	1.233662
33.C	5.360368	9.648232	2.579682
34.C	4.941350	10.992762	2.503802
35.H	4.005223	11.303378	2.964070
36.C	5.682223	11.964657	1.819725
37.H	5.311413	12.983647	1.797624
38.C	6.860831	11.605882	1.155003
39.C	7.281959	10.267402	1.195265
40.H	8.195404	9.988346	0.675179
41.C	6.554714	9.310495	1.895095
42.H	6.910127	8.285759	1.919942
43.H	7.220318	14.295728	1.393170
44.H	2.560780	10.310007	1.392518
45.C	2.171556	8.750381	-0.035780
46.H	2.685094	9.274386	-0.833953
47.C	4.905355	7.305144	3.105186
48.C	4.405591	6.653580	1.962822
49.H	3.820883	7.220303	1.248852
50.C	4.646490	5.302273	1.748921
51.H	4.247275	4.797369	0.873166

52.C	5.392748	4.561809	2.682415
53.C	5.901159	5.197688	3.824095
54.H	6.473753	4.651625	4.565186
55.C	5.658454	6.563114	4.020063
56.H	6.050642	7.048223	4.907880
57.H	5.806823	2.424306	4.322491
58.C	1.587516	7.493745	-0.247744
59.C	0.936400	6.842707	0.815004
60.H	0.494765	5.864793	0.642016
61.C	0.200749	9.770677	4.086464
62.C	0.020364	10.084137	5.455781
63.H	0.817109	9.899365	6.173892
64.C	-1.177029	10.602101	5.938370
65.H	-1.290554	10.830096	6.995183
66.C	-2.263060	10.807826	5.074837
67.C	-2.116280	10.492412	3.718350
68.H	-2.933426	10.634758	3.019104
69.C	-0.902443	9.989728	3.235003
70.H	-0.812802	9.761910	2.178178
71.O	5.558874	3.222864	2.393832
72.C	6.297461	2.423887	3.340802
73.H	6.302961	1.412479	2.931516
74.H	7.327738	2.787117	3.444413
75.O	7.661895	12.478655	0.433256
76.C	7.255141	13.858285	0.386250
77.H	8.011883	14.370746	-0.210293
78.H	6.272722	13.966508	-0.092815
79.O	1.608337	6.813291	-1.448005
80.C	2.306175	7.428441	-2.550331
81.H	2.217480	6.728259	-3.382399
82.H	1.846787	8.387140	-2.822527
83.O	-1.068800	3.918462	3.912620
84.C	-0.737566	2.805497	3.057095
85.H	-0.247976	3.148771	2.136805
86.H	-0.086220	2.089739	3.574368
87.O	-3.419570	11.308301	5.655067
88.C	-4.553095	11.511198	4.791126
89.H	-4.326298	12.243164	4.004491
90.H	-4.873849	10.567507	4.329998
91.O	6.159730	5.981246	10.219213
92.C	5.819054	4.853059	11.045477
93.H	6.590960	4.805447	11.815705
94.H	4.836029	4.988499	11.516016

1-Ph (-19342.6, -18767.4)

Bi	16.83580000	-11.87570000	-6.81710000
N	16.46550000	-10.02110000	-5.69810000
N	18.92560000	-11.56000000	-7.26840000
N	15.66700000	-11.32250000	-8.63490000
C	15.45650000	-10.26000000	-4.73740000
C	15.57660000	-11.37670000	-3.91450000
H	16.39100000	-11.86510000	-3.90690000
C	14.52580000	-11.79200000	-3.10290000
H	14.62080000	-12.57460000	-2.57340000
C	13.32330000	-11.06310000	-3.05760000
C	13.24800000	-9.88050000	-3.83330000
H	12.47230000	-9.33440000	-3.77960000
C	14.28430000	-9.51000000	-4.66190000
H	14.19670000	-8.72730000	-5.19350000
C	12.17110000	-11.54890000	-2.24980000
C	11.21260000	-10.68320000	-1.73640000
H	11.33560000	-9.74620000	-1.82720000
C	10.08070000	-11.16480000	-1.09090000
H	9.43960000	-10.55510000	-0.74380000
C	9.87850000	-12.54090000	-0.95130000
H	9.08800000	-12.87540000	-0.54590000
C	10.86130000	-13.40930000	-1.42120000
H	10.76440000	-14.34620000	-1.29460000
C	11.94990000	-12.92520000	-2.05540000
H	12.59490000	-13.53940000	-2.38600000
C	16.77890000	-8.70780000	-6.14160000
C	17.02660000	-8.40750000	-7.44960000
H	16.88370000	-9.06750000	-8.11780000
C	17.48180000	-7.15640000	-7.81770000
H	17.65550000	-6.98170000	-8.73530000
C	17.69320000	-6.14610000	-6.89280000
C	17.38970000	-6.43240000	-5.55840000
H	17.49290000	-5.75330000	-4.90320000
C	16.94740000	-7.67190000	-5.17720000
H	16.75110000	-7.84070000	-4.26330000
C	18.23260000	-4.82620000	-7.32880000
C	17.77750000	-4.23110000	-8.49520000
H	17.06940000	-4.63330000	-8.98320000
C	18.34890000	-3.05200000	-8.95770000
H	18.03850000	-2.66280000	-9.76750000
C	19.37270000	-2.43370000	-8.24420000
H	19.74460000	-1.61390000	-8.54550000
C	19.84180000	-3.03110000	-7.09100000
H	20.54860000	-2.62350000	-6.60380000
C	19.29250000	-4.21860000	-6.63610000
H	19.63780000	-4.62700000	-5.85070000
C	19.67470000	-10.35460000	-7.26090000
C	19.74740000	-9.54560000	-6.14730000
H	19.28760000	-9.80060000	-5.35670000
C	20.48130000	-8.36780000	-6.16050000
H	20.53030000	-7.83750000	-5.37390000
C	21.14600000	-7.95570000	-7.30990000
C	21.07850000	-8.77740000	-8.44430000
H	21.53030000	-8.51920000	-9.23970000
C	20.36170000	-9.96220000	-8.41790000
H	20.33540000	-10.51430000	-9.19040000
C	21.94540000	-6.71080000	-7.34010000
C	21.88080000	-5.84830000	-8.45750000
H	21.30890000	-6.06070000	-9.18500000
C	22.64840000	-4.69600000	-8.49520000
H	22.61680000	-4.13270000	-9.26000000
C	23.45170000	-4.36040000	-7.44210000
H	23.97250000	-3.56730000	-7.46520000
C	23.49290000	-5.20390000	-6.32660000
H	24.06600000	-4.99150000	-5.59880000
C	22.73590000	-6.30950000	-6.27190000
H	22.74120000	-6.83450000	-5.47880000
C	19.62200000	-12.71690000	-7.78180000
C	20.88810000	-12.99050000	-7.30050000
H	21.26210000	-12.43420000	-6.62630000
C	21.62670000	-14.06850000	-7.78370000
H	22.49390000	-14.23870000	-7.43530000
C	21.10160000	-14.90650000	-8.78400000
C	19.79930000	-14.62260000	-9.22190000
H	19.39980000	-15.18820000	-9.87260000
C	19.07990000	-13.55140000	-8.74440000
H	18.20510000	-13.38430000	-9.07520000
C	21.94580000	-15.97340000	-9.37100000
C	22.97190000	-16.57460000	-8.61980000
H	23.10710000	-16.31130000	-7.71600000
C	23.79510000	-17.55600000	-9.18600000
H	24.50480000	-17.92750000	-8.67520000
C	23.59050000	-17.97820000	-10.46000000
H	24.13890000	-18.66210000	-10.82760000
C	22.57350000	-17.40900000	-11.22630000
H	22.44040000	-17.70570000	-12.11910000
C	21.74420000	-16.40490000	-10.69780000
H	21.05650000	-16.02120000	-11.22910000
C	16.05640000	-10.96080000	-9.92400000
C	17.41220000	-10.76570000	-10.24680000
H	18.06460000	-10.82170000	-9.55810000
C	17.82320000	-10.49240000	-11.54720000
H	18.74680000	-10.38290000	-11.73690000
C	16.87820000	-10.37430000	-12.58340000
C	15.53290000	-10.53800000	-12.25680000
H	14.88060000	-10.46670000	-12.94430000
C	15.11590000	-10.80340000	-10.96020000

H	14.18790000	-10.87990000	-10.77100000
C	17.32010000	-10.10830000	-13.97250000
C	16.56430000	-10.58880000	-15.05020000
H	15.78230000	-11.10200000	-14.87900000
C	16.93610000	-10.32550000	-16.36200000
H	16.40370000	-10.65210000	-17.07760000
C	18.07520000	-9.59080000	-16.63190000
H	18.32620000	-9.41180000	-17.53070000
C	18.85280000	-9.11540000	-15.57680000
H	19.64420000	-8.62320000	-15.75940000
C	18.48340000	-9.35440000	-14.26510000
H	19.01260000	-9.01010000	-13.55450000
C	14.33860000	-11.08750000	-8.17820000
C	13.74340000	-9.83320000	-8.24420000
H	14.20910000	-9.11140000	-8.64960000
C	12.47220000	-9.63120000	-7.72330000
H	12.07270000	-8.77190000	-7.80250000
C	11.76000000	-10.65530000	-7.08530000
C	12.37730000	-11.89620000	-6.97020000
H	11.93780000	-12.59720000	-6.50170000
C	13.62550000	-12.12570000	-7.53080000
H	14.00900000	-12.99250000	-7.48010000
C	10.39220000	-10.42930000	-6.54370000
C	9.43210000	-9.70000000	-7.25330000
H	9.66380000	-9.32380000	-8.09450000
C	8.14820000	-9.51010000	-6.75880000
H	7.50020000	-9.05230000	-7.28160000
C	7.81410000	-9.98770000	-5.50370000
H	6.94040000	-9.84640000	-5.15580000
C	8.76860000	-10.67890000	-4.74870000
H	8.54710000	-10.99990000	-3.88260000
C	10.04370000	-10.89610000	-5.26780000
H	10.68530000	-11.36600000	-4.74860000

1-Br (-9911.0, -9656.1)

Bi	2.646855	1.610391	20.269467
N	2.756740	3.608098	21.247998
C	1.742811	4.590952	21.029872
Br	-1.629103	7.788731	20.173077
Br	7.492558	4.888364	24.977821
N	3.691819	2.237712	18.405113
C	0.472165	4.453222	21.605215
H	0.256949	3.597228	22.235938
Br	5.363130	-2.040097	14.296307
C	-0.240767	6.495686	20.550671
Br	4.897535	8.195981	17.452485
N	0.593641	1.904426	19.460425
C	-0.528938	5.399481	21.364772
H	-1.515280	5.277236	21.800500
Br	-0.165507	4.598466	13.980475
C	1.024592	6.669051	19.985279
H	1.236890	7.525277	19.353089
C	3.819731	5.042512	22.936895
H	2.958646	5.701804	22.936454
C	3.837127	3.910746	22.087074
Br	-4.224031	-0.161194	22.700005
C	2.009382	5.712213	20.228234
H	2.994203	5.832450	19.795791
C	4.891580	5.329563	23.782444
H	4.852116	6.206384	24.421770
C	6.002263	4.485631	23.807715
C	6.053454	3.359069	22.986911
H	6.921216	2.706858	22.994719
C	4.986427	3.086449	22.131240
H	5.076998	2.222842	21.474762
C	5.028544	4.251683	18.871561
H	5.605919	3.695554	19.602422
C	4.002779	3.611254	18.163033
C	4.556754	6.310767	17.719168
C	5.307734	5.605385	18.660382
H	6.091682	6.098432	19.226082
C	3.547260	5.689361	16.980552
H	2.969802	6.248371	16.251226
C	4.063449	1.272346	17.460544
C	3.275709	4.340843	17.209200
H	2.494570	3.846648	16.646209
C	4.963497	1.572344	16.410164
H	5.371144	2.573305	16.321230
C	5.342652	0.602037	15.482259
H	6.032935	0.861164	14.685048
C	4.840108	-0.695083	15.588429
C	3.953043	-1.028458	16.611825
H	3.549999	-2.033356	16.690044
C	3.563963	-0.050111	17.526410
H	2.838648	-0.333518	18.287056
C	0.385720	2.509563	18.182876
C	0.688981	1.818414	17.001741
H	1.071551	0.804719	17.054747
C	0.519634	2.424918	15.753368
H	0.773568	1.889433	14.844281
C	0.028630	3.730131	15.698036
C	-0.305675	4.431379	16.858724
H	-0.686235	5.446194	16.803000
C	-0.122824	3.815207	18.096507
H	-0.374254	4.347517	19.004752
C	-0.509134	1.453795	20.197016
C	-1.793244	1.336828	19.612922
H	-1.938440	1.613247	18.574310
C	-2.882211	0.866787	20.347486
H	-3.856539	0.788919	19.874365
C	-2.711744	0.491852	21.680592
C	-1.461378	0.594565	22.290096
H	-1.328317	0.318023	23.331346
C	-0.380220	1.082170	21.556424
H	0.571136	1.190339	22.074449

1-CF_3 (-12586.8, -12283.7)

