Supporting Information

Jonas, Bresien, Alexander Hinz, Axel Schulz, and Alexander Villinger*

This file includes:

1. General Information

All manipulations were carried out under oxygen- and moisture free conditions using standard Schlenk and Drybox techniques.

All solvents were obtained from commercial sources. THF was dried over Na/benzophenone and freshly distilled prior to use. Benzene and toluene were dried over Na/benzophenone/tetraglyme ($Me(OCH_2CH_2)_4OMe$) and freshly distilled. $[TerNAs]_2$,[1] $[TerNSbCl]_2$, $[TerNBiCl]_2$[2] were prepared according to the published procedures and C_2Ph_2, C_2H_2, Mg were commercially obtained and used as received.

NMR: $^{13}C\{^1H\}$ and ^1H NMR spectra were recorded on BRUKER spectrometers AVANCE 250, AVANCE 300 and AVANCE 500, respectively. The ^1H and ^{13}C NMR chemical shifts were referenced to the solvent signals.[3] CD_2Cl_2 was dried over P_4O_{10} and was degassed prior to use. C_6D_6 was dried over Na and freshly distilled prior to use.

CHN analysis: Analysator Flash EA 1112 from Thermo Quest.

IR: Nicolet 380 FT-IR with a Smart Orbit ATR module.

RAMAN: LabRAM HR 800 Horiba Jobin YVON equipped with a High Stability BX40 Microscope (Focus 1 μm) or an Olympus Mplan 50xNA 0.70 lens, the laser is variable and was chosen prior to the measurement.

DSC: DSC 823e from Mettler-Toledo (Heating rate 5 °C/min).

MS: Finnigan MAT 95-XP from Thermo Electron was used.

2. Structure Elucidation

X-Ray quality crystals were selected in Fomblin YR-1800 perfluoroether (Alfa Aesar) at ambient temperature. The samples were cooled to 123(2) K during measurement. The data were collected on a Bruker-Nonius Apex X8 or Bruker Kappa Apex II diffractometer using Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods (SHELXS-2013)[4] and refined by full matrix least squares procedures (SHELXL-2013).[5] Semi-empirical absorption corrections were applied (SADABS).[6] All non-hydrogen atoms were refined anisotropically, hydrogen atoms were included in the refinement at calculated positions using a riding model.

The phenyl group at As in **4As** was found to be disordered and was split in two parts, which were restrained to adopt similar structures using the SAME command. Additionally, the ADPs of corresponding atoms in A and B part were made equal using EADP.

In **4Sb**·C_6H_6, the co-crystallized benzene molecule was found to be heavily disordered. The disorder was modelled by splitting the solvent molecule in two parts, which were fixed at an idealized geometry using AFIX 66. Additionally, the ADPs of corresponding atoms in A and B part were made equal using EADP.

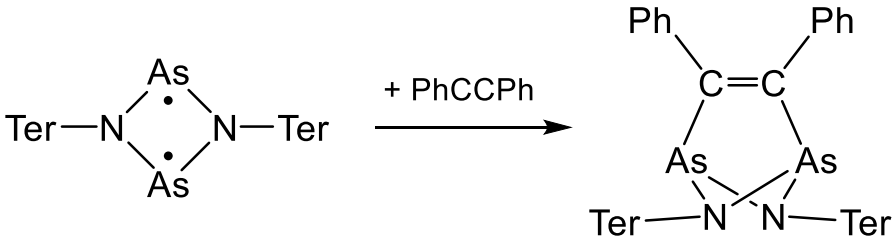
The crystal structure of **4Bi**·C_6H_6 exhibited one disordered phenyl group at Bi, which was split in two parts. Both parts were fixed at an idealized geometry using AFIX 66. Additionally, the ADPs of corresponding atoms in A and B part were made equal using EADP.

Table S1: Crystallographic details of **4As**, **4Sb**·C_6H_6, **4Bi**·C_6H_6 and **4BiH**.

Compound	**4As**	**4Sb**·C_6H_6	**4Bi**·C_6H_6	**4BiH**
Chem. Formula	$C_{62}H_{60}As_2N_2$	$C_{62}H_{60}N_2Sb_2 \cdot C_6H_6$	$C_{62}H_{60}Bi_2N_2 \cdot C_6H_6$	$C_{50}H_{52}Bi_2N_2$
Formula weight [g/mol]	982.96	1154.73	1329.18	1098.89
Colour	red	yellow	orange	orange
Crystal system	monoclinic	triclinic	triclinic	Monoclinic
Space group	*C*2/*c*	$P\bar{1}$	$P\bar{1}$	$P2_1/n$
a [Å]	18.1246(3)	12.0121(9)	12.0269(8)	12.7008(5)
b [Å]	11.4075(2)	12.3543(9)	12.4083(8)	21.1286(9)
c [Å]	23.8632(4)	19.479(1)	19.558(1)	16.6191(7)
α [°]	90	98.965(4)	98.920(2)	90
β [°]	99.146(1)	101.551(4)	101.713(3)	110.843(2)
γ [°]	90	90.870(4)	90.533(2)	90
V [Å^3]	4871.1(1)	2794.3(4)	2820.8(3)	4167.9(3)
Z	4	2	2	4
$\rho_{calc.}$ [g/cm^3]	1.340	1.372	1.565	1.751
μ [mm^{-1}]	1.415	1.009	6.272	8.469
T [K]	173(2)	173(2)	173(2)	173(2)
Measured reflections	44970	84759	91771	86216
Independent reflections	8809	17736	20308	15080
Reflections with $I > 2\sigma(I)$	6399	12399	15876	11970
R_{int}	0.0496	0.0761	0.0445	0.0563
F(000)	2048	1180	1308	2128
$R_1(R[F^2>2\sigma(F^2)])$	0.0366	0.0387	0.0262	0.0312
$wR_2(F^2)$	0.0912	0.0837	0.0531	0.0627
GooF	1.009	1.011	1.022	1.014
No. of Parameters	323	656	656	499
CCDC #	1812918	1812919	1812920	1812921

3. Syntheses

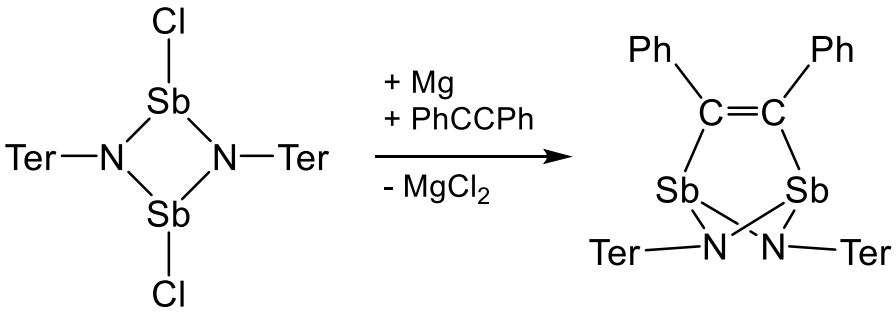
3.1. [(TerNAsCPh)$_2$] (4As)



To a stirred solution of [As(μ-NTer)]$_2$ (220 mg, 0.274 mmol) in 5 ml of toluene a solution of tolan (55 mg, 0.310 mmol) in 1.5 ml of toluene was added dropwise at ambient temperature. The initially purple solution immediately turned yellow. After completion of the addition the solution was concentrated to incipient crystallisation and left undisturbed overnight, after which yellow crystals deposited. The supernatant was removed via syringe and the crystals were dried in vacuo (241 mg, 0.245 mmol, 89%).

Mp. 185 °C (dec.). **EA** found (calc.): C 74.92 (75.75), H 6.18 (6.15), N 3.16 (2.85). **^{1}H NMR** (298 K, CD_2Cl_2, 250.1 MHz): 1.89 (s, 24 H, *o*-CH_3), 2.30 (s, 12 H, *p*-CH_3), 6.53-6.64 (m, 6 H), 6.97 (s, 8 H, *m*-CH_{Mes}), 7.15-7.25 (m, 6 H), 7.51-7.59 (m, 4 H). **^{13}C NMR** (298 K, CD_2Cl_2, 62.9 MHz): 21.31 (*C*H$_3$), 21.61 (*C*H$_3$), 117.67 (s, *C*H), 123.64 (s), 127.26 (s), 127.43 (s, *C*H), 127.86 (s, *C*H), 128.44 (s, *C*H), 128.76 (s, *C*H), 128.84 (s, *C*H), 129.06 (s, *C*H), 130.54 (s, *C*H), 131.94 (s, *C*H), 137.15 (s), 137.30 (s), 137.61 (s), 137.69 (s), 141.81 (s), 176.48 (s, As-*C*=*C*-As). **IR** (ATR, cm^{-1}): 538 (m), 547 (m), 570 (s), 588 (m), 607 (m), 624 (m), 644 (m), 667 (s), 675 (s), 694 (vs), 715 (s), 725 (s), 750 (s), 775 (s), 790 (s), 802 (m), 844 (vs), 869 (s), 906 (w), 921 (w), 954 (w), 981 (w), 1004 (m), 1027 (m), 1085 (m), 1151 (w), 1226 (vs), 1247 (m), 1268 (w), 1322 (w), 1375 (s), 1398 (vs), 1434 (m), 1454 (m), 1479 (m), 1579 (m), 1610 (w), 1646 (w), 2726 (w), 2848 (w), 2908 (m), 2937 (m), 2960 (w), 3014 (w), 3052 (w), 3074 (w). **Raman** (784 nm): 215 (6), 228 (21), 243 (47), 260 (29), 270 (12), 284 (6), 312 (5), 342 (97), 361 (3), 408 (4), 417 (14), 425 (34), 460 (19), 483 (2), 500 (2), 515 (14), 525 (20), 541 (11), 557 (26), 563 (22), 577 (50), 589 (19), 611 (17), 671 (2), 691 (3), 743 (14), 753 (6), 769 (4), 793 (2), 844 (3), 872 (4), 907 (3), 948 (8), 958 (3), 986 (5), 1001 (100), 1031 (20), 1094 (12), 1103 (12), 1154 (35), 1160 (22), 1185 (12), 1191 (8), 1243 (29), 1250 (25), 1275 (30), 1307 (44), 1377 (20), 1382 (20), 1405 (20), 1437 (17), 1490 (11), 1539 (7), 1563 (86), 1587 (54), 1597 (98), 1613 (29), 2730 (1), 2854 (3), 2917 (13), 2976 (3), 3017 (4), 3060 (10). **MS** (CI, pos., isobutane) *m*/*z* (%): 153 (86) [PhAsH]$^+$, 179 (16) [PhCCPh+H]$^+$, 235 (77) [PhCCPh+C_4H_9]$^+$, 326 (14), 330 (95) [TerNH$_3$]$^+$, 372 (11), 386 (73) [TerNH$_2$+C_4H_9]$^+$, 402 (30) [TerNAs]$^+$, 731 (36) [Ter$_2$N$_2$AsH$_2$]$^+$, 804 (100) [(TerNAs)$_2$]$^+$, 983 (15) [M]$^+$, 1039 (4) [M+C_4H_9]$^+$.

3.2. [(TerNSbCPh)$_2$] (4Sb)

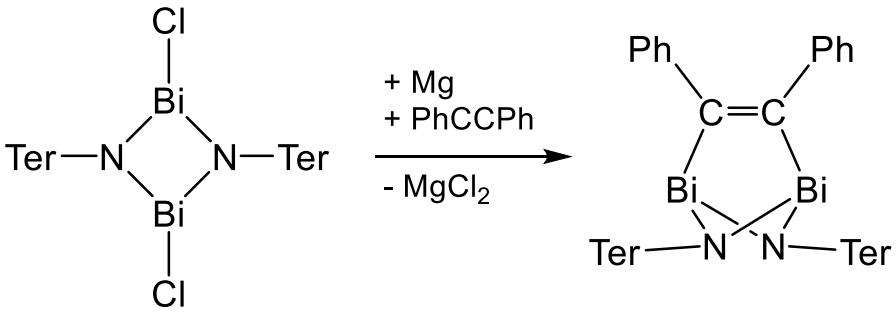


In a flask, 180 mg [ClSb(μ-NTer)]$_2$ (0.186 mmol), 61 mg PhCCPh (0.343 mmol) and magnesium turnings (88 mg) were combined as solids. To the mixture, 8 ml of THF were added and the suspension was stirred for three days. Subsequently, volatiles were removed in vacuo and the residue was extracted with 4 ml of benzene. The solution was filtered over a glass frit padded with celite, and the procedure was repeated with a second portion of 2 ml benzene. The combined extracts were concentrated to incipient crystallisation (approx. 1 ml) and left undisturbed overnight. Yellow crystals formed and the supernatant was removed via syringe. The crystals were washed with 1 ml of *n*-hexane and dried in vacuo, yielding 62 mg (0.058 mmol, 31%) of the product.

Mp. 143 °C (dec.). **EA** found (calc.): C 69.20 (69.16), H 5.67 (5.62), N 2.72 (2.60). **^{1}H NMR** (298 K, C_6D_6, 250.1 MHz): 2.09 (br s, 24 H, C*H*$_3$), 2.17 (s, 12 H, C*H*$_3$), 6.47 (br s, 8 H, C*H*$_{Mes}$), 6.67, 6.75 (*m*-/*p*-C*H*, AB$_2$-Spinsystem, J_{HH} = 7.4 Hz), 7.02-7.14 (m, 10 H, C*H*$_{Ph}$). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 62.9 MHz): 21.53 (s, *o*-*C*H$_3$), 21.91 (s, *p*-*C*H$_3$), 116.46 (s, *C*H), 126.51 (s, *C*H), 127.38 (s), 128.56 (s, *C*H), 128.89 (s, *C*H), 128.92 (s, *C*H), 130.16 (s, *C*H), 130.58 (s, *C*H), 137.88 (s), 138.40 (s), 141.94 (s), 145.94 (s), 188.92 (s, Sb-*C*). **IR** (ATR, cm^{-1}): 545 (m), 565 (m), 574 (m), 599 (m), 644 (m), 661 (s), 676 (vs), 692 (m), 709 (m), 742 (s), 771 (m), 786 (m), 796 (m), 848 (s), 867 (m), 894 (w), 919 (w), 945 (w), 962 (w), 1002 (m), 1025 (m), 1079 (m), 1095 (w), 1155 (m), 1182 (m), 1240 (s), 1274 (m), 1334 (w), 1371 (s), 1390 (s), 1434 (m), 1454 (w), 1479 (w), 1581 (m), 1608 (w), 2725 (w), 2848 (w), 2910 (w), 2941 (w), 2968 (w), 3020 (w), 3033 (w), 3049 (w), 3070 (w), 3089 (vw). **Raman** (632 nm, cm^{-1}): 123 (31), 144 (29), 160 (11), 170 (13), 197 (13), 211 (5), 232 (43), 256 (19), 265 (30), 331 (4), 378 (2), 418 (12), 453 (3), 464 (2), 510 (5), 520 (11), 536 (3), 555 (33), 573 (62), 599 (4), 661 (3), 678 (3), 740 (8), 754 (5), 789 (7), 868 (4), 893 (4), 943 (7), 997 (93), 1027 (13), 1082 (19), 1093 (5), 1100 (5), 1157 (47), 1182 (7), 1228 (27), 1242 (29), 1275 (23), 1303 (24), 1380 (20), 1393 (23), 1402 (12), 1438 (11), 1480 (6), 1488 (5), 1526 (3), 1550 (78), 1592 (100), 1610 (11), 2726 (2), 2853 (5), 2914 (21), 2974 (4), 3034 (9), 3056 (18). **MS** (CI, pos., isobutane) m/z (%): 179 (7)