1.Bi	3.231201	9.355346	5.021698
2.N	2.841265	7.325750	5.861500
3.N	4.763110	8.666330	3.553785
4.N	1.532521	9.293534	3.574853
5.C	3.571048	6.882667	6.966493
6.C	4.700862	7.598906	7.432684
7.H	5.049553	8.488130	6.910843
8.C	5.419032	7.178080	8.544272
9.H	6.282751	7.749845	8.869743
10.C	5.050014	6.008402	9.223705
11.C	3.937288	5.283862	8.776183
12.H	3.635261	4.378152	9.293119
13.C	3.207403	5.709929	7.671829
14.H	2.347741	5.133556	7.350013
15.C	5.808666	5.578741	10.441965
16.F	5.685559	4.238766	10.701026
17.F	5.378146	6.229925	11.587017
18.F	7.154153	5.846819	10.347362
19.C	1.860695	6.465925	5.278419
20.C	2.263456	5.343486	4.536875
21.H	3.318540	5.129271	4.431434
22.C	1.318733	4.509365	3.949064
23.H	1.642983	3.648639	3.372323
24.C	-0.047199	4.791725	4.095550
25.C	-0.459423	5.899788	4.844101
26.H	-1.515525	6.116992	4.964784
27.C	0.494157	6.726897	5.439813
28.H	0.176015	7.580474	6.027785
29.C	-1.055767	3.932111	3.380159
30.F	-2.318621	4.056887	3.887004
31.F	-0.732466	2.601297	3.421309
32.F	-1.137301	4.265919	2.039801
33.C	5.487256	9.607344	2.818702

34.C	5.117811	10.974212	2.813496
35.H	4.233226	11.313128	3.349525
36.C	5.848621	11.921423	2.107305
37.H	5.535053	12.960479	2.125798
38.C	6.972429	11.536685	1.363850
39.C	7.347566	10.185945	1.346337
40.H	8.216739	9.870889	0.776706
41.C	6.627273	9.237836	2.063604
42.H	6.948310	8.202713	2.046343
43.C	7.718474	12.543184	0.542418
44.F	9.048126	12.233976	0.403777
45.F	7.654272	13.809601	1.069088
46.F	7.218134	12.644957	-0.746286
47.C	5.010161	7.274610	3.347105
48.C	4.579315	6.654157	2.163591
49.H	4.081332	7.245465	1.406915
50.C	4.794659	5.295305	1.959365
51.H	4.449196	4.825740	1.043624
52.C	5.447390	4.537878	2.942467
53.C	5.895064	5.149944	4.118861
54.H	6.406521	4.568125	4.878577
55.C	5.682950	6.515752	4.313333
56.H	6.036910	6.992679	5.220385
57.C	5.592189	3.050786	2.752686
58.F	6.584980	2.509692	3.520703
59.F	5.854987	2.710603	1.452437
60.F	4.427452	2.386662	3.095937
61.C	0.277396	9.770883	3.958141
62.C	0.008456	10.127847	5.301760
63.H	0.765758	10.001461	6.073254
64.C	-1.231319	10.620198	5.689241
65.H	-1.401676	10.878624	6.729649
66.C	-2.262791	10.755834	4.750400
67.C	-2.016600	10.408377	3.414690
68.H	-2.802748	10.511917	2.672663
69.C	-0.772954	9.928744	3.020900
70.H	-0.609041	9.672371	1.980699
71.C	-3.591485	11.317203	5.155096
72.F	-4.629529	10.804319	4.417640
73.F	-3.655114	12.691587	4.989883
74.F	-3.885701	11.084875	6.475866
75.C	1.705102	8.745069	2.267080
76.C	2.429466	9.441690	1.291405
77.H	2.849207	10.413548	1.525836
78.C	2.618616	8.891736	0.022488
79.H	3.190766	9.434337	-0.722827
80.C	2.065531	7.642975	-0.282790
81.C	1.319988	6.948739	0.681114
82.H	0.886292	5.981193	0.447777
83.C	1.143728	7.498264	1.946549
84.H	0.564878	6.970289	2.692534
85.C	2.322430	6.998243	-1.619517
86.F	1.228290	6.324840	-2.095077
87.F	3.341680	6.065664	-1.538343
88.F	2.694920	7.894347	-2.581490

1-HH (-10188.9, -9881.8)

1.Bi	0.792993	8.788250	10.475474
2.N	-0.815262	7.510109	11.238220
3.C	0.304284	5.332647	11.322770
4.H	1.168756	5.812867	11.772397
5.C	-1.541739	8.953402	7.541243
6.C	-3.091366	10.133513	12.616527
7.H	-3.319355	11.182147	12.444912
8.C	-1.526252	8.571919	6.194594
9.H	-0.744322	8.917766	5.530340
10.C	-2.586247	8.528856	8.374215
11.H	-2.613135	8.830988	9.414861
12.C	2.939787	11.089987	6.039160
13.H	3.827317	11.430009	5.513067
14.C	0.326975	6.172114	8.146292
15.H	-0.414498	6.899609	8.455362
16.C	0.872539	4.151789	6.930284
17.H	0.566625	3.310747	6.314568
18.C	1.010832	11.563281	7.428090
19.H	0.394422	12.274553	7.974675
20.C	-0.835244	6.100036	11.039908
21.C	-1.833941	8.132553	11.998824
22.C	-3.460968	8.065287	13.806360
23.H	-3.968436	7.501585	14.585164
24.N	2.037208	7.424691	9.336311
25.C	-2.508487	7.424352	13.016660
26.H	-2.267234	6.381106	13.190701
27.C	-3.756401	9.421930	13.618658
28.H	-4.500365	9.913480	14.238877
29.C	2.161064	11.997630	6.764108
30.H	2.437651	13.047579	6.803928
31.C	1.438261	9.292843	6.679499
32.H	1.181274	8.240226	6.672881
33.C	2.571585	9.740709	5.999269
34.H	3.178854	9.024917	5.452080
35.C	-3.594882	7.708460	7.868213
36.H	-4.400684	7.387293	8.522745
37.C	-1.976171	5.475945	10.503911
38.H	-2.855232	6.071869	10.282513
39.C	2.616882	5.380977	8.097452
40.H	3.659103	5.482084	8.378046
41.C	1.669128	6.327044	8.543862
42.C	-3.567116	7.297960	6.531677
43.H	-4.345530	6.648513	6.140953
44.C	-2.535464	7.741769	5.700040
45.H	-2.512955	7.448467	4.653963
46.C	-2.153857	9.492840	11.803800
47.H	-1.691657	10.056372	10.995357
48.C	-0.067256	5.096442	7.359330
49.H	-1.112225	5.001754	7.079000
50.C	-1.958724	4.109885	10.231869
51.H	-2.839294	3.636656	9.805275
52.C	0.321314	3.967798	11.032011
53.H	1.213279	3.384061	11.242360
54.N	-0.502563	9.777647	8.134453
55.C	0.642533	10.211878	7.378602
56.C	3.414668	7.660170	9.698042
57.C	5.405254	9.040784	9.556239
58.H	5.923669	9.899348	9.137482
59.C	4.092605	8.763135	9.157168
60.H	3.592349	9.386899	8.423701
61.C	2.212911	4.309691	7.299295
62.H	2.956874	3.589408	6.967597
63.C	4.057659	6.838553	10.640496
64.H	3.524651	5.989405	11.058533
65.C	-0.806830	3.353150	10.481302
66.H	-0.791969	2.291157	10.252545
67.C	5.372454	7.110533	11.020146
68.H	5.867339	6.468838	11.744398
69.C	6.047946	8.214120	10.481387
70.H	7.068964	8.427388	10.786189
71.H	-0.931964	10.577560	8.600256

1-MeH (-12406.1, -12004.6)

1.Bi	2.777329	9.032447	5.037707
2.N	2.635467	7.031818	5.910307
3.N	5.401064	8.458081	4.188895
4.N	1.166150	8.798208	3.589047
5.C	3.691237	6.553835	6.712180
6.C	4.625200	7.459026	7.267349
7.H	4.468500	8.534637	7.185273
8.C	5.734836	7.009802	7.979279
9.H	6.431763	7.739419	8.386469
10.C	5.952668	5.639669	8.205682
11.C	4.991556	4.748002	7.706781
12.H	5.113143	3.680884	7.881673

13.C	3.882751	5.182234	6.978812
14.H	3.174080	4.455217	6.600562
15.C	7.142792	5.155923	9.000771
16.H	7.417438	4.133527	8.721275
17.H	6.920604	5.154381	10.076714
18.H	8.013877	5.802163	8.847931
19.C	1.594280	6.151995	5.462927
20.C	1.846385	5.139833	4.524887
21.H	2.848659	5.015904	4.129667
22.C	0.810032	4.318498	4.087892
23.H	1.020982	3.539452	3.359384
24.C	-0.504812	4.498798	4.547006
25.C	-0.746063	5.522331	5.474853
26.H	-1.755727	5.682586	5.846656
27.C	0.289830	6.339776	5.933847
28.H	0.095231	7.123278	6.661737
29.C	-1.631729	3.648884	4.009434
30.H	-2.493539	3.651179	4.684015
31.H	-1.312855	2.612280	3.855944
32.H	-1.969508	4.033105	3.036988
33.C	5.751412	9.809932	3.834907
34.C	5.001397	10.504146	2.872705
35.H	4.195027	10.004396	2.340822
36.C	5.299829	11.835823	2.584272
37.H	4.713281	12.359136	1.832738
38.C	6.333212	12.512744	3.254151
39.C	7.057170	11.808829	4.228357
40.H	7.857076	12.310079	4.768314
41.C	6.777568	10.470013	4.516454
42.H	7.359074	9.939369	5.267250
43.C	6.666688	13.947093	2.914947
44.H	7.178119	14.444644	3.744657
45.H	5.764923	14.517576	2.668565
46.H	7.330782	13.991384	2.041338
47.C	5.567517	7.365866	3.264821
48.C	5.795015	7.556000	1.898280
49.H	5.918010	8.552339	1.490014
50.C	5.873178	6.447735	1.048837
51.H	6.048257	6.613034	-0.011725
52.C	5.732351	5.139096	1.528991
53.C	5.535293	4.969884	2.910806
54.H	5.442163	3.966759	3.321697
55.C	5.451557	6.061423	3.769593
56.H	5.294854	5.902996	4.831695
57.C	5.777372	3.947255	0.601081
58.H	4.802340	3.443655	0.562298
59.H	6.507943	3.205042	0.943885
60.H	6.043678	4.245058	-0.417366
61.C	0.323219	9.929316	3.496111
62.C	-0.165737	10.536633	4.669866
63.H	-0.007165	10.048027	5.629434
64.C	-0.912593	11.717025	4.601267
65.H	-1.279970	12.167492	5.520431
66.C	-1.229949	12.301359	3.369106
67.C	-0.763368	11.667554	2.196874
68.H	-0.995953	12.105111	1.227961
69.C	0.003366	10.511006	2.249426
70.H	0.374619	10.053045	1.337193
71.C	-2.068254	13.554530	3.281304
72.H	-3.038618	13.343748	2.813284
73.H	-1.573801	14.316219	2.666102
74.H	-2.255473	13.980160	4.271510
75.C	1.074038	7.751280	2.641326
76.C	2.224142	7.213257	2.047555
77.H	3.194948	7.649600	2.259257
78.C	2.131186	6.134149	1.168695
79.H	3.040691	5.733208	0.730101
80.C	0.889737	5.576273	0.837990
81.C	-0.262469	6.147900	1.410530
82.H	-1.239377	5.735015	1.167946
83.C	-0.181276	7.211566	2.301218
84.H	-1.077900	7.615600	2.760932
85.C	0.781241	4.386860	-0.086832
86.H	0.453233	3.494861	0.463773
87.H	1.742613	4.156918	-0.556172
88.H	0.044883	4.562973	-0.879720
89.H	5.783471	8.200270	5.100328

Table S8. Cartesian coordinates and ADF total electronic and Gibbs energies (in parentheses and in kcal mol^{-1}) of compounds **1-X** under analysis computed at the ZORA-BLYP(D3BJ)/TZ2P level of theory in the gas phase.