[PhCCPh+H]$^+$, 235 (53) [PhCCPh+C_4H_9]$^+$, 330 (38) [$TerNH_3$]$^+$, 386 (12) [$TerNH_2$+C_4H_9]$^+$, 448 (1) [TerNSb]$^+$, 776 (1) [Ter_2N_2SbH]$^+$, 896 (87) [$(TerNSb)_2$]$^+$, 1075 (3) [M+H]$^+$.

3.3. [(TerNBiCPh)$_2$] (4Bi)

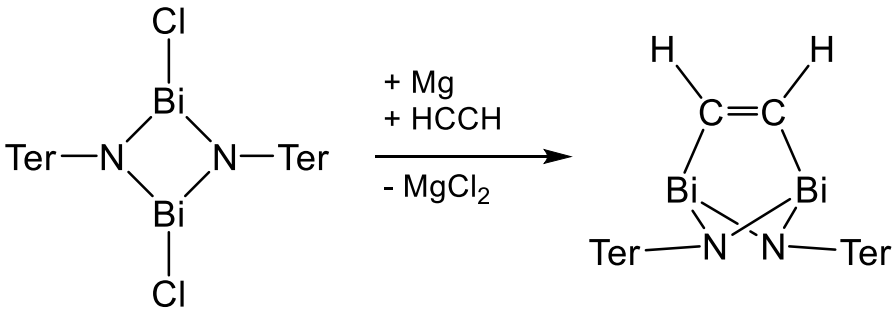


In a flask 155 mg [ClBi(μ-NTer)]$_2$ (0.136 mmol), 35 mg PhCCPh (0.196 mmol) and mangesium turnings (109 mg) were combined. To this, 8 ml of THF were added and the mixture was stirred for one day, resulting in a red solution and the deposition of a black precipitate. Volatiles were evaporated in vacuo and to the residue 3 ml of benzene were added. The suspension was filtered over a celite-padded glass frit, the residue washed with another 1 ml portion of benzene and the combined filtrate was concentrated to incipient crystallisation (approx. 1 ml). The solution was left undisturbed overnight which afforded red crystals. The crystals were washed with 1 ml of *n*-hexane and dried in vacuo, yielding 44 mg (0.035 mmol, 26%) of the product.

Mp. 133 °C (dec.). **EA** found (calc.): C 60.16 (59.52), H 5.54 (4.83), N 2.70 (2.24). **^{1}H NMR** (298 K, C_6D_6, 250.1 MHz): 1.99 (br s, 12 H, CH_3), 2.15 (s, 12 H, CH_3), 2.33 (br s, 12 H, CH_3), 6.22 (br s, 4 H, CH_{Mes}), 6.58 (dd, J_{HH} = 7.6, 7.0 Hz, 2 H, *p*-C*H*), 6.75 (br s, 4 H, CH_{Mes}), 6.83 (d, $^3J_{HH}$ = 7.4 Hz, 4 H, *m*-C*H*), 6.97-7.09 (m, 6 H, CH_{Ph}), 7.13-7.20 (m, 4 H, CH_{Ph}). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 62.9 MHz): 21.26 (br s, *C*H$_3$), 21.82 (s, *C*H$_3$), 114.72 (s, *C*H), 125.84 (s, *C*H), 128.56 (s, *C*H), 129.00 (s, *C*H), 129.16 (s, *C*H), 130.16 (br s, *C*H), 131.71 (s, *C*H), 131.79 (s), 137.77 (s), 138.35 (s), 145.90 (s), 153.99 (s). **IR** (ATR, cm^{-1}): 545 (m), 553 (m), 565 (m), 574 (w), 590 (w), 640 (m), 651 (s), 678 (s), 698 (m), 740 (m), 769 (m), 784 (w), 794 (w), 808 (w), 850 (m), 860 (m), 879 (w), 892 (w), 902 (w), 910 (w), 945 (w), 981 (s), 1027 (m), 1078 (s), 1124 (s), 1147 (vs), 1180 (s), 1228 (vs), 1307 (m), 1380 (m), 1436 (w), 1452 (w), 1479 (w), 1579 (w), 1608 (vw), 2725 (vw), 2848 (w), 2908 (w), 2941 (w), 3031 (w), 3070 (vw), 3087 (vw). **Raman** (632 nm, cm^{-1}): 150 (19), 165 (18), 180 (73), 202 (6), 245 (26), 254 (40), 333 (1), 417 (7), 460 (4), 497 (3), 512 (3), 520 (8), 538 (3), 559 (82), 570 (10), 577 (16), 653 (7), 664 (7), 741 (4), 752 (6), 778 (16), 862 (9), 880 (4), 943 (6), 998 (96), 1028 (9), 1081 (21), 1102 (4), 1149 (70), 1157 (18), 1180 (7), 1223 (17), 1247 (32), 1273 (24), 1304 (14), 1385 (34), 1396 (17), 1440 (7), 1482 (3), 1563 (40), 1582 (53), 1593 (100), 1611 (8), 2729 (1), 2854 (2), 2917 (10), 3034 (5), 3061 (8). **MS** (CI, pos., isobutane) *m*/*z* (%): 179 (18) [PhCCPh+H]$^+$, 235 (69),

330 (30) $[TerNH_3]^+$, 387 (19) $[PhCCPh+Bi]^+$, 538 (16) $[TerNHBi+H]^+$, 867 (10) $[(TerNH)_2Bi]^+$.

3.4. [(TerNBiCH)$_2$] (4BiH)



[ClBi(μ-NTer)]$_2$ (148 mg, 0.129 mmol) was suspended with magnesium turnings (105 mg) in 5 ml of THF and cooled to –80 °C. Separately, THF was saturated with acetylene at –60 °C. Of this solution, 5 ml were added to the suspension via syringe. The mixture was stirred vigorously at –80 °C for three hours, then warmed to ambient temperature and then stirred overnight. The resulting brownish suspension was evaporated in vacuo. The residue was extracted twice with 10 ml of benzene. The combined extract was concentrated to incipient crystallisation and stored in fridge overnight, affording few orange crystals. In solution, the compound slowly decomposes under formation of a dark brown amorphous precipitate, precluding full spectroscopic characterisation.