1-H (-10205.8, -9907.8)

1.Bi	1.008864	8.966165	9.952143
2.N	-0.457437	7.899634	11.277174
3.C	0.733784	5.836472	11.829577
4.H	1.624238	6.417504	12.045908
5.C	-1.079180	8.374652	7.470927
6.C	-2.823352	10.728397	11.851306
7.H	-3.142319	11.634841	11.341928
8.C	-1.107643	8.102800	6.086869
9.H	-0.347907	8.536229	5.444710
10.C	-2.052522	7.774802	8.291144
11.H	-2.053591	7.977930	9.353163
12.C	1.549130	12.483583	5.877724
13.H	1.961852	13.339573	5.350457
14.C	0.579296	5.623216	8.175316
15.H	0.077774	5.497773	9.127065
16.C	0.783501	5.089543	5.820775
17.H	0.429753	4.555053	4.942784
18.C	-0.379355	11.206113	6.622790
19.H	-1.455346	11.069272	6.684505
20.C	-0.450518	6.496573	11.464908
21.C	-1.457815	8.699474	11.858013
22.C	-2.957160	9.202885	13.713901
23.H	-3.370982	8.926605	14.681373
24.N	2.153212	7.219099	9.220274
25.C	-2.016617	8.368953	13.115302
26.H	-1.695646	7.458729	13.612713
27.C	-3.362384	10.394670	13.095236
28.H	-4.093838	11.041919	13.571447
29.C	0.159621	12.292741	5.939648
30.H	-0.507119	13.008482	5.463626
31.C	1.860676	10.445352	7.154272
32.H	2.526278	9.684401	7.556797
33.C	2.393960	11.556767	6.490264
34.H	3.473211	11.677615	6.431245
35.C	-3.009889	6.918361	7.747321
36.H	-3.746875	6.460864	8.403630
37.C	-1.608947	5.729616	11.224735
38.H	-2.531403	6.232416	10.951669
39.C	2.321077	6.654770	6.846040
40.H	3.168876	7.331405	6.781002
41.C	1.676343	6.490436	8.080775
42.C	-3.037374	6.658004	6.374092
43.H	-3.788381	5.995202	5.952192
44.C	-2.081100	7.263529	5.550395
45.H	-2.076735	7.061329	4.481529
46.C	-1.898404	9.885638	11.227543
47.H	-1.559068	10.129357	10.222711
48.C	0.135363	4.928898	7.047958
49.H	-0.727448	4.273774	7.129140
50.C	-1.565380	4.339564	11.319584
51.H	-2.464977	3.760949	11.121919
52.C	0.779054	4.442886	11.899142
53.H	1.714899	3.953899	12.156158
54.N	-0.072772	9.202002	8.014688
55.C	0.465378	10.264152	7.250887
56.C	3.235355	6.711519	9.954632
57.C	4.947298	7.006818	11.678777
58.H	5.442533	7.656210	12.397163
59.C	3.913838	7.520292	10.895716
60.H	3.647668	8.571164	11.005280
61.C	1.877899	5.955376	5.721622
62.H	2.381050	6.093608	4.767403
63.C	3.671271	5.375530	9.804104
64.H	3.169901	4.731472	9.090057
65.C	-0.368163	3.686571	11.642547
66.H	-0.334270	2.601530	11.697377
67.C	4.719707	4.877994	10.577941
68.H	5.029876	3.844019	10.441267
69.C	5.361682	5.678642	11.529349
70.H	6.172899	5.281387	12.133074

1-Me (-12416.35, -12023.1)

1.Bi	3.216614	9.278600	4.983989
2.N	2.862540	7.259273	5.823010
3.N	4.730275	8.628178	3.502149
4.N	1.507559	9.218396	3.576028
5.C	3.577016	6.854308	6.960090
6.C	4.728601	7.548290	7.395163
7.H	5.125488	8.377874	6.811574
8.C	5.412529	7.170439	8.551611
9.H	6.295818	7.734358	8.846913
10.C	5.007297	6.069404	9.318161
11.C	3.877603	5.364050	8.872455
12.H	3.534489	4.496703	9.435091
13.C	3.171517	5.739715	7.731566
14.H	2.298777	5.171970	7.427033
15.C	5.741998	5.663841	10.577367
16.H	5.858346	4.575088	10.640157
17.H	5.199537	5.984454	11.477912
18.H	6.740292	6.113238	10.617419
19.C	1.888359	6.380866	5.254813
20.C	2.295568	5.264637	4.507420
21.H	3.353784	5.079951	4.370663
22.C	1.350416	4.410599	3.943441
23.H	1.688252	3.559691	3.354338
24.C	-0.026898	4.640917	4.100529
25.C	-0.424046	5.757879	4.849792
26.H	-1.483539	5.969781	4.979161
27.C	0.518346	6.614152	5.425615
28.H	0.189240	7.476294	5.996167
29.C	-1.045361	3.704872	3.488002
30.H	-2.025764	4.184433	3.400293
31.H	-1.171161	2.802999	4.102732
32.H	-0.733932	3.375536	2.489873
33.C	5.467156	9.593794	2.801037
34.C	5.072550	10.950626	2.777089
35.H	4.147331	11.264445	3.258648
36.C	5.830237	11.917302	2.115043
37.H	5.488086	12.950882	2.126371
38.C	7.000591	11.584019	1.419527
39.C	7.384747	10.233392	1.429320
40.H	8.290048	9.932923	0.903110
41.C	6.650074	9.258496	2.101245
42.H	6.989649	8.228254	2.094589
43.C	7.796072	12.623568	0.660418
44.H	8.874609	12.454651	0.763924
45.H	7.575669	13.634444	1.020545
46.H	7.565581	12.599128	-0.414172
47.C	4.997337	7.241341	3.280603
48.C	4.552183	6.615314	2.106535
49.H	4.011094	7.197464	1.370856
50.C	4.803376	5.261524	1.890423
51.H	4.440837	4.793928	0.976664
52.C	5.497107	4.488444	2.835942
53.C	5.946706	5.125418	4.002336
54.H	6.487772	4.553126	4.753451
55.C	5.706204	6.483872	4.221578
56.H	6.060536	6.957035	5.131340
57.C	5.713955	3.006467	2.623052
58.H	6.602234	2.652213	3.156860
59.H	5.832958	2.768633	1.560200
60.H	4.856363	2.427906	2.994098
61.C	0.279220	9.771678	3.965785

62.C	-0.002033	10.065865	5.318559
63.H	0.711705	9.806214	6.099241
64.C	-1.208193	10.656330	5.699564
65.H	-1.380430	10.864788	6.754212
66.C	-2.206397	10.957293	4.763955
67.C	-1.936635	10.643889	3.421356
68.H	-2.688674	10.856910	2.662602
69.C	-0.730914	10.072987	3.021440
70.H	-0.559602	9.855302	1.972596
71.C	-3.518212	11.590494	5.173738
72.H	-4.375429	11.009116	4.810693
73.H	-3.618822	12.604551	4.763470
74.H	-3.599440	11.663656	6.263523
75.C	1.653347	8.683916	2.257899
76.C	2.351942	9.388157	1.267029
77.H	2.789217	10.352281	1.504667
78.C	2.503826	8.850031	-0.011385
79.H	3.066016	9.406659	-0.759026
80.C	1.952845	7.601307	-0.343386
81.C	1.244870	6.910826	0.651901
82.H	0.815496	5.936432	0.426225
83.C	1.097431	7.438222	1.935354
84.H	0.555218	6.888726	2.694921
85.C	2.124512	7.024761	-1.731609
86.H	1.746137	5.998876	-1.785854
87.H	3.180120	7.015264	-2.030056
88.H	1.583556	7.621673	-2.477668

1-OMe (-13226.8, -12820.7)

1.Bi	3.215146	9.361544	4.853302
2.N	2.934350	7.366074	5.777086
3.N	4.613677	8.683250	3.278016
4.N	1.407808	9.267261	3.577815
5.C	3.724474	6.998980	6.880320
6.C	4.904108	7.709732	7.211328
7.H	5.252978	8.523346	6.577357
8.C	5.670282	7.381681	8.324800
9.H	6.571966	7.941293	8.559451
10.C	5.307141	6.303994	9.145268
11.C	4.158580	5.569278	8.825208
12.H	3.847572	4.725373	9.432090
13.C	3.379830	5.916427	7.715440
14.H	2.488478	5.338622	7.495552
15.H	5.789698	3.999020	10.522983
16.H	-5.323388	11.951881	5.452525
17.C	0.843144	7.416107	2.060322
18.H	0.342984	6.920563	2.883212
19.C	1.935244	6.460609	5.301725
20.C	2.296400	5.360769	4.514623
21.H	3.340420	5.205555	4.274854
22.C	1.336908	4.466481	4.033741
23.H	1.656381	3.636820	3.413022
24.C	-0.017307	4.672240	4.337416
25.C	-0.391216	5.768190	5.132655
26.H	-1.443403	5.921316	5.355937
27.C	0.577645	6.645284	5.611760
28.H	0.279315	7.492362	6.220172
29.H	-1.659337	2.278036	2.802869
30.H	3.304807	7.517549	-2.330568
31.C	1.444220	8.669589	2.281718
32.C	2.075764	9.304403	1.208405
33.C	5.361446	9.649844	2.583059
34.C	4.931304	10.989318	2.493820
35.H	3.965769	11.282855	2.901966
36.C	5.699046	11.974338	1.858889
37.H	5.320378	12.990228	1.824731
38.C	6.914577	11.631865	1.255940
39.C	7.343396	10.295856	1.303948
40.H	8.284914	10.032949	0.828053
41.C	6.590725	9.327001	1.956452
42.H	6.951694	8.304535	1.991781
43.H	7.248643	14.314167	1.550473
44.H	2.544132	10.271320	1.359614
45.C	2.135299	8.706226	-0.057276
46.H	2.651730	9.220774	-0.859868
47.C	4.891861	7.297895	3.069122
48.C	4.392694	6.644472	1.927715
49.H	3.801936	7.208396	1.216671
50.C	4.641011	5.295063	1.712076
51.H	4.243453	4.787357	0.837453
52.C	5.395048	4.558614	2.641913
53.C	5.904091	5.196937	3.781931
54.H	6.482199	4.654432	4.521482
55.C	5.652806	6.560130	3.980851
56.H	6.043750	7.046034	4.868642
57.H	5.845332	2.420411	4.273666
58.C	1.540116	7.453352	-0.259137
59.C	0.885747	6.816020	0.809594
60.H	0.433478	5.842316	0.641816
61.C	0.186493	9.761497	4.072647
62.C	0.007815	10.050684	5.446832
63.H	0.798193	9.832249	6.162870
64.C	-1.181016	10.581362	5.936085
65.H	-1.297080	10.792200	6.995911
66.C	-2.260603	10.820773	5.073938
67.C	-2.115585	10.525180	3.712573
68.H	-2.929127	10.692100	3.014438
69.C	-0.909683	10.011973	3.222618
70.H	-0.819052	9.800816	2.162452
71.O	5.565074	3.221058	2.351480
72.C	6.321023	2.429847	3.283582
73.H	6.332119	1.419007	2.871541
74.H	7.350477	2.801200	3.377006
75.O	7.747522	12.514957	0.588973
76.C	7.343408	13.889505	0.540775
77.H	8.132595	14.413073	-0.002805
78.H	6.389503	14.008497	0.007004
79.O	1.552318	6.761936	-1.452652
80.C	2.242058	7.362967	-2.561228
81.H	2.144555	6.656422	-3.387616
82.H	1.785965	8.322361	-2.840695
83.O	-1.048636	3.870548	3.895998
84.C	-0.711594	2.762213	3.045639
85.H	-0.223889	3.103527	2.122456
86.H	-0.054604	2.049107	3.561812
87.O	-3.407364	11.329627	5.661208
88.C	-4.533584	11.565419	4.805038
89.H	-4.298358	12.308088	4.029425
90.H	-4.873008	10.636269	4.325486
91.O	6.144165	6.047269	10.219389
92.C	5.795295	4.950308	11.074206
93.H	6.565460	4.919133	11.847742
94.H	4.811792	5.103566	11.540793

1-Ph (-19338.6, -18759.6)

1.Bi	16.950289	-12.104777	-6.891129
2.N	16.381387	-10.168526	-5.923797
3.N	19.132107	-11.796065	-7.273380
4.N	15.800391	-11.842019	-8.899481
5.C	15.357049	-10.327652	-4.964010
6.C	15.457475	-11.332675	-3.978766
7.H	16.381688	-11.900626	-3.887386
8.C	14.413383	-11.569776	-3.085033
9.H	14.531868	-12.339268	-2.326619
10.C	13.243731	-10.790106	-3.106609
11.C	13.165337	-9.762263	-4.070313
12.H	12.257693	-9.170651	-4.143627
13.C	14.186314	-9.540090	-4.983103
14.H	14.080183	-8.773435	-5.742044
15.C	12.124718	-11.043113	-2.172179
16.C	11.333848	-9.985970	-1.683108
17.H	11.579384	-8.964009	-1.958696