Mp. 117 °C (dec.). **^{1}H NMR** (298 K, C_6D_6, 250.1 MHz): 12.90 (s, BiC*H*). **IR** (ATR, cm^{-1}): 532 (s), 545 (s), 551 (s), 567 (s), 626 (m), 648 (s), 676 (m), 746 (s), 784 (m), 796 (m), 848 (vs), 879 (m), 914 (w), 946 (m), 985 (w), 1004 (m), 1029 (m), 1074 (m), 1159 (m), 1180 (m), 1224 (s), 1234 (s), 1253 (m), 1380 (s), 1448 (s), 1484 (w), 1579 (m), 1604 (m), 2728 (w), 2854 (w), 2914 (m), 2931 (m), 2942 (m), 2964 (m). **Raman** (632 nm, cm^{-1}): 172 (100), 258 (78), 283 (14), 319 (6), 341 (9), 357 (6), 421 (69), 454 (16), 516 (6), 525 (4), 559 (34), 574 (19), 582 (22), 742 (10), 753 (6), 880 (8), 949 (15), 964 (11), 1005 (24), 1082 (42), 1096 (15), 1121 (5), 1128 (6), 1152 (7), 1164 (13), 1186 (14), 1242 (20), 1254 (36), 1270 (83), 1305 (36), 1387 (24), 1397 (65), 1438 (7), 1483 (6), 1555 (5), 1585 (83), 1613 (14), 2732 (1), 2855 (2), 2919 (15), 2936 (11), 2983 (8), 3011 (9), 3030 (9), 3040 (9).

4. Computational Details

All computations were carried out using the Gaussian09 program package[7] and the standalone version of NBO 6.0.[8–11] To gain insight in the observed reactivity of **2E** (E = P, As, Sb, Bi), the structures of **2E**, **4E** and tolan were fully optimized utilizing the pure DFT functional PBE (including the exchange and gradient-corrected correlation functionals as defined by Perdew, Burke and Ernzerhof)[12,13] as well as the def2svp basis set,[14] which includes fully relativistic effective core potentials for Sb and Bi[15] (notation PBE/def2svp). All structures were confirmed as minima by frequency analyses. Partial charges were derived by NBO analysis. The pure DFT functional PBE was chosen over the hybrid functional PBE0,[16] as HF exchange has been shown to impair the results obtained for systems with multiconfigurational character.[17] Still, it is important to note that the results obtained by any "common" DFT method can only be considered a rough estimate due to the single-determinantal nature of Kohn-Sham theory.

To estimate the biradical character of **2E**, CASSCF(6,4)[18–26] single point calculations were run (CAS(6,4)/def2svp) using the optimized molecular structures obtained from the DFT calculations. To that end, the SCF guess was modified to include the three highest-lying occupied π-type MOs and the lowest-lying unoccupied π-type MO centred at the N_2E_2 scaffold in the active space. These MOs always comprised the HOMO and LUMO of the HF wave function, which would serve as active space for a CAS(2,2) calculation. The biradical character was estimated using the β scale as proposed by Miliordos *et al*.[27]

Moreover, the model systems **2E**H were optimized at the CAS(6,4)/def2svp and CCSD/def2tzvp level of theory. The ST energy gaps compare well at both levels of theory (ΔE_{max} = 7.7 kJ/mol = 1.8 kcal/mol for E = Bi). The CASSCF and CCSD densities were used to run subsequent NBO/NRT analyses (vide infra).

It should be emphasized that all computations were carried out for single, isolated molecules in the gas phase. There may well be differences between gas phase, solution and solid state properties of the considered species.

Table S2: Summary of DFT calculations (PBE/def2svp, energies given in a.u.).

Compound	Point group	E_{tot}	E_0	E_{298}	H_{298}	G_{298}
2P	D_2	-2647.0306	-2646.2089	-2646.1539	-2646.1530	-2646.3013
2As	D_2	-6435.3884	-6434.5686	-6434.5130	-6434.5120	-6434.6608
2Sb	D_2	-2445.3496	-2444.5315	-2444.4754	-2444.4745	-2444.6253
2Bi	D_2	-2394.1791	-2393.3620	-2393.3056	-2393.3047	-2393.4584
4P	C_2	-3185.4503	-3184.4373	-3184.3721	-3184.3711	-3184.5383
4As	C_2	-6973.8069	-6972.7970	-6972.7305	-6972.7296	-6972.8997
4Sb	C_2	-2983.7726	-2982.7667	-2982.7002	-2982.6993	-2982.8705
4Bi	C_2	-2932.5972	-2931.5915	-2931.5232	-2931.5223	-2931.6989
tolan	D_{2h}	-538.3827	-538.1960	-538.1846	-538.1837	-538.2339

Table S3: NPA partial charges *q* of **2E** and **4E** as well as charge transfer onto the tolan unit in **4E** (PBE/def2svp).

Compound	*q*(N)	*q*(E)	*q*(C)	CT = *q*(tolan)
2P	-0.92	0.74		
2As	-0.94	0.79		
2Sb	-1.01	0.91		
2Bi	-0.96	0.91		
4P	-0.95	1.13	-0.26	-0.55
4As	-0.97	1.21	-0.29	-0.63
4Sb	-1.05	1.43	-0.37	-0.83
4Bi	-1.01	1.44	-0.36	-0.85
tolan			0.01	0

Table S4: Wiberg bond indices of **2E**, **4E** and tolan (PBE/def2svp).

Compound	N-E	E-E	N-N	C-E	C-C
2P	0.86	0.47	0.06		
2As	0.81	0.45	0.06		
2Sb	0.72	0.45	0.05		
2Bi	0.70	0.42	0.05		

Compound	N-E	E-E	N-N	C-E	C-C
4P	0.75	0.03	0.04	0.84	1.72
4As	0.71	0.03	0.03	0.80	1.75
4Sb	0.62	0.04	0.03	0.72	1.79
4Bi	0.61	0.04	0.03	0.69	1.81
tolan					2.61

Table S5: Configuration state function coefficients and biradical characters (CAS(6,4)/def2svp).

Compound	c_1[a]	c_2[a]	c_3[a]	c_4[a]	β[b]
2P	0.9269	-0.3691	-0.0680	-0.0042	0.274
2As	0.9095	-0.4102	-0.0675	-0.0015	0.338
2Sb	0.8729	-0.4848	-0.0544	-0.0088	0.471
2Bi	0.8529	-0.5194	-0.0518	-0.0075	0.541

[a] CSFs: $\Psi_1 = |\pi_1^2\pi_2^2\pi_3^2\rangle$, $\Psi_2 = |\pi_1^2\pi_2^2\pi_4^2\rangle$, $\Psi_3 = |\pi_1^2\pi_3^2\pi_4^2\rangle$, $\Psi_4 = |\pi_2^2\pi_3^2\pi_4^2\rangle$;
CAS wave function $\Phi \approx \sum_i c_i\Psi_i$

[b] $\beta = 2c_1^2/(c_1^2 + c_2^2)$

Figure S1: Schematic depiction of the four leading configuration state functions.