18.C	10.250877	-10.229008	-0.837782
19.H	9.656837	-9.394964	-0.471382
20.C	9.931375	-11.536758	-0.457730
21.H	9.085891	-11.726789	0.198783
22.C	10.710992	-12.598314	-0.929941
23.H	10.467908	-13.620230	-0.647797
24.C	11.793887	-12.353793	-1.776133
25.H	12.371202	-13.190266	-2.161810
26.C	16.720593	-8.891636	-6.413369
27.C	17.141957	-8.705860	-7.740303
28.H	17.133943	-9.536427	-8.435121
29.C	17.606776	-7.472566	-8.182752
30.H	17.969669	-7.392626	-9.203169
31.C	17.644776	-6.353577	-7.331896
32.C	17.189994	-6.537957	-6.010438
33.H	17.180787	-5.694133	-5.325635
34.C	16.744654	-7.773067	-5.553873
35.H	16.422709	-7.884113	-4.522903
36.C	18.143462	-5.039592	-7.796462
37.C	17.984220	-4.632486	-9.135526
38.H	17.466203	-5.283122	-9.835130
39.C	18.452112	-3.391537	-9.570956
40.H	18.309255	-3.097031	-10.608343
41.C	19.086060	-2.523271	-8.676813
42.H	19.449605	-1.555960	-9.014985
43.C	19.255783	-2.915337	-7.345380
44.H	19.771554	-2.261711	-6.646548
45.C	18.795058	-4.157583	-6.912768
46.H	18.977994	-4.464855	-5.887424
47.C	19.797240	-10.545055	-7.234252
48.C	19.706822	-9.719269	-6.102170
49.H	19.157807	-10.070854	-5.233489
50.C	20.262122	-8.443257	-6.107535
51.H	20.124599	-7.806074	-5.239424
52.C	20.942763	-7.945864	-7.233277
53.C	21.070061	-8.799250	-8.347136
54.H	21.620833	-8.460018	-9.220275
55.C	20.510244	-10.071080	-8.352624
56.H	20.618034	-10.707447	-9.225989
57.C	21.497027	-6.573211	-7.259824
58.C	21.497455	-5.820148	-8.449995
59.H	21.042980	-6.235066	-9.344883
60.C	22.029377	-4.532526	-8.485390
61.H	21.996940	-3.963206	-9.410372
62.C	22.569523	-3.961240	-7.329266
63.H	22.979170	-2.954563	-7.355726
64.C	22.565301	-4.689739	-6.136268
65.H	22.985575	-4.256431	-5.231328
66.C	22.035076	-5.981000	-6.102023
67.H	22.064166	-6.548380	-5.175385
68.C	19.773710	-12.911749	-7.858341
69.C	21.134905	-13.177644	-7.591392
70.H	21.698932	-12.478233	-6.981285
71.C	21.749888	-14.313603	-8.101892
72.H	22.804547	-14.477670	-7.895933
73.C	21.046163	-15.247762	-8.892454
74.C	19.695273	-14.975916	-9.161194
75.H	19.117743	-15.667318	-9.768858
76.C	19.073903	-13.824902	-8.673880
77.H	18.048912	-13.620188	-8.979489
78.C	21.712574	-16.457406	-9.430334
79.C	22.676933	-17.150010	-8.672865
80.H	22.916503	-16.805868	-7.669962
81.C	23.306389	-18.288590	-9.179090
82.H	24.042080	-18.811520	-8.572196
83.C	22.986195	-18.763224	-10.455338
84.H	23.476891	-19.649543	-10.849960
85.C	22.030138	-18.086322	-11.219854
86.H	21.780722	-18.439914	-12.217739
87.C	21.402019	-16.946901	-10.714007
88.H	20.682186	-16.413503	-11.329584
89.C	16.259222	-11.252170	-10.087399
90.C	17.632922	-11.005326	-10.291766
91.H	18.341779	-11.258043	-9.515247
92.C	18.097683	-10.421693	-11.464028
93.H	19.165453	-10.251426	-11.574601
94.C	17.224456	-10.063005	-12.507151
95.C	15.858237	-10.351305	-12.321042
96.H	15.146080	-10.089283	-13.099740
97.C	15.381136	-10.929191	-11.148688
98.H	14.319065	-11.125435	-11.044132
99.C	17.719928	-9.399846	-13.734547
100.C	17.143694	-9.663415	-14.992907
101.H	16.339767	-10.391033	-15.069804
102.C	17.609286	-9.027810	-16.145383
103.H	17.152436	-9.254133	-17.106318
104.C	18.666025	-8.114025	-16.070734
105.H	19.028822	-7.619530	-16.968464
106.C	19.251073	-7.842793	-14.829260
107.H	20.067645	-7.127660	-14.756854
108.C	18.782799	-8.475973	-13.676786
109.H	19.227402	-8.234626	-12.714561
110.C	14.475970	-11.616924	-8.445505
111.C	13.844485	-10.355153	-8.496320
112.H	14.346699	-9.528820	-8.989388
113.C	12.625387	-10.150189	-7.865408
114.H	12.189115	-9.154779	-7.879463
115.C	11.984922	-11.173413	-7.131919
116.C	12.603181	-12.434493	-7.106392
117.H	12.119495	-13.259181	-6.590480
118.C	13.814888	-12.658577	-7.759621
119.H	14.256831	-13.652967	-7.766391
120.C	10.741753	-10.909285	-6.374333
121.C	9.788706	-9.975575	-6.826440
122.H	9.934439	-9.479520	-7.782558
123.C	8.645672	-9.697456	-6.074571
124.H	7.919607	-8.977788	-6.446112
125.C	8.429419	-10.344270	-4.852530
126.H	7.543547	-10.119962	-4.263401
127.C	9.364000	-11.277201	-4.392319
128.H	9.222934	-11.767732	-3.433241
129.C	10.502983	-11.556982	-5.146580
130.H	11.241663	-12.248056	-4.754771

1-Br (-9906.1, -9650.6)

1.Bi	2.640392	1.628876	20.258068
2.N	2.754374	3.615601	21.242452
3.C	1.749144	4.607522	21.022441
4.Br	-1.590791	7.831968	20.151203
5.Br	7.467818	4.825889	25.020587
6.N	3.688724	2.244733	18.400012
7.C	0.475480	4.481436	21.593700
8.H	0.249517	3.626550	22.222095
9.Br	5.393388	-2.067164	14.343486
10.C	-0.216365	6.530432	20.536191
11.Br	4.874369	8.198542	17.406130
12.N	0.590603	1.912724	19.456656
13.C	-0.515790	5.436924	21.350123
14.H	-1.505213	5.324014	21.781394
15.Br	-0.198306	4.640017	13.999443
16.C	1.053060	6.691714	19.976037
17.H	1.275435	7.546340	19.345104
18.C	3.807942	5.015426	22.965406
19.H	2.942376	5.668860	22.975927
20.C	3.835072	3.905394	22.089073
21.Br	-4.187449	-0.226909	22.703099
22.C	2.028597	5.726759	20.222551
23.H	3.016098	5.838609	19.794160
24.C	4.874359	5.286046	23.822331
25.H	4.829428	6.146209	24.483538
26.C	5.989682	4.447350	23.834199
27.C	6.050127	3.343537	22.984161

28.H	6.922821	2.697896	22.980374
29.C	4.989342	3.088520	22.114739
30.H	5.089760	2.248030	21.429682
31.C	5.021904	4.265901	18.849791
32.H	5.600644	3.717523	19.585407
33.C	3.996905	3.617435	18.147556
34.C	4.542557	6.316124	17.683377
35.C	5.297003	5.618523	18.627835
36.H	6.079484	6.119051	19.189026
37.C	3.534315	5.685258	16.950806
38.H	2.954510	6.237157	16.217889
39.C	4.064368	1.270043	17.463614
40.C	3.266946	4.337815	17.189083
41.H	2.486738	3.837266	16.630474
42.C	4.988432	1.556190	16.431549
43.H	5.407758	2.552940	16.348948
44.C	5.375599	0.577956	15.516167
45.H	6.084667	0.824538	14.731650
46.C	4.858464	-0.714277	15.615992
47.C	3.945870	-1.032089	16.621305
48.H	3.530504	-2.032511	16.692369
49.C	3.546790	-0.044997	17.522660
50.H	2.796306	-0.313380	18.264618
51.C	0.373419	2.523683	18.183076
52.C	0.673966	1.841595	16.996015
53.H	1.062500	0.829757	17.040328
54.C	0.496747	2.455975	15.752772
55.H	0.749407	1.928741	14.838491
56.C	0.001818	3.760262	15.707306
57.C	-0.330524	4.451273	16.874851
58.H	-0.715352	5.464929	16.827561
59.C	-0.140997	3.827606	18.107551
60.H	-0.390988	4.352629	19.020381
61.C	-0.505973	1.449260	20.198464
62.C	-1.782808	1.292554	19.610083
63.H	-1.927371	1.551480	18.566781
64.C	-2.862462	0.805123	20.346067
65.H	-3.832869	0.695634	19.871233
66.C	-2.690740	0.450852	21.685051
67.C	-1.446776	0.595724	22.298324
68.H	-1.314822	0.337735	23.344469
69.C	-0.374830	1.103091	21.563683
70.H	0.569298	1.252286	22.085432

1-CF_3 (-12578.5, -12276.4)

1.Bi	3.222584	9.315153	5.018416
2.N	2.847513	7.294058	5.862057
3.N	4.762402	8.652482	3.558038
4.N	1.527805	9.259087	3.581812
5.C	3.574036	6.867742	6.979067
6.C	4.709114	7.580794	7.432655
7.H	5.075885	8.447006	6.884153
8.C	5.413707	7.182189	8.563600
9.H	6.282068	7.750012	8.882756
10.C	5.027407	6.036508	9.268861
11.C	3.912297	5.310798	8.827958
12.H	3.600674	4.419704	9.365092
13.C	3.194379	5.715529	7.708561
14.H	2.331175	5.141067	7.392362
15.C	5.762261	5.614936	10.510063
16.F	5.807742	4.251720	10.650583
17.F	5.164272	6.099446	11.655168
18.F	7.056408	6.066631	10.531171
19.C	1.879996	6.420165	5.276635
20.C	2.301160	5.298548	4.544626
21.H	3.359375	5.095132	4.449410
22.C	1.370448	4.452308	3.951436
23.H	1.709217	3.592115	3.382008
24.C	0.000567	4.720643	4.083219
25.C	-0.429638	5.825973	4.825284
26.H	-1.489653	6.031279	4.933517
27.C	0.509323	6.666787	5.425514
28.H	0.176486	7.521291	6.004287
29.C	-0.993343	3.853467	3.351661
30.F	-2.260111	3.966204	3.847902
31.F	-0.655045	2.529245	3.389680
32.F	-1.060111	4.200356	2.015211
33.C	5.472612	9.608654	2.823861
34.C	5.079431	10.968201	2.814657
35.H	4.180800	11.290069	3.338708
36.C	5.801118	11.928499	2.114811
37.H	5.472644	12.963145	2.129674
38.C	6.935316	11.563403	1.379707
39.C	7.332134	10.219600	1.365287
40.H	8.211197	9.921684	0.801483
41.C	6.623194	9.258748	2.077529
42.H	6.960510	8.228637	2.063927
43.C	7.670705	12.585347	0.559754
44.F	9.003012	12.293360	0.432319
45.F	7.581031	13.845584	1.093124
46.F	7.170375	12.674393	-0.724140
47.C	5.015180	7.263924	3.333666
48.C	4.587427	6.656728	2.142203
49.H	4.087577	7.255286	1.392377
50.C	4.807803	5.301191	1.921651
51.H	4.465814	4.842098	0.999142
52.C	5.461700	4.533279	2.895471
53.C	5.907372	5.132918	4.078638
54.H	6.419622	4.541642	4.830715
55.C	5.690346	6.495561	4.290600
56.H	6.039790	6.961779	5.205102
57.C	5.604830	3.045622	2.690811
58.F	6.596786	2.500196	3.454246
59.F	5.865036	2.721345	1.388755
60.F	4.437856	2.386904	3.031182
61.C	0.284286	9.774253	3.963140
62.C	0.007139	10.099380	5.312401
63.H	0.739250	9.899256	6.093156
64.C	-1.212959	10.647138	5.691984
65.H	-1.393507	10.883169	6.736171
66.C	-2.216698	10.864099	4.740396
67.C	-1.965852	10.535152	3.401662
68.H	-2.735200	10.696105	2.652360
69.C	-0.740767	10.003954	3.014588
70.H	-0.569357	9.765113	1.971195
71.C	-3.522525	11.491052	5.140071
72.F	-4.564633	11.072830	4.354789
73.F	-3.488928	12.866672	5.036376
74.F	-3.859031	11.213421	6.440587
75.C	1.688221	8.708417	2.272382
76.C	2.405942	9.399371	1.287747
77.H	2.834562	10.368963	1.515740
78.C	2.580001	8.844169	0.018914
79.H	3.147897	9.380172	-0.734736
80.C	2.020051	7.596171	-0.276932
81.C	1.280075	6.909423	0.695693
82.H	0.838156	5.943891	0.469143
83.C	1.117312	7.464358	1.960915
84.H	0.542446	6.942037	2.713763
85.C	2.272171	6.943070	-1.613128
86.F	1.193923	6.228687	-2.055364
87.F	3.325651	6.051290	-1.534958
88.F	2.594549	7.842679	-2.588304

Table S9. Cartesian coordinates and ADF total electronic and Gibbs energies (in parentheses and in kcal mol^{-1}) of compounds **3-X** under analysis computed at the ZORA-BLYP(D3BJ)/TZ2P level of theory in benzene.

3-H (-6736.8, -6540.5)

C	0.167970	7.064558	4.635863
C	0.814328	7.579374	3.506545
N	4.930368	8.323977	3.704049
H	0.293177	7.625083	2.553189
C	5.331128	9.533666	3.086658
C	4.548420	10.692457	3.239732
H	3.627730	10.647265	3.811437
C	4.961053	11.897185	2.668904
H	4.342797	12.782782	2.795718
C	6.152025	11.971196	1.937960
C	6.938361	10.820988	1.799849
H	7.877414	10.864904	1.253062
C	6.543361	9.613349	2.376090
H	7.173024	8.734891	2.282335
H	6.467797	12.910858	1.492705
C	2.128297	8.042689	3.586006
H	2.623393	8.432102	2.702981
H	-0.856284	6.707503	4.569857
C	5.228274	7.019285	3.241527
C	5.373070	6.757299	1.866337
H	5.273458	7.565293	1.149317
C	5.636607	5.460215	1.425209
H	5.746940	5.275477	0.359186
C	5.737516	4.401168	2.335415
C	5.565194	4.658420	3.700099
H	5.629550	3.846373	4.420580
C	5.313443	5.953243	4.155495
H	5.172865	6.141152	5.214498
H	5.936340	3.391606	1.985845
H	2.718247	7.376571	6.879255
C	0.863941	7.003010	5.849157
N	4.167968	8.427471	4.875624
H	0.384599	6.586606	6.732115
C	4.812410	8.961202	6.018099
C	6.202872	8.813044	6.171988
H	6.771040	8.269150	5.424940
C	6.849603	9.374128	7.273973
H	7.924727	9.248494	7.378120
C	6.129554	10.087223	8.238960
C	4.748190	10.247701	8.076542
H	4.175823	10.816834	8.805455
C	4.091579	9.702417	6.972865
H	3.024975	9.854231	6.845788
H	6.637052	10.519851	9.096987
C	2.181842	7.451752	5.939270
C	2.821124	7.995634	4.809437

3-Me (-8209.4, -7949.5)

H	6.445870	2.352719	2.535949
H	6.628653	2.979801	0.884753
N	4.930921	8.311792	3.700084
H	5.035782	2.494329	1.477682
C	5.320537	9.528170	3.089412
C	4.543855	10.686533	3.264453
H	3.632052	10.638873	3.850447
C	4.951349	11.897781	2.705289
H	4.333504	12.780836	2.858534
C	6.132081	12.002757	1.953769
C	6.907005	10.841329	1.802348
H	7.842857	10.890670	1.248317
C	6.522555	9.625042	2.365703
H	7.157423	8.752296	2.252913
C	6.545982	13.311298	1.317205
H	6.180446	14.167920	1.894030
H	6.138545	13.402792	0.300441
H	7.636261	13.389129	1.239834
C	5.227905	7.013202	3.221327
C	5.358646	6.759174	1.844086
H	5.253570	7.571238	1.132171
C	5.620756	5.467167	1.390066
H	5.722561	5.297980	0.319458
C	5.736665	4.382838	2.275365
C	5.579914	4.647659	3.644457
H	5.658807	3.831169	4.360113
C	5.330987	5.936030	4.118221
H	5.207811	6.108932	5.182173
C	5.979151	2.978335	1.767370
H	-1.539497	6.228325	3.621541
H	-1.961374	7.343735	4.927679
N	4.187900	8.401264	4.884791
H	-1.439719	5.699664	5.313939
C	4.847576	8.926431	6.022100
C	6.239719	8.790497	6.156587
H	6.804261	8.261112	5.396190
C	6.898570	9.349831	7.252100
H	7.977856	9.232878	7.331239
C	6.205690	10.054693	8.247946
C	4.817155	10.198516	8.090649
H	4.250023	10.762305	8.829500
C	4.143994	9.658039	6.996071
H	3.074836	9.809825	6.890204
C	6.920249	10.626224	9.452709
H	7.981138	10.798010	9.241390
H	6.861796	9.940604	10.309765
H	6.474127	11.577004	9.766338
C	2.841409	7.967123	4.837329
C	2.218906	7.408260	5.968255
H	2.768100	7.322146	6.900163
C	0.902821	6.954329	5.893168
H	0.444486	6.524352	6.782190
C	0.167841	7.015477	4.697792
C	0.812790	7.545875	3.570015
H	0.280607	7.593556	2.621652
C	2.124480	8.017547	3.629612
H	2.600586	8.411483	2.737876
C	-1.267890	6.542718	4.635084

3-OMe (-8752.34, -8484.6)

C	0.265705	7.126551	4.508876
C	0.953079	7.638049	3.396324
N	5.091267	8.208830	3.694238
H	0.438343	7.698030	2.440920
C	5.530373	9.379216	3.028681
C	4.805986	10.574878	3.139046
H	3.890247	10.596384	3.720031
C	5.255610	11.749867	2.526496
H	4.668289	12.654416	2.638902
C	6.442629	11.743319	1.782741
C	7.181215	10.552557	1.681587
H	8.113339	10.557064	1.122652
C	6.740397	9.391307	2.305394
H	7.336576	8.487553	2.234763
H	6.158868	14.414498	2.265736
C	2.270522	8.064707	3.514739
H	2.789866	8.449330	2.643528
H	-1.852039	6.897906	6.222454
C	5.329912	6.878063	3.268650
C	5.434059	6.551405	1.908932
H	5.349741	7.330141	1.157917
C	5.646564	5.230232	1.500363
H	5.727954	5.018210	0.440049
C	5.727541	4.205584	2.453549
C	5.591777	4.522754	3.814933

H	5.643689	3.723550	4.549722
C	5.399893	5.839005	4.217619
H	5.289702	6.066664	5.272566
H	6.196783	1.425780	0.759586
H	2.769429	7.345662	6.804271
C	0.929756	7.033363	5.739934
N	4.303060	8.377874	4.839634
H	0.434954	6.626249	6.614784
C	4.943404	8.891730	5.993643
C	6.328564	8.705981	6.174435
H	6.896551	8.150349	5.436054
C	6.978520	9.242745	7.279835
H	8.047487	9.098431	7.413145
C	6.265177	9.974852	8.242139
C	4.889111	10.176437	8.065856
H	4.310346	10.751636	8.780137
C	4.241457	9.649777	6.942968
H	3.180365	9.833768	6.810546
H	5.864185	12.130819	9.869655
C	2.261797	7.447152	5.850580
C	2.944153	7.985615	4.749818
O	7.002577	10.454575	9.309037
C	6.303531	11.224376	10.306261
H	5.515406	10.628314	10.784823
H	7.055877	11.500926	11.046727
O	5.928087	2.869819	2.159745
C	6.045905	2.506425	0.770188
H	5.131177	2.757780	0.217749
H	6.905718	3.004369	0.303058
O	-1.043393	6.741060	4.287678
C	-1.766284	6.176653	5.399149
H	-2.759320	5.938306	5.014748
H	-1.280505	5.261388	5.761674
O	6.971098	12.842201	1.130552
C	6.240761	14.081172	1.222918
H	6.818246	14.807807	0.649073
H	5.236945	13.981285	0.789753

3-Ph (-12819.5, -12437.2)

C	0.190319	6.993211	4.751831
C	0.834150	7.515035	3.613469
N	4.950442	8.272682	3.713608
H	0.307045	7.542391	2.663753
C	5.339860	9.489274	3.106757
C	4.562534	10.647102	3.286121
H	3.644170	10.595353	3.861181
C	4.964654	11.856859	2.728336
H	4.330539	12.729219	2.860856
C	6.147232	11.964661	1.971199
C	6.921954	10.798188	1.813497
H	7.864373	10.849016	1.274786
C	6.538519	9.584945	2.376795
H	7.175212	8.713398	2.266004
H	5.820142	14.469039	3.001486
C	2.146362	7.976530	3.663256
H	2.620064	8.354955	2.763827
H	-0.909114	4.877122	6.079521
C	5.226467	6.976618	3.221649
C	5.351236	6.736004	1.841072
H	5.244114	7.554754	1.137377
C	5.589962	5.448025	1.371898
H	5.658737	5.287297	0.299330
C	5.689133	4.348368	2.247272
C	5.535068	4.602978	3.623632
H	5.619839	3.784604	4.333511
C	5.310408	5.888085	4.108083
H	5.198697	6.052285	5.174506
H	7.248478	3.601093	0.139030
H	2.798231	7.322787	6.942771
C	0.934401	6.941001	5.946832
N	4.216601	8.362082	4.904980
H	0.474231	6.548301	6.849503
C	4.889060	8.884042	6.034463
C	6.279980	8.723614	6.163402
H	6.829866	8.167820	5.411202
C	6.952814	9.272132	7.251149
H	8.023581	9.109515	7.339095
C	6.274547	9.995264	8.251236
C	4.883543	10.160503	8.098284
H	4.330730	10.751338	8.823772
C	4.200425	9.629113	7.008734
H	3.134976	9.804326	6.902503
H	8.789380	11.053059	8.307472
C	2.250181	7.389949	6.008966
C	2.869732	7.932431	4.868303
C	6.994703	10.567624	9.412523
C	6.387465	10.630069	10.682954
C	7.065092	11.169174	11.778560
C	8.368735	11.656620	11.632478
C	8.985868	11.600992	10.377594
C	8.307068	11.064686	9.281378
H	5.385623	10.230643	10.817525
H	6.577980	11.199284	12.750619
H	8.896995	12.074917	12.485724
H	9.995254	11.985352	10.249454
C	5.932681	2.978647	1.738296
C	5.342361	1.858341	2.357085
C	5.572456	0.567368	1.877146
C	6.396719	0.363676	0.764577
C	6.988919	1.466107	0.137971
C	6.760860	2.756874	0.619679
H	4.678111	2.003222	3.205051
H	5.098802	-0.280613	2.366739
H	6.574877	-0.641465	0.390325
H	7.638168	1.319923	-0.722368
C	-1.209166	6.508282	4.691438
C	-2.160750	7.141868	3.867331
C	-3.478962	6.684569	3.807295
C	-3.879855	5.583100	4.571905
C	-2.947040	4.943815	5.396370
C	-1.628328	5.399964	5.454474
H	-1.870214	8.013678	3.286912
H	-4.196916	7.195140	3.169407
H	-4.906226	5.227347	4.525884
H	-3.244463	4.081270	5.988461
C	6.565248	13.254569	1.374372
C	7.231075	13.298370	0.132872
C	7.624562	14.514338	-0.429945
C	7.359351	15.718107	0.232795
C	6.698285	15.691489	1.466036
C	6.307990	14.475355	2.030342
H	7.419645	12.373764	-0.406475
H	8.130083	14.522691	-1.392944
H	7.664099	16.664930	-0.206149
H	6.494793	16.619726	1.995209

3-Br (-6535.7, -6368.4)

C	0.190903	7.055837	4.677719
C	0.805668	7.566937	3.534424
N	4.924786	8.316653	3.701255
H	0.269186	7.611401	2.591997
C	5.326913	9.529503	3.091512
C	4.548261	10.689286	3.252401
H	3.625513	10.648168	3.820962
C	4.958071	11.901437	2.696170
H	4.348691	12.790245	2.825237
C	6.149265	11.956131	1.971905
C	6.944005	10.819717	1.811959
H	7.880300	10.873231	1.265560
C	6.538562	9.612760	2.381448
H	7.170104	8.736908	2.277477
Br	6.716699	13.633528	1.192013

C	2.119862	8.029381	3.610082
H	2.599834	8.420952	2.719766
Br	-1.635588	6.424963	4.578661
C	5.218736	7.016397	3.225300
C	5.349369	6.766340	1.846999
H	5.241624	7.576814	1.134087
C	5.610987	5.477457	1.382776
H	5.711372	5.295331	0.317500
C	5.718505	4.427106	2.295860
C	5.561976	4.648434	3.664496
H	5.636268	3.826122	4.369016
C	5.314439	5.941415	4.126771
H	5.186324	6.112949	5.190098
Br	6.074911	2.637786	1.651453
H	2.738545	7.353355	6.895884
C	0.879221	6.983249	5.890015
N	4.172923	8.412041	4.880190
H	0.403281	6.564138	6.770915
C	4.820993	8.954321	6.016274
C	6.211569	8.809883	6.167382
H	6.782983	8.260443	5.426937
C	6.869250	9.379401	7.258123
H	7.942669	9.260802	7.365976
C	6.135072	10.093593	8.205570
C	4.756335	10.261439	8.066618
H	4.194024	10.837102	8.795030
C	4.104156	9.702794	6.967507
H	3.036966	9.856101	6.848112
Br	7.041654	10.876592	9.724968
C	2.197485	7.433522	5.959033
C	2.825895	7.980492	4.825185

3-CF$_3$ (-8320.0, -8120.5)

F	6.627470	2.239771	2.672198
F	6.649610	2.993097	0.600049
N	4.925503	8.310348	3.698743
F	4.755045	2.360431	1.523398
C	5.332860	9.524050	3.098576
C	4.564641	10.687385	3.280464
H	3.647150	10.646981	3.856666
C	4.982294	11.895526	2.730520
H	4.378613	12.785540	2.875562
C	6.172167	11.963317	1.995707
C	6.947183	10.807874	1.824185
H	7.882961	10.854918	1.276119
C	6.540063	9.599927	2.379302
H	7.162862	8.719654	2.266034
C	6.598453	13.253059	1.353552
F	6.098904	14.355173	1.995459
F	6.168249	13.343956	0.041923
F	7.962724	13.395439	1.313278
C	5.213452	7.012043	3.219415
C	5.348487	6.769988	1.840155
H	5.244554	7.584175	1.131701
C	5.606779	5.483688	1.378606
H	5.710241	5.309974	0.312276
C	5.717240	4.417033	2.280618
C	5.550115	4.649814	3.651694
H	5.625020	3.828962	4.357838
C	5.301407	5.935675	4.120349
H	5.173340	6.106088	5.183305
C	5.943774	3.020327	1.775261
F	-1.719396	6.437943	3.377342
F	-2.079789	7.427370	5.311700
N	4.179146	8.402852	4.881596
F	-1.395842	5.338418	5.260240
C	4.837796	8.925792	6.018187
C	6.230143	8.777845	6.150446
H	6.792813	8.240567	5.395302
C	6.890390	9.321850	7.247304
H	7.963839	9.192975	7.342634
C	6.174481	10.018503	8.229269
C	4.790558	10.187041	8.088482
H	4.230220	10.746138	8.831127
C	4.126170	9.653690	6.989099
H	3.058604	9.808362	6.879839
C	6.897756	10.641260	9.389735
F	7.337876	11.919824	9.100907
F	8.011997	9.931343	9.758260
F	6.107511	10.754314	10.504347
C	2.834765	7.968222	4.830404
C	2.217508	7.411297	5.966776
H	2.767207	7.324210	6.897321
C	0.906227	6.957532	5.895820
H	0.442491	6.525665	6.777702
C	0.194655	7.030064	4.689021
C	0.814251	7.559245	3.551866
H	0.275765	7.612466	2.611631
C	2.125294	8.023715	3.618689
H	2.600147	8.423831	2.729929
C	-1.231745	6.560007	4.649216

Table S10. Cartesian coordinates and ADF total electronic and Gibbs (in parentheses and in kcal mol^{-1}) of compounds of the potential steps for the formation of **3-Me** from **1-Me** computed at the ZORA-BLYP(D3BJ)/TZ2P level of theory in benzene. R = 4-Me-C_6H_4.