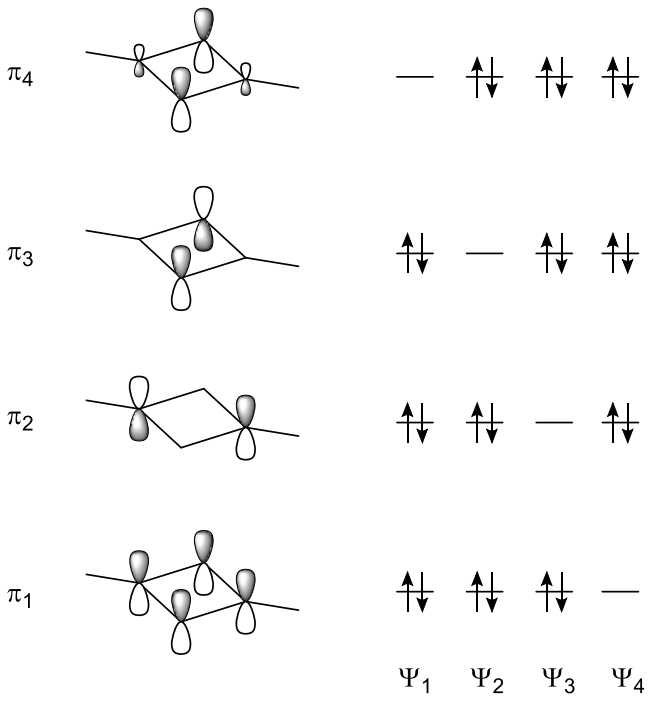


Table S6: Singlet-triplet gaps (CAS(6,4)/def2svp).

Compound	E_{tot} (S) [a.u.]	E_{tot} (T) [a.u.]	ΔE_{ST} [kJ/mol]
2P	-2635.5414	-2635.5103	81.9
2As	-6422.1135	-6422.0925	55.2
2Sb	-2432.7750	-2432.7654	25.4
2Bi	-2381.3628	-2381.3564	16.9

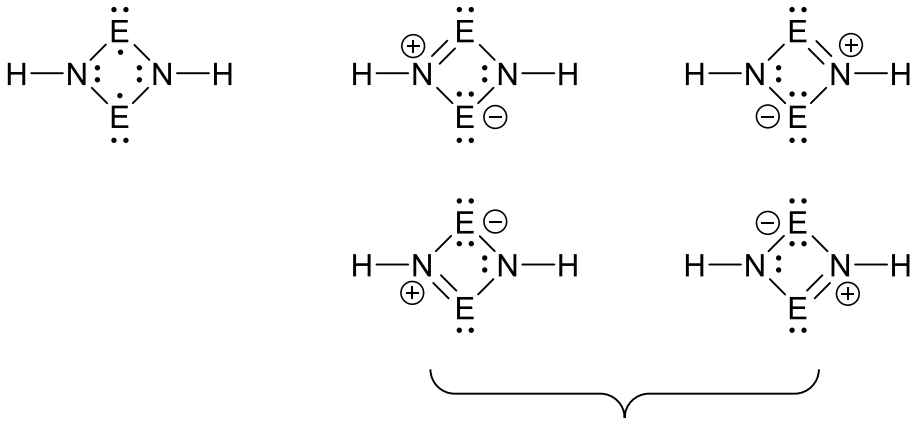
Table S7: Summary of CASSCF calculations on model compounds (CAS(6,4)/def2svp).

Compound	Point group	E_{tot} (S) [a.u.]	E_{tot} (T) [a.u.]	ΔE_{ST} [kJ/mol]
2PH	D_{2h}	-791.2336	-791.1872	121.7
2AsH	D_{2h}	-4577.8035	-4577.7678	93.9
2SbH	D_{2h}	-588.4613	-588.4401	55.6
2BiH	D_{2h}	-537.0332	-537.0157	45.9

Table S8: Summary of CCSD calculations on model compounds (CCSD/def2svp).

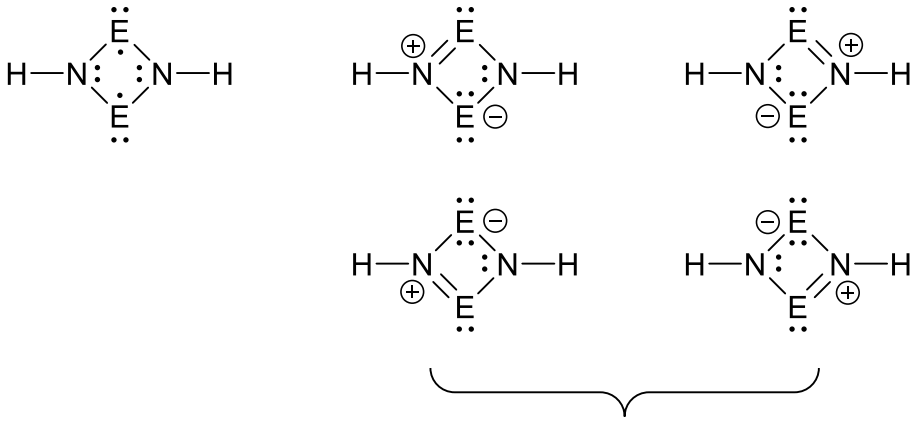
Compound	Point group	E_{tot} (S) [a.u.]	E_{tot} (T) [a.u.]	ΔE_{ST} [kJ/mol]
2PH	D_{2h}	-792.2969	-792.2501	122.9
2AsH	D_{2h}	-4579.4049	-4579.3685	95.5
2SbH	D_{2h}	-589.6806	-589.6617	49.5
2BiH	D_{2h}	-538.5283	-538.5138	38.3

Figure S2: NRT analysis using the CAS density.



68 %	**2P**H	29 %
68 %	**2As**H	29 %
67 %	**2Sb**H	28 %
66 %	**2Bi**H	29 %

Figure S3: NRT analysis using the CCSD density.



56 %	**2P**H	29 %
57 %	**2As**H	28 %
59 %	**2Sb**H	26 %
58 %	**2Bi**H	27 %

Optimized structure of **2P** (PBE/def2svp):

```
N                  0.00000000    0.00000000   -1.12598400
N                  0.00000000    0.00000000    1.12598400
P                  1.36031800    0.00000000    0.00000000
P                 -1.36031800    0.00000000    0.00000000
C                  0.00000000    0.00000000    2.53321300
C                  1.16250800    0.40684600    3.25741000
C                 -1.16250800   -0.40684600    3.25741000
C                  1.13783600    0.39748300    4.66551600
C                 -1.13783600   -0.39748300    4.66551600
C                  0.00000000    0.00000000    5.37788300
H                  2.04334100    0.72247800    5.20151700
```