^{3}[Bi(NR$_2$)] (-4150.7, -4031.5)

Bi	3.367523	10.390514	4.458485
H	2.375266	5.660026	-1.337041
H	3.108540	7.072140	-2.120442
N	1.555927	9.729443	3.330261
C	0.271113	10.016131	3.836384
C	0.006400	9.966116	5.218360
H	0.787140	9.626130	5.895587
C	-1.248510	10.319905	5.721525
H	-1.421285	10.267575	6.795057
C	-2.292802	10.714106	4.873713
C	-2.028467	10.749113	3.491168
H	-2.815133	11.058756	2.804526
C	-0.779059	10.415151	2.977805
H	-0.597974	10.469647	1.908187
C	-3.657044	11.083775	5.412553
H	-4.437326	10.427954	5.004626
H	-3.926566	12.112579	5.139568
H	-3.686818	11.005357	6.504112
C	1.695794	9.027530	2.115834
C	2.732552	9.334119	1.213491
H	3.386950	10.177468	1.424435
C	2.910949	8.588337	0.045244
H	3.720927	8.853402	-0.632067
C	2.056771	7.526766	-0.283825
C	1.012660	7.232318	0.613530
H	0.335292	6.408425	0.393126
C	0.832940	7.956093	1.788312
H	0.030411	7.693371	2.471418
C	2.236929	6.727023	-1.555122
H	1.356887	6.810729	-2.206356

^{3}[Bi(NR$_2$)(benzene)] (-5838.0, -5664.7)

Bi	-1.009079822	-0.338408958	0.399763674
H	3.756662385	5.175582939	2.360938872
H	2.978474167	5.830938143	0.908168682
N	1.232117782	-0.147064805	0.286559772
C	2.021771264	-1.281644774	0.017086683
C	1.680621772	-2.543396398	0.542842833
H	0.841365050	-2.619635890	1.231093234
C	2.418589223	-3.683206442	0.212575502
H	2.128994548	-4.642226484	0.638785001
C	3.534586424	-3.613714300	-0.632694906
C	3.882010566	-2.349121465	-1.145380356
H	4.738720481	-2.260296353	-1.812148026
C	3.147366962	-1.208305969	-0.836546670
H	3.427548779	-0.249138154	-1.262473022
C	4.344708085	-4.842846781	-0.981251835
H	5.386113176	-4.741802081	-0.648294490
H	4.368627387	-5.009015010	-2.066286077
H	3.926362350	-5.739140811	-0.511773189
C	1.840510749	1.107117853	0.482891631
C	1.220439693	2.291708322	0.037549169
H	0.301364919	2.223056917	-0.540736411
C	1.782149521	3.542568011	0.306253722
H	1.276390623	4.436992634	-0.053630838
C	2.991071581	3.668299682	1.004461052
C	3.617712738	2.482646130	1.433179233
H	4.554676972	2.543413811	1.985265987
C	3.061503176	1.231063644	1.186772276
H	3.558160696	0.335455542	1.548650338
C	3.610638012	5.019844689	1.283996350
H	4.596424671	5.112648300	0.809225838
C	-4.385937772	-0.263045461	1.063674280
C	-4.401424770	-1.160985022	-0.012201227
C	-4.429807805	-0.677538015	-1.326881214
C	-4.446097354	0.701332547	-1.565817807
C	-4.426594914	1.598416153	-0.491635752
C	-4.394099400	1.117311706	0.822587743
H	-4.391139560	-2.232010735	0.174056422
H	-4.437174348	-1.374628519	-2.161044109
H	-4.465594007	1.075408248	-2.586397271
H	-4.430872663	2.669610725	-0.677462175
H	-4.373573987	1.813621870	1.657094086
H	-4.364653858	-0.637110178	2.084124302

^{3}[Bi(NR$_2$)(benzene)$_2$] (-7528.7, -7299.3)

BI	0.379322457	1.303900103	-0.908230034
H	-5.618635564	-2.073212406	1.830150853
H	-4.904878136	-1.417564174	3.315487439
N	0.054163799	-0.872867705	-0.458851239
C	0.975237732	-1.852395691	-0.845838094
C	1.154764189	-3.043943785	-0.106520953
H	0.523025981	-3.238816854	0.754153411
C	2.157475743	-3.952056710	-0.445836209
H	2.276533426	-4.851751280	0.156247315
C	3.028711086	-3.726906252	-1.523491670
C	2.836128068	-2.550864715	-2.269067388
H	3.479322112	-2.346872817	-3.123994675
C	1.829368327	-1.642752294	-1.951999235
H	1.695075476	-0.751217230	-2.561893567
C	4.122685510	-4.709029737	-1.880941924
H	5.108462390	-4.225849088	-1.883987453
H	3.968929509	-5.132339808	-2.882646393
H	4.156605274	-5.539838557	-1.168362655
C	-1.084345738	-1.220840545	0.300650988
C	-1.443901050	-0.481520642	1.440829440
H	-0.789556642	0.318752717	1.775421205
C	-2.620724643	-0.767174046	2.138614326
H	-2.877169363	-0.171327047	3.012892563
C	-3.469812158	-1.809131935	1.742665837
C	-3.093974907	-2.562427141	0.613052138
H	-3.736942431	-3.373441914	0.274073031
C	-1.931504841	-2.277834739	-0.097196607
H	-1.674419644	-2.856504438	-0.980049471
C	-4.745237048	-2.122514493	2.493269829
H	-4.720056257	-3.135293353	2.916557456
C	-3.236799591	0.868657652	-2.335448090
C	-2.874394663	2.052235258	-2.989169941
C	-2.778682211	3.248255689	-2.268512317
C	-3.046983030	3.259590190	-0.893917073
C	-3.410408777	2.075519536	-0.242797999
C	-3.506113491	0.880138557	-0.962988601
H	-3.297330247	-0.063849881	-2.891220320
H	-2.657567472	2.040805425	-4.054727457
H	-2.492292986	4.167249392	-2.774772564
H	-2.967572663	4.187637461	-0.332329320
H	-3.604484496	2.077472787	0.826650502
H	-3.769909895	-0.040281047	-0.452553122
C	3.919632482	0.737611472	0.836216645
C	3.591078720	1.906252167	1.534207562
C	2.602566580	1.874375813	2.524305029
C	1.944311024	0.673461198	2.815273088
C	2.273396767	-0.492543662	2.116626994
C	3.262394471	-0.462461434	1.128216208
H	4.680775607	0.764079954	0.059937368
H	4.098853625	2.839704559	1.302296025
H	2.342062629	2.782518747	3.063143567
H	1.171245204	0.648430982	3.579876815
H	1.746819260	-1.419616233	2.324568821
H	3.500487564	-1.365139167	0.573536065

[Bi$_2$(NR$_2$)$_4$] (-16614.9, -16092.4)

BI	-1.253886431	-0.039059629	-0.913814777

Bi	1.143886071	0.501384120	0.853047202
N	-1.709636245	-2.246107054	-0.789084248
N	-2.222225227	0.727816382	1.002271308
N	2.947044914	-0.497748266	-0.033111135
N	0.874687669	2.312683969	-0.545663669
C	-2.932408958	-2.601648436	-1.414209132
C	-4.077243592	-1.790326076	-1.293823807
C	-3.022399704	-3.753091324	-2.224661252
C	-5.254305290	-2.101444451	-1.984511497
H	-4.060068229	-0.922006787	-0.638306628
C	-4.205310556	-4.064225483	-2.889624296
H	-2.150958499	-4.394518785	-2.326435720
C	-5.344750395	-3.241783474	-2.792181821
H	-6.120476523	-1.452023001	-1.871634699
H	-4.244820018	-4.958663006	-3.509487940
C	-1.068272614	-3.160454000	0.068366035
C	-1.766139796	-4.212945953	0.697180913
C	0.299185174	-3.013777643	0.387659686
C	-1.140312870	-5.019910560	1.649279793
H	-2.815415867	-4.371165184	0.469309949
C	0.901574950	-3.803390146	1.363718353
H	0.898101163	-2.283918496	-0.143546211
C	0.193040111	-4.817293981	2.030113171
H	-1.719825208	-5.805369434	2.132466857
H	1.948895130	-3.631785467	1.603808631
C	3.912516659	-0.751771357	0.982154210
C	4.397271016	0.298057805	1.785422768
C	4.360923388	-2.057660420	1.257274503
C	5.273228221	0.044508565	2.843689623
H	4.092743753	1.319091241	1.566311060
C	5.250389153	-2.297763504	2.303903584
H	4.005804181	-2.878806991	0.641154460
C	5.717755278	-1.256317037	3.124694005
H	5.627472712	0.876703349	3.449584448
H	5.578528529	-3.317496460	2.497575748
C	3.179099647	-0.955143414	-1.342576852
C	4.488992474	-1.217398970	-1.807289527
C	2.134546409	-1.104212379	-2.271782883
C	4.716963680	-1.610475634	-3.125144222
H	5.330342690	-1.091775527	-1.133873505
C	2.373447935	-1.488131816	-3.587593802
H	1.117965632	-0.881572080	-1.969196870
C	3.669991126	-1.756239629	-4.048387190
H	5.741924390	-1.789436151	-3.447160035
H	1.531290933	-1.566071858	-4.272422383
C	1.611642732	2.250186222	-1.771830124
C	3.013934585	2.209347809	-1.797025743
C	0.916639645	2.152708247	-2.986772433
C	3.695774228	2.017146596	-2.997338191
H	3.563505650	2.285817679	-0.863462692
C	1.605649153	1.965526432	-4.187071420
H	-0.169360728	2.210486201	-2.979410908
C	3.004843749	1.874498972	-4.210815575
H	4.780745454	1.941846953	-2.987780018
H	1.045309812	1.862770433	-5.114377656
C	0.679904671	3.559990085	0.076884643
C	-0.198004680	3.649968768	1.180687836
C	1.286113008	4.751398759	-0.375734825
C	-0.426016187	4.864846795	1.821296313
H	-0.754095859	2.767878851	1.485747731
C	1.033582208	5.965233372	0.269494408
H	1.948109694	4.725486329	-1.235448323
C	0.188239932	6.051912784	1.385965507
H	-1.120856271	4.896100642	2.659127489
H	1.512582229	6.867854517	-0.107686627
C	-3.335676941	1.573981239	0.887676218
C	-4.445983757	1.501074000	1.756076918
C	-3.358310102	2.563315371	-0.121823810
C	-5.527595264	2.371851316	1.602148937
H	-4.459391511	0.757591168	2.547027165
C	-4.452433338	3.410818788	-0.272595805
H	-2.490993553	2.688038676	-0.766745378
C	-5.562933735	3.338237768	0.586064848
H	-6.370042036	2.287531741	2.287518328
H	-4.433459537	4.160946663	-1.061675110
C	-2.064037955	-0.087151855	2.169431952
C	-2.605613949	-1.377257298	2.261358736
C	-1.269243967	0.378175792	3.234045840
C	-2.307128321	-2.196984197	3.349653620
H	-3.232076255	-1.748702307	1.458440829
C	-0.969695404	-0.451043265	4.318643879
H	-0.882201379	1.393015028	3.203373201
C	-1.467849414	-1.760905408	4.385181409
H	-2.704890763	-3.207458047	3.375195939
H	-0.326265881	-0.077694487	5.113230910
C	-0.046662202	7.365025441	2.100872871
H	-1.075732932	7.438633897	2.471796657
H	0.619611416	7.471352217	2.968843222
H	0.139612562	8.217698429	1.438712690
C	-6.726777092	4.295733929	0.446123105
H	-7.644958774	3.869110150	0.865101625
H	-6.532644147	5.239577304	0.975405979
H	-6.914370330	4.545724164	-0.604548231
C	-1.122996826	-2.676623588	5.538458993
H	-1.874104467	-2.607246621	6.337189562
H	-1.085983003	-3.721107110	5.210935359
H	-0.152867507	-2.417427736	5.975771102
C	0.853087509	-5.655348067	3.102632160
H	0.129786039	-6.320099397	3.586524733
H	1.656553089	-6.279948424	2.689131195
H	1.303523439	-5.023120110	3.878515754
C	-6.610579617	-3.572174842	-3.552099813
H	-6.542720381	-3.236881750	-4.596504322
H	-6.794892176	-4.652472452	-3.569571711
H	-7.481929753	-3.082070157	-3.104851548
C	3.925112566	-2.186212873	-5.475715848
H	4.921839390	-1.879430769	-5.812067366
H	3.866112265	-3.278665586	-5.581888266
H	3.186573953	-1.751947681	-6.158767132
C	3.754382604	1.624354492	-5.499346253
H	4.160380901	2.558707409	-5.910120112
H	4.595386782	0.942919836	-5.333447412
H	3.101241419	1.182920324	-6.258865165
C	6.664521360	-1.522323542	4.274612011
H	7.563936428	-0.898173935	4.201083503
H	6.190888082	-1.293394684	5.238335527
H	6.979306330	-2.570505369	4.295380855

$[Bi_2(NR_2)_2]$ (-8360.6, -8106.5)

Bi	-0.821819766	1.239334451	-0.041418631
H	-0.790349182	-5.898271896	0.119623220
H	-2.180310790	-6.156599908	-0.943667208
N	-2.709337578	0.021534629	0.017334466
C	-3.999239879	0.556234456	0.038668988
C	-4.212684936	1.953051410	0.120679942
H	-3.360318687	2.627234394	0.179754441
C	-5.498191061	2.488363051	0.135611178
H	-5.615289036	3.569112477	0.201713391
C	-6.641602548	1.672677586	0.076936293
C	-6.431599233	0.287517371	0.006276187
H	-7.290275379	-0.381635739	-0.033667341
C	-5.151099919	-0.267719340	-0.015232412
H	-5.038271593	-1.345404387	-0.072703008
C	-8.034203337	2.264847654	0.060099376
H	-8.758027955	1.595374571	0.538821536
H	-8.382312583	2.439656889	-0.968190554
H	-8.063688906	3.228165686	0.581837704
C	-2.550252676	-1.398964422	0.007605440
C	-2.407641796	-2.098157897	-1.202719357
H	-2.462134019	-1.546525845	-2.137661685
C	-2.201023367	-3.481727563	-1.202407626
H	-2.094734724	-4.004131225	-2.151267387

C	-2.130631402	-4.206294828	-0.002228511
C	-2.283863262	-3.501133346	1.203313612
H	-2.240901623	-4.039534479	2.148256764
C	-2.485633141	-2.119175715	1.213053696
H	-2.594697451	-1.581064102	2.151072791
C	-1.863256636	-5.694944134	-0.002792820
H	-2.385334837	-6.193557374	0.821182968
N	2.655386889	0.044046597	-0.056545297
Bl	0.771181530	-1.175081478	-0.189397735
H	0.740640645	5.965104565	-0.020585093
C	6.367468385	-0.240335486	0.184014434
H	7.234173413	0.417403032	0.130854770
C	5.096295181	0.316822892	0.038272964
H	4.997384556	1.384543920	-0.128408621
C	7.943459567	-2.212814830	0.509497329
H	8.645105922	-1.506883565	0.968495152
H	8.348804661	-2.480271902	-0.477068958
H	7.932808776	-3.125851399	1.115521781
C	2.499524872	1.463722847	-0.080306553
C	2.341185145	2.151356337	-1.295384554
H	2.144448815	6.215438478	-1.066847015
H	2.380470402	1.589233920	-2.224719559
C	2.136398344	3.534073863	-1.306787319
H	2.020312517	4.047138696	-2.259613722
C	2.081494525	4.271710949	-0.112960361
C	2.249289619	3.579353206	1.097375785
H	2.217304650	4.127210612	2.037272335
C	2.450391466	2.196716400	1.119016970
H	2.572829794	1.669156063	2.061382267
C	1.815048082	5.760428621	-0.126863122
H	2.326601146	6.264494429	0.700276014
C	3.934821125	-0.492669028	0.102508027
C	4.127881496	-1.876372543	0.328467584
H	3.264860652	-2.533972014	0.414602638
C	5.405278709	-2.415416232	0.461321198
H	5.507354140	-3.485387636	0.637043742
C	6.558439871	-1.614761762	0.391914255

$[Bi_4(NR_2)_4]$ (-16783.0, -16267.9)

Bl	-0.396951135	1.803020974	0.277441185
Bl	-1.685228987	-0.968491405	0.018298810
Bl	1.115212568	-1.991440407	0.788252564
Bl	2.087432346	0.377692095	-0.958963072
C	2.434855153	-3.224045787	-1.852959324
C	3.650967505	-2.946684977	-1.185857043
C	2.524239876	-3.561199413	-3.227080525
C	4.873287966	-2.970479876	-1.858282834
H	3.648836017	-2.724800010	-0.122354521
C	3.754188545	-3.581561322	-3.882292283
H	1.624840200	-3.813127621	-3.778754024
C	4.957861263	-3.276334633	-3.223205181
H	5.781034391	-2.744454003	-1.301072280
H	3.776435301	-3.845148305	-4.939063925
H	6.424558702	-4.208705825	-4.522260645
C	-0.009089024	-3.214186877	-1.884688883
C	-0.317926113	-2.237886358	-2.853663145
C	-0.999082905	-4.154523388	-1.555637955
C	-1.575299310	-2.207507955	-3.462959260
H	0.434096234	-1.500960450	-3.127457888
C	-2.256897771	-4.110910340	-2.162459904
H	-0.772970896	-4.906115348	-0.803588464
C	-2.570107327	-3.139898257	-3.126953690
H	-1.791937505	-1.434318032	-4.196307696
H	-3.008415932	-4.845894167	-1.879890065
H	-4.682143146	-2.699478166	-3.034188907
C	3.727911229	0.320932188	1.661670261
C	4.809244297	-0.521477962	1.357897705
C	2.987131682	0.055636944	2.830882336
C	5.131179520	-1.600447187	2.184898427
H	5.377863049	-0.331770115	0.451188273
C	3.328467619	-1.013551940	3.660619686
H	2.127125669	0.672166653	3.072780290
C	4.398221681	-1.869748787	3.350825672
H	5.966642872	-2.244751382	1.917348201
H	2.736919585	-1.204456518	4.553335995
H	4.165664769	-3.954012564	3.875080599
C	3.085111647	2.631102060	1.105203396
C	3.268015559	3.120818487	2.421640548
C	2.647538597	3.565265507	0.137541392
C	2.958072062	4.442481921	2.741710982
H	3.657475886	2.467989512	3.194004143
C	2.330253998	4.880160487	0.475032567
H	2.594222497	3.256828148	-0.902994020
C	2.458215809	5.347541004	1.790507916
H	3.108646835	4.777276450	3.767238774
H	1.979298254	5.551815332	-0.306124392
H	2.843000430	7.227754777	2.801476130
C	-1.245527238	3.357730900	-2.462032455
C	0.129231049	3.639358314	-2.596066274
C	-2.122858988	4.002158891	-3.369612177
C	0.605188854	4.512809814	-3.574178526
H	0.831588493	3.166845164	-1.918735702
H	-3.192303691	3.834581958	-3.289449639
C	-0.260473962	5.142117268	-4.479742266
H	1.676000248	4.702585171	-3.633433115
H	-2.340731149	5.346399225	-5.021377263
H	1.192190190	6.546841398	-5.262015696
C	-2.945644504	1.848416794	-1.554023331
C	-3.813453120	1.743419524	-0.448674689
C	-3.294845443	1.150194553	-2.729545031
C	-4.970094097	0.960536869	-0.506778603
H	-3.569084269	2.285605142	0.460827228
C	-4.466989060	0.399419726	-2.787929314
H	-2.635652045	1.200231578	-3.591183893
C	-5.325561021	0.281359789	-1.680158415
H	-5.600741808	0.876544993	0.374851234
H	-4.711788268	-0.124260587	-3.709387689
H	-7.148966368	-0.351613408	-2.662220561
C	-3.975413512	-1.144881503	2.168973123
C	-4.585446453	-2.058818395	1.272860476
C	-4.828992857	-0.484654900	3.081388984
C	-5.961567714	-2.251343511	1.253339021
H	-3.961403556	-2.630978243	0.589134575
C	-6.211496648	-0.693515553	3.050951461
H	-4.415598246	0.196092098	3.816797147
C	-6.815216921	-1.562190399	2.132009825
H	-6.383947289	-2.956736611	0.539787623
H	-6.834846948	-0.155068125	3.763672089
H	-8.701556754	-1.733874602	1.075423642
C	-1.910320443	-0.112923576	3.033791461
C	-0.825119919	-0.612795525	3.772410186
C	-2.203910979	1.261849794	3.144829119
C	-0.045634725	0.234330486	4.564852759
H	-0.599974922	-1.674797009	3.711224614
C	-1.421040259	2.100600280	3.940090127
H	-3.038383306	1.672661771	2.585964004
C	-0.314270826	1.608438467	4.651599944
H	0.785759082	-0.181227873	5.129169983
H	-1.660270572	3.161268001	3.988641837
H	1.201306241	1.982850140	6.152285093
N	-2.581622858	-0.986154854	2.132427896
N	-1.724184470	2.546764908	-1.425598659
N	3.348673047	1.313228857	0.714039496
N	1.217014530	-3.208443467	-1.158465638
C	-1.632677474	4.864335712	-4.348388354
C	0.578385986	2.537096732	5.442849210
H	1.247981471	3.090549558	4.770762081
H	-0.006955610	3.276171074	6.001592570
C	-8.312208776	-1.779228801	2.100417020
H	-8.584746821	-2.764189913	2.504468802
H	-8.834573173	-1.021733039	2.694511126
C	-6.575378125	-0.564945544	-1.752335002

H	-6.328233688	-1.634630181	-1.765860956
H	-7.219434395	-0.392186296	-0.885756869
C	0.259528709	6.058451077	-5.565992662
H	0.467888757	5.503151627	-6.491789049
H	-0.469924779	6.838554858	-5.812406732
C	2.074249735	6.759420843	2.174571963
H	1.930237215	7.385725816	1.287806271
H	1.136297591	6.775326688	2.747139392
C	4.716169790	-3.066798084	4.218133607
H	5.783194009	-3.311441538	4.184811205
H	4.434567714	-2.889875951	5.261658907
C	-3.945491588	-3.085630359	-3.750036753
H	-3.960709257	-2.431149641	-4.626638404
H	-4.281338735	-4.082191885	-4.059077404
C	6.279314513	-3.277140434	-3.960612684
H	6.334399193	-2.452479557	-4.684588701
H	7.119272148	-3.166565475	-3.266577553

$[Bi(NR_2)_2]^-$ (-8287.0, -8030.3)

Bi	1.665228	9.410389	6.550132
N	2.225273	7.256729	6.383166
H	4.135436	6.317701	0.237812
N	0.779642	9.459038	4.502999
C	3.506287	6.834912	6.797269
C	4.638721	7.661502	6.671514
H	4.540266	8.625935	6.179395
C	5.887221	7.248717	7.147336
H	6.742083	7.912837	7.031146
C	6.066143	5.992758	7.741535
C	4.934691	5.160943	7.851587
H	5.035924	4.179909	8.313839
C	3.683559	5.566942	7.399605
H	2.824523	4.911140	7.509920
C	7.418596	5.534102	8.240656
H	7.753531	4.632676	7.710694
H	7.384990	5.284933	9.309327
H	8.177733	6.310055	8.098604
C	1.390771	6.370922	5.670693
C	1.926202	5.443554	4.751686
H	3.001486	5.390898	4.617577
C	1.089341	4.634378	3.990487
H	1.531851	3.943588	3.274755
C	-0.309460	4.718589	4.093120
C	-0.837997	5.632956	5.016489
H	-1.917410	5.716115	5.130689
C	-0.009457	6.436653	5.799658
H	-0.442629	7.128241	6.518182
C	-1.207168	3.891775	3.200473
H	-2.212341	3.793369	3.624517
H	-0.800823	2.886041	3.042379
H	-1.311363	4.359014	2.210516
C	-0.462619	10.097168	4.300304
C	-1.474534	10.082329	5.278552
H	-1.325563	9.505039	6.187611
C	-2.672584	10.777425	5.084551
H	-3.434709	10.742770	5.861329
C	-2.922688	11.491080	3.905215
C	-1.915246	11.489719	2.920536
H	-2.073846	12.038969	1.993444
C	-0.712125	10.817577	3.108423
H	0.054119	10.844388	2.338645
C	-4.223115	12.231866	3.684139
H	-4.760956	11.840464	2.810608
H	-4.046289	13.299777	3.500664
H	-4.882661	12.143399	4.553520
C	1.348204	8.686533	3.470045
C	2.745330	8.587813	3.326200
H	3.387324	9.177342	3.976149
C	3.307495	7.744054	2.368767
H	4.391477	7.680684	2.290502
C	2.506695	6.983073	1.503816
C	1.113213	7.108096	1.630852
H	0.463066	6.522925	0.982625
C	0.539667	7.931597	2.594053
H	-0.539297	7.972948	2.700382
C	3.116203	6.021248	0.509019
H	2.519859	5.961044	-0.408504
H	3.170063	5.006364	0.929110