H	-2.04334100	-0.72247800	5.20151700
H	0.00000000	0.00000000	6.47820400
C	0.00000000	0.00000000	-2.53321300
C	1.16250800	-0.40684600	-3.25741000
C	-1.16250800	0.40684600	-3.25741000
C	1.13783600	-0.39748300	-4.66551600
C	-1.13783600	0.39748300	-4.66551600
C	0.00000000	0.00000000	-5.37788300
H	2.04334100	-0.72247800	-5.20151700
H	-2.04334100	0.72247800	-5.20151700
H	0.00000000	0.00000000	-6.47820400
C	-2.41811600	0.87654500	-2.58734300
C	-3.53103500	0.00252900	-2.46388200
C	-2.52312400	2.22981500	-2.15802700
C	-4.72155000	0.49532200	-1.89605200
C	-3.73283400	2.67580000	-1.60177900
C	-4.84436600	1.82366400	-1.45443200
H	-5.58121600	-0.18683900	-1.79244000
H	-3.80853800	3.72467000	-1.26979600
C	2.41811600	-0.87654500	-2.58734300
C	3.53103500	-0.00252900	-2.46388200
C	2.52312400	-2.22981500	-2.15802700
C	4.72155000	-0.49532200	-1.89605200
C	3.73283400	-2.67580000	-1.60177900
C	4.84436600	-1.82366400	-1.45443200
H	5.58121600	0.18683900	-1.79244000
H	3.80853800	-3.72467000	-1.26979600
C	-2.41811600	-0.87654500	2.58734300
C	-3.53103500	-0.00252900	2.46388200
C	-2.52312400	-2.22981500	2.15802700
C	-4.72155000	-0.49532200	1.89605200
C	-3.73283400	-2.67580000	1.60177900
C	-4.84436600	-1.82366400	1.45443200
H	-5.58121600	0.18683900	1.79244000
H	-3.80853800	-3.72467000	1.26979600
C	2.41811600	0.87654500	2.58734300
C	2.52312400	2.22981500	2.15802700
C	3.53103500	0.00252900	2.46388200
C	3.73283400	2.67580000	1.60177900
C	4.72155000	0.49532200	1.89605200
C	4.84436600	1.82366400	1.45443200
H	3.80853800	3.72467000	1.26979600
H	5.58121600	-0.18683900	1.79244000
C	-3.43944900	1.43832300	2.90575900
H	-4.38404700	1.97957300	2.70335900
H	-3.21639000	1.52717900	3.98868100
H	-2.62237900	1.96589200	2.37051800
C	-1.34882600	-3.16813600	2.28655100
H	-0.97070700	-3.20951600	3.32870700
H	-1.61758700	-4.19507200	1.97210600
H	-0.49850400	-2.82994300	1.65670000
C	-6.12165000	-2.32853200	0.82864000
H	-5.97451700	-2.56176500	-0.24787400
H	-6.47009400	-3.26487900	1.31181000
H	-6.93717100	-1.58272800	0.90085700
C	3.43944900	-1.43832300	2.90575900
H	4.38404700	-1.97957300	2.70335900
H	3.21639000	-1.52717900	3.98868100
H	2.62237900	-1.96589200	2.37051800
C	1.34882600	3.16813600	2.28655100
H	0.49850400	2.82994300	1.65670000

H	0.97070700	3.20951600	3.32870700
H	1.61758700	4.19507200	1.97210600
C	6.12165000	2.32853200	0.82864000
H	5.97451700	2.56176500	-0.24787400
H	6.47009400	3.26487900	1.31181000
H	6.93717100	1.58272800	0.90085700
C	6.12165000	-2.32853200	-0.82864000
H	5.97451700	-2.56176500	0.24787400
H	6.47009400	-3.26487900	-1.31181000
H	6.93717100	-1.58272800	-0.90085700
C	-6.12165000	2.32853200	-0.82864000
H	-5.97451700	2.56176500	0.24787400
H	-6.47009400	3.26487900	-1.31181000
H	-6.93717100	1.58272800	-0.90085700
C	-1.34882600	3.16813600	-2.28655100
H	-0.97070700	3.20951600	-3.32870700
H	-1.61758700	4.19507200	-1.97210600
H	-0.49850400	2.82994300	-1.65670000
C	1.34882600	-3.16813600	-2.28655100
H	0.97070700	-3.20951600	-3.32870700
H	1.61758700	-4.19507200	-1.97210600
H	0.49850400	-2.82994300	-1.65670000
C	3.43944900	1.43832300	-2.90575900
H	4.38404700	1.97957300	-2.70335900
H	3.21639000	1.52717900	-3.98868100
H	2.62237900	1.96589200	-2.37051800
C	-3.43944900	-1.43832300	-2.90575900
H	-4.38404700	-1.97957300	-2.70335900
H	-3.21639000	-1.52717900	-3.98868100
H	-2.62237900	-1.96589200	-2.37051800

Optimized structure of **2As** (PBE/def2svp):

N	0.00000000	0.00000000	-1.19616000
N	0.00000000	0.00000000	1.19616000
As	1.48031900	0.00000000	0.00000000
As	-1.48031900	0.00000000	0.00000000
C	0.00000000	0.00000000	2.59540700
C	1.17591100	0.35860100	3.33156600
C	-1.17591100	-0.35860100	3.33156600
C	1.15133400	0.35137200	4.73912400
C	-1.15133400	-0.35137200	4.73912400
C	0.00000000	0.00000000	5.45407300
H	2.06954600	0.64059900	5.27442100
H	-2.06954600	-0.64059900	5.27442100
H	0.00000000	0.00000000	6.55428500
C	0.00000000	0.00000000	-2.59540700
C	1.17591100	-0.35860100	-3.33156600
C	-1.17591100	0.35860100	-3.33156600
C	1.15133400	-0.35137200	-4.73912400
C	-1.15133400	0.35137200	-4.73912400
C	0.00000000	0.00000000	-5.45407300
H	2.06954600	-0.64059900	-5.27442100
H	-2.06954600	0.64059900	-5.27442100
H	0.00000000	0.00000000	-6.55428500
C	-2.45347200	0.77908000	-2.67134100
C	-3.53661200	-0.13479800	-2.56285900
C	-2.61813500	2.13067700	-2.25145100
C	-4.75514500	0.31635700	-2.01891500
C	-3.85422400	2.53427900	-1.72052200