$[Bi_2(NR_2)_3]^-$ (-12484.2, -12091.9)

Bi	-0.888471	-0.796771	-0.402530
Bi	1.034062	-1.272306	1.952037
N	-2.376442	-2.324404	0.444635
N	-1.552943	1.117158	0.590149
N	2.593048	-1.710722	0.322774
H	2.771001	-7.964843	0.115638
C	-3.763195	-2.139901	0.332262
C	-4.314162	-0.883549	0.003398
C	-4.663130	-3.223930	0.480704
C	-5.689846	-0.725830	-0.184728
H	-3.671697	-0.014361	-0.084138
C	-6.032973	-3.045676	0.307027
H	-4.273486	-4.208998	0.720221
C	-6.582062	-1.795024	-0.031945
H	-6.072154	0.260943	-0.440737
H	-6.692836	-3.904586	0.424268
C	-1.842756	-3.300111	1.308939
C	-2.305259	-3.475809	2.632611
C	-0.723366	-4.056133	0.903847
C	-1.654730	-4.347767	3.503267
H	-3.166294	-2.908470	2.974604
C	-0.072789	-4.921439	1.788801
H	-0.367305	-3.965688	-0.118734
C	-0.522113	-5.083241	3.104430
H	-2.022381	-4.445833	4.523744
H	0.804264	-5.462963	1.444990
C	2.901211	-3.100288	0.268110
C	3.679656	-3.660828	1.295907
C	2.367257	-3.970380	-0.703598
C	3.908574	-5.037605	1.354120
H	4.092215	-3.002739	2.057362
C	2.615335	-5.340848	-0.647114
H	1.735291	-3.571736	-1.491368
C	3.387131	-5.905365	0.383213
H	4.505261	-5.442728	2.169411
H	2.178134	-5.989510	-1.404399
C	2.621997	-0.898160	-0.808745
C	3.127449	-1.309514	-2.070640
C	2.155807	0.442629	-0.725189
C	3.075388	-0.463670	-3.175645
H	3.560816	-2.296669	-2.181330
C	2.108170	1.273875	-1.846945
H	1.878477	0.850700	0.244018
C	2.539381	0.835652	-3.105218
H	3.464415	-0.827260	-4.125932
H	1.743511	2.292230	-1.726872
C	-3.986195	5.081717	-2.828761
H	-5.077708	4.974710	-2.840987
H	-3.765345	6.100595	-2.481693
H	-3.623341	4.995855	-3.858309
C	-1.052661	1.504965	6.326193
H	-1.276373	0.551595	6.815797
H	-0.023015	1.784761	6.585660
H	-1.712069	2.269561	6.756983
C	0.175818	-6.023883	4.061515
H	0.278625	-5.575264	5.056925
H	-0.389081	-6.958248	4.184594
H	1.175199	-6.284707	3.698198
C	-8.075301	-1.616668	-0.201554
H	-8.502318	-2.403074	-0.836479
H	-8.595887	-1.664597	0.765044
H	-8.309141	-0.648415	-0.656729

C	2.443610	1.716311	-4.330800
H	3.357606	1.664322	-4.934524
H	1.610684	1.407685	-4.978118
H	2.276569	2.762732	-4.054206
C	-2.119437	2.125026	-0.214776
C	-3.271699	2.834766	0.189907
C	-1.592495	2.401553	-1.491673
C	-3.857967	3.778021	-0.650972
H	-3.707362	2.627664	1.163147
C	-2.203381	3.334352	-2.333273
H	-0.690646	1.890509	-1.820421
C	-3.342812	4.046816	-1.931949
H	-4.749026	4.304951	-0.312560
H	-1.774015	3.520934	-3.316159
C	-1.529378	1.237247	1.989659
C	-1.785377	0.126263	2.821147
C	-1.159427	2.450444	2.614202
C	-1.621484	0.211366	4.210442
H	-2.152619	-0.792288	2.378491
C	-1.018628	2.523549	3.996650
H	-0.961408	3.323801	1.999074
C	-1.232527	1.405104	4.827533
H	-1.818752	-0.671141	4.816379
H	-0.714577	3.468523	4.444787
C	3.651831	-7.393875	0.431315
H	4.476176	-7.670869	-0.240233
H	3.926962	-7.716454	1.441002

$[Bi(NR_2)_3]_2$ (-24866.4, -24061.2)

Bl	2.250386	0.608840	-0.451638
N	4.133554	1.511572	0.360547
C	4.522464	4.398399	-1.943561
H	3.871558	5.127493	-2.423482
C	3.960405	3.440714	-1.101175
H	2.889500	3.465863	-0.906544
C	6.513255	5.487772	-3.090501
H	5.968740	6.438271	-3.048033
H	6.481080	5.141251	-4.133388
H	7.562108	5.683847	-2.842659
C	4.835592	0.811046	1.387876
C	5.812075	-0.165291	1.127106
N	2.969044	-1.432167	-1.066343
H	6.113202	-0.365918	0.107314
C	6.363859	-0.906935	2.172692
H	7.099699	-1.675931	1.944241
C	5.964750	-0.703925	3.503384
C	5.007593	0.290248	3.756817
H	4.674782	0.466137	4.778163
C	4.456116	1.041718	2.719069
H	3.697130	1.790080	2.922418
C	6.556758	-1.525297	4.626961
H	5.889053	-1.550230	5.494548
N	1.464425	0.193138	1.638672
H	7.516302	-1.105546	4.959337
H	6.745787	-2.556394	4.307614
C	2.039831	-2.440381	-1.368719
C	0.908948	-2.648639	-0.555537
H	0.793899	-2.080474	0.359232
C	-0.025914	-3.635225	-0.864073
H	-0.858991	-3.793369	-0.186701
C	0.103483	-4.447410	-1.996975
C	1.227192	-4.232659	-2.815153
H	1.361430	-4.838507	-3.710520
C	4.759987	2.473733	-0.447506
C	2.176485	-3.257477	-2.515267
H	3.030173	-3.113525	-3.170686
C	-0.925392	-5.505458	-2.326863
H	-1.459904	-5.260941	-3.253842
H	-1.669869	-5.590656	-1.528569
H	-0.459993	-6.489288	-2.466533
C	4.300149	-1.523334	-1.530816
C	5.106491	-2.624800	-1.178100
H	4.667388	-3.430765	-0.596668
C	6.449757	-2.663959	-1.539605
C	6.156200	2.556270	-0.637580
H	7.054393	-3.519944	-1.244362
C	7.051757	-1.605116	-2.247636
C	6.241850	-0.522086	-2.613928
H	6.670993	0.308865	-3.169193
C	4.883896	-0.490499	-2.284028
H	4.277353	0.349781	-2.612488
C	8.528124	-1.631234	-2.576453
H	8.775475	-0.898580	-3.351555
H	8.842249	-2.621465	-2.926710
H	9.132741	-1.393918	-1.690189
H	6.810465	1.854069	-0.133920
C	0.967061	1.343983	2.283343
C	0.365228	2.387808	1.544553
H	0.193269	2.281595	0.475503
C	-0.070755	3.556998	2.167974
H	-0.533850	4.332221	1.563030
C	0.024264	3.729571	3.553224
C	0.621764	2.692829	4.289610
H	0.721569	2.794713	5.369043
C	1.095673	1.534800	3.678088
H	1.570944	0.763212	4.274648
C	6.705914	3.534978	-1.467647
C	-0.574242	4.937177	4.235490
H	-0.021403	5.201232	5.143986
H	-1.613513	4.730861	4.526341
H	-0.584225	5.808685	3.571827
C	1.563486	-1.035213	2.329151
C	0.494156	-1.510490	3.117810
H	-0.368658	-0.872675	3.288414
C	0.535447	-2.779557	3.692502
H	-0.309070	-3.117882	4.289865
C	1.634119	-3.632619	3.499891
H	7.787636	3.569092	-1.589549
C	2.710664	-3.140182	2.746848
H	3.591624	-3.762694	2.601181
C	2.690040	-1.864933	2.185629
H	3.542045	-1.519048	1.615171
C	1.641459	-5.037832	4.059127
H	2.659741	-5.371657	4.287207
H	1.220440	-5.750253	3.335341
H	1.042670	-5.108524	4.973718
C	5.909181	4.464131	-2.154362
Bl	-1.963355	-0.272721	0.423874
N	-3.840323	-1.433232	0.849425
C	-2.258157	-4.623339	1.905218
H	-1.364639	-4.917901	2.452363
C	-2.539029	-3.267078	1.762240
H	-1.877736	-2.545615	2.233992
C	-2.771422	-7.076036	1.480182
H	-2.334415	-7.314218	2.457011
H	-2.039169	-7.374164	0.716347
H	-3.661772	-7.698990	1.343124
C	-5.096857	-0.870408	0.462502
C	-5.690702	-1.088423	-0.794244
N	-1.873741	-0.273552	-1.815569
H	-5.211389	-1.744201	-1.509662
C	-6.870432	-0.429937	-1.142138
H	-7.301719	-0.602497	-2.126785
C	-7.488398	0.476201	-0.265162
C	-6.892495	0.684419	0.987236
H	-7.338398	1.390373	1.685120
C	-5.722574	0.015675	1.350692
H	-5.261317	0.201953	2.315069
C	-8.759973	1.194404	-0.659320
H	-8.914138	2.092205	-0.051616
N	-3.049781	1.672954	0.670196
H	-9.636918	0.546646	-0.522433

H	-8.737276	1.491697	-1.714101
C	-0.762606	0.347467	-2.426526
C	-0.501507	1.725703	-2.270298
H	-1.192562	2.338253	-1.702077
C	0.604464	2.316112	-2.891679
H	0.769777	3.384745	-2.768218
C	1.490989	1.565348	-3.685702
C	1.233330	0.187606	-3.820630
H	1.917722	-0.428556	-4.399802
C	-3.667911	-2.815345	1.038849
C	0.135647	-0.412871	-3.209781
H	-0.032128	-1.479703	-3.315497
C	2.661165	2.211573	-4.391824
H	3.314822	1.456587	-4.839886
H	3.260198	2.819745	-3.706451
H	2.315029	2.872487	-5.197411
C	-2.656144	-1.147671	-2.611662
C	-3.221482	-0.669968	-3.812145
H	-3.023418	0.354444	-4.113730
C	-4.034158	-1.490594	-4.590025
C	-4.547407	-3.801780	0.542596
H	-4.462429	-1.095667	-5.510162
C	-4.327765	-2.811252	-4.202030
C	-3.753769	-3.281529	-3.013741
H	-3.951396	-4.298854	-2.684429
C	-2.922660	-2.471004	-2.237444
H	-2.482645	-2.873202	-1.335449
C	-5.249137	-3.679438	-5.030329
H	-5.147588	-4.735953	-4.760971
H	-5.039928	-3.576334	-6.101618
H	-6.300126	-3.397818	-4.877052
H	-5.445063	-3.506931	0.011834
C	-3.314020	2.112089	1.978291
C	-2.619535	1.588525	3.086833
H	-1.770143	0.926938	2.940356
C	-2.945392	1.957989	4.390981
H	-2.371317	1.535813	5.213191
C	-3.958917	2.888134	4.657519
C	-4.644937	3.421511	3.552252
H	-5.447597	4.139006	3.717895
C	-4.342231	3.045054	2.246097
H	-4.915964	3.451170	1.419696
C	-4.263293	-5.158983	0.711448
C	-4.272363	3.334557	6.068762
H	-5.347124	3.502956	6.205069
H	-3.763571	4.278523	6.311771
H	-3.947708	2.589169	6.802995
C	-3.342042	2.501352	-0.438524
C	-2.889456	3.835617	-0.486821
H	-2.372050	4.247553	0.373736
C	-3.095271	4.617287	-1.622230
H	-2.731196	5.643371	-1.634890
C	-3.745722	4.099674	-2.756351
H	-4.959444	-5.891296	0.305217
C	-4.214216	2.779270	-2.690742
H	-4.743999	2.355709	-3.542136
C	-4.029530	1.993987	-1.552442
H	-4.419846	0.985011	-1.523792
C	-3.911237	4.928340	-4.011002
H	-4.822158	4.651984	-4.553664
H	-3.064660	4.777544	-4.695702
H	-3.958908	5.998349	-3.780624
C	-3.106119	-5.605120	1.368818

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Conflicts of Interest

The authors declare no conflicts of interest

Acknowledgements

We thank Hannah Dengel, Benedikt Ritschel, and Dr. Conor Pranckevicius for their contributions. Financial support by the FCI, the DFG, the University of Würzburg, the Cusanuswerk, the Netherlands Organisation of Scientific Research (NWO), and the Spanish Government (PID2019-106830GB-I100 and MDM-2017-0767) is gratefully acknowledged. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No946184). C. L. thanks Prof. Holger Braunschweig for continuous support.