C	-4.93606100	1.64214400	-1.58912500
H	-5.59086900	-0.39666200	-1.92737900
H	-3.97469800	3.58130000	-1.39629400
C	2.45347200	-0.77908000	-2.67134100
C	3.53661200	0.13479800	-2.56285900
C	2.61813500	-2.13067700	-2.25145100
C	4.75514500	-0.31635700	-2.01891500
C	3.85422400	-2.53427900	-1.72052200
C	4.93606100	-1.64214400	-1.58912500
H	5.59086900	0.39666200	-1.92737900
H	3.97469800	-3.58130000	-1.39629400
C	-2.45347200	-0.77908000	2.67134100
C	-3.53661200	0.13479800	2.56285900
C	-2.61813500	-2.13067700	2.25145100
C	-4.75514500	-0.31635700	2.01891500
C	-3.85422400	-2.53427900	1.72052200
C	-4.93606100	-1.64214400	1.58912500
H	-5.59086900	0.39666200	1.92737900
H	-3.97469800	-3.58130000	1.39629400
C	2.45347200	0.77908000	2.67134100
C	2.61813500	2.13067700	2.25145100
C	3.53661200	-0.13479800	2.56285900
C	3.85422400	2.53427900	1.72052200
C	4.75514500	0.31635700	2.01891500
C	4.93606100	1.64214400	1.58912500
H	3.97469800	3.58130000	1.39629400
H	5.59086900	-0.39666200	1.92737900
C	-3.39038400	1.56975000	3.01003800
H	-4.30198400	2.15457200	2.77980000
H	-3.20034900	1.64370800	4.10062700
H	-2.53141100	2.06073400	2.50749600
C	-1.48095100	-3.11392700	2.37586000
H	-1.11332300	-3.17920800	3.42064000
H	-1.78645800	-4.12664500	2.04930000
H	-0.61442600	-2.80025700	1.75610900
C	-6.24526100	-2.10473400	0.99773500
H	-6.11807200	-2.41943600	-0.05996400
H	-6.65051100	-2.98202400	1.54402700
H	-7.01142400	-1.30542400	1.02124200
C	3.39038400	-1.56975000	3.01003800
H	4.30198400	-2.15457200	2.77980000
H	3.20034900	-1.64370800	4.10062700
H	2.53141100	-2.06073400	2.50749600
C	1.48095100	3.11392700	2.37586000
H	0.61442600	2.80025700	1.75610900
H	1.11332300	3.17920800	3.42064000
H	1.78645800	4.12664500	2.04930000
C	6.24526100	2.10473400	0.99773500
H	6.11807200	2.41943600	-0.05996400
H	6.65051100	2.98202400	1.54402700
H	7.01142400	1.30542400	1.02124200
C	6.24526100	-2.10473400	-0.99773500
H	6.11807200	-2.41943600	0.05996400
H	6.65051100	-2.98202400	-1.54402700
H	7.01142400	-1.30542400	-1.02124200
C	-6.24526100	2.10473400	-0.99773500
H	-6.11807200	2.41943600	0.05996400
H	-6.65051100	2.98202400	-1.54402700
H	-7.01142400	1.30542400	-1.02124200
C	-1.48095100	3.11392700	-2.37586000
H	-1.11332300	3.17920800	-3.42064000

H	-1.78645800	4.12664500	-2.04930000
H	-0.61442600	2.80025700	-1.75610900
C	1.48095100	-3.11392700	-2.37586000
H	1.11332300	-3.17920800	-3.42064000
H	1.78645800	-4.12664500	-2.04930000
H	0.61442600	-2.80025700	-1.75610900
C	3.39038400	1.56975000	-3.01003800
H	4.30198400	2.15457200	-2.77980000
H	3.20034900	1.64370800	-4.10062700
H	2.53141100	2.06073400	-2.50749600
C	-3.39038400	-1.56975000	-3.01003800
H	-4.30198400	-2.15457200	-2.77980000
H	-3.20034900	-1.64370800	-4.10062700
H	-2.53141100	-2.06073400	-2.50749600

Optimized structure of **2Sb** (PBE/def2svp):

N	0.00000000	0.00000000	1.31567800
N	0.00000000	0.00000000	-1.31567800
Sb	1.67352200	0.00000000	0.00000000
Sb	-1.67352200	0.00000000	0.00000000
C	0.00000000	0.00000000	-2.70757500
C	-1.18619800	0.31005400	-3.46223300
C	1.18619800	-0.31005400	-3.46223300
C	-1.16141900	0.30626100	-4.86937000
C	1.16141900	-0.30626100	-4.86937000
C	0.00000000	0.00000000	-5.58821700
H	-2.09109600	0.55903500	-5.40399500
H	2.09109600	-0.55903500	-5.40399500
H	0.00000000	0.00000000	-6.68827200
C	0.00000000	0.00000000	2.70757500
C	-1.18619800	-0.31005400	3.46223300
C	1.18619800	0.31005400	3.46223300
C	-1.16141900	-0.30626100	4.86937000
C	1.16141900	0.30626100	4.86937000
C	0.00000000	0.00000000	5.58821700
H	-2.09109600	-0.55903500	5.40399500
H	2.09109600	0.55903500	5.40399500
H	0.00000000	0.00000000	6.68827200
C	2.49271500	0.67215300	2.82451400
C	3.53732600	-0.29303700	2.74203700
C	2.74184000	2.02021800	2.43527600
C	4.79539100	0.10423600	2.25063700
C	4.01839900	2.37044100	1.95841300
C	5.05676600	1.42748200	1.84790100
H	5.60003300	-0.64726200	2.18756700
H	4.20415000	3.41512700	1.65938200
C	-2.49271500	-0.67215300	2.82451400
C	-3.53732600	0.29303700	2.74203700
C	-2.74184000	-2.02021800	2.43527600
C	-4.79539100	-0.10423600	2.25063700
C	-4.01839900	-2.37044100	1.95841300
C	-5.05676600	-1.42748200	1.84790100
H	-5.60003300	0.64726200	2.18756700
H	-4.20415000	-3.41512700	1.65938200
C	2.49271500	-0.67215300	-2.82451400
C	3.53732600	0.29303700	-2.74203700
C	2.74184000	-2.02021800	-2.43527600
C	4.79539100	-0.10423600	-2.25063700
C	4.01839900	-2.37044100	-1.95841300

C	5.05676600	-1.42748200	-1.84790100
H	5.60003300	0.64726200	-2.18756700
H	4.20415000	-3.41512700	-1.65938200
C	-2.49271500	0.67215300	-2.82451400
C	-2.74184000	2.02021800	-2.43527600
C	-3.53732600	-0.29303700	-2.74203700
C	-4.01839900	2.37044100	-1.95841300
C	-4.79539100	0.10423600	-2.25063700
C	-5.05676600	1.42748200	-1.84790100
H	-4.20415000	3.41512700	-1.65938200
H	-5.60003300	-0.64726200	-2.18756700
C	3.31021900	1.71805700	-3.18680400
H	4.17839800	2.35837500	-2.93784100
H	3.13925200	1.77956300	-4.28157000
H	2.41009700	2.15127500	-2.70469800
C	1.65785200	-3.06185000	-2.55760100
H	1.32425400	-3.17201000	-3.61032600
H	2.00470700	-4.04898900	-2.19622200
H	0.76029900	-2.77399000	-1.97163000
C	6.40336900	-1.81546000	-1.28826900
H	6.44264000	-1.62979400	-0.19268300
H	6.61881700	-2.89095300	-1.44465900
H	7.22357200	-1.22717200	-1.74624200
C	-3.31021900	-1.71805700	-3.18680400
H	-4.17839800	-2.35837500	-2.93784100
H	-3.13925200	-1.77956300	-4.28157000
H	-2.41009700	-2.15127500	-2.70469800
C	-1.65785200	3.06185000	-2.55760100
H	-0.76029900	2.77399000	-1.97163000
H	-1.32425400	3.17201000	-3.61032600
H	-2.00470700	4.04898900	-2.19622200
C	-6.40336900	1.81546000	-1.28826900
H	-6.44264000	1.62979400	-0.19268300
H	-6.61881700	2.89095300	-1.44465900
H	-7.22357200	1.22717200	-1.74624200
C	-6.40336900	-1.81546000	1.28826900
H	-6.44264000	-1.62979400	0.19268300
H	-6.61881700	-2.89095300	1.44465900
H	-7.22357200	-1.22717200	1.74624200
C	6.40336900	1.81546000	1.28826900
H	6.44264000	1.62979400	0.19268300
H	6.61881700	2.89095300	1.44465900
H	7.22357200	1.22717200	1.74624200
C	1.65785200	3.06185000	2.55760100
H	1.32425400	3.17201000	3.61032600
H	2.00470700	4.04898900	2.19622200
H	0.76029900	2.77399000	1.97163000
C	-1.65785200	-3.06185000	2.55760100
H	-1.32425400	-3.17201000	3.61032600
H	-2.00470700	-4.04898900	2.19622200
H	-0.76029900	-2.77399000	1.97163000
C	-3.31021900	1.71805700	3.18680400
H	-4.17839800	2.35837500	2.93784100
H	-3.13925200	1.77956300	4.28157000
H	-2.41009700	2.15127500	2.70469800
C	3.31021900	-1.71805700	3.18680400
H	4.17839800	-2.35837500	2.93784100
H	3.13925200	-1.77956300	4.28157000
H	2.41009700	-2.15127500	2.70469800

Optimized structure of **2Bi** (PBE/def2svp):

N	0.00000000	0.00000000	1.38159200
N	0.00000000	0.00000000	-1.38159200
Bi	1.76485600	0.00000000	0.00000000
Bi	-1.76485600	0.00000000	0.00000000
C	0.00000000	0.00000000	-2.76407300
C	-1.19524800	0.27446200	-3.52678600
C	1.19524800	-0.27446200	-3.52678600
C	-1.17061300	0.26991700	-4.93314600
C	1.17061300	-0.26991700	-4.93314600
C	0.00000000	0.00000000	-5.65306200
H	-2.10727700	0.49386700	-5.46900400
H	2.10727700	-0.49386700	-5.46900400
H	0.00000000	0.00000000	-6.75305000
C	0.00000000	0.00000000	2.76407300
C	-1.19524800	-0.27446200	3.52678600
C	1.19524800	0.27446200	3.52678600
C	-1.17061300	-0.26991700	4.93314600
C	1.17061300	0.26991700	4.93314600
C	0.00000000	0.00000000	5.65306200
H	-2.10727700	-0.49386700	5.46900400
H	2.10727700	0.49386700	5.46900400
H	0.00000000	0.00000000	6.75305000
C	2.51133400	0.60230700	2.88969100
C	3.52778100	-0.39169800	2.79521100
C	2.79882400	1.94521300	2.50559200
C	4.79794200	-0.02669800	2.30653300
C	4.08679100	2.26379400	2.03486900
C	5.09892700	1.29286800	1.91844200
H	5.58060700	-0.80060300	2.23770500
H	4.30287500	3.30572400	1.74681400
C	-2.51133400	-0.60230700	2.88969100
C	-3.52778100	0.39169800	2.79521100
C	-2.79882400	-1.94521300	2.50559200
C	-4.79794200	0.02669800	2.30653300
C	-4.08679100	-2.26379400	2.03486900
C	-5.09892700	-1.29286800	1.91844200
H	-5.58060700	0.80060300	2.23770500
H	-4.30287500	-3.30572400	1.74681400
C	2.51133400	-0.60230700	-2.88969100
C	3.52778100	0.39169800	-2.79521100
C	2.79882400	-1.94521300	-2.50559200
C	4.79794200	0.02669800	-2.30653300
C	4.08679100	-2.26379400	-2.03486900
C	5.09892700	-1.29286800	-1.91844200
H	5.58060700	0.80060300	-2.23770500
H	4.30287500	-3.30572400	-1.74681400
C	-2.51133400	0.60230700	-2.88969100
C	-2.79882400	1.94521300	-2.50559200
C	-3.52778100	-0.39169800	-2.79521100
C	-4.08679100	2.26379400	-2.03486900
C	-4.79794200	-0.02669800	-2.30653300
C	-5.09892700	1.29286800	-1.91844200
H	-4.30287500	3.30572400	-1.74681400
H	-5.58060700	-0.80060300	-2.23770500
C	3.26154400	1.81096700	-3.23774800
H	4.09075300	2.48435000	-2.94636100
H	3.13948100	1.87294900	-4.33928500
H	2.32210900	2.20259100	-2.79752600
C	1.74218600	-3.01376900	-2.63620700

H	1.42949800	-3.13909900	-3.69367400
H	2.10585000	-3.98981500	-2.26142300
H	0.82905000	-2.73922400	-2.06818700
C	6.45806300	-1.64925000	-1.36791900
H	7.25593000	-1.01331200	-1.80074100
H	6.48827900	-1.50459600	-0.26588200
H	6.71493400	-2.70907800	-1.56415300
C	-3.26154400	-1.81096700	-3.23774800
H	-4.09075300	-2.48435000	-2.94636100
H	-3.13948100	-1.87294900	-4.33928500
H	-2.32210900	-2.20259100	-2.79752600
C	-1.74218600	3.01376900	-2.63620700
H	-0.82905000	2.73922400	-2.06818700
H	-1.42949800	3.13909900	-3.69367400
H	-2.10585000	3.98981500	-2.26142300
C	-6.45806300	1.64925000	-1.36791900
H	-7.25593000	1.01331200	-1.80074100
H	-6.48827900	1.50459600	-0.26588200
H	-6.71493400	2.70907800	-1.56415300
C	-6.45806300	-1.64925000	1.36791900
H	-7.25593000	-1.01331200	1.80074100
H	-6.48827900	-1.50459600	0.26588200
H	-6.71493400	-2.70907800	1.56415300
C	6.45806300	1.64925000	1.36791900
H	7.25593000	1.01331200	1.80074100
H	6.48827900	1.50459600	0.26588200
H	6.71493400	2.70907800	1.56415300
C	1.74218600	3.01376900	2.63620700
H	1.42949800	3.13909900	3.69367400
H	2.10585000	3.98981500	2.26142300
H	0.82905000	2.73922400	2.06818700
C	-1.74218600	-3.01376900	2.63620700
H	-1.42949800	-3.13909900	3.69367400
H	-2.10585000	-3.98981500	2.26142300
H	-0.82905000	-2.73922400	2.06818700
C	-3.26154400	1.81096700	3.23774800
H	-4.09075300	2.48435000	2.94636100
H	-3.13948100	1.87294900	4.33928500
H	-2.32210900	2.20259100	2.79752600
C	3.26154400	-1.81096700	3.23774800
H	4.09075300	-2.48435000	2.94636100
H	3.13948100	-1.87294900	4.33928500
H	2.32210900	-2.20259100	2.79752600

Optimized structure of **4P** (PBE/def2svp):

N	-1.03977800	0.48806800	-0.71759800
N	1.03977800	-0.48806800	-0.71759800
P	0.56247700	1.17340000	-0.24622300
P	-0.56247700	-1.17340000	-0.24622300
C	2.27999100	-1.05875500	-1.02135600
C	3.49144000	-0.29636900	-0.92896400
C	2.38377800	-2.41557900	-1.47824600
C	4.71533900	-0.85902400	-1.34041200
C	3.63570300	-2.93203500	-1.86792000
C	4.80594600	-2.16840600	-1.82285300
H	5.61963300	-0.23531600	-1.25643800
H	3.66917900	-3.97295700	-2.22689900
H	5.77009000	-2.58947200	-2.14373800
C	-2.27999100	1.05875500	-1.02135600

C	-2.38377800	2.41557900	-1.47824600
C	-3.49144000	0.29636900	-0.92896400
C	-3.63570300	2.93203500	-1.86792000
C	-4.71533900	0.85902400	-1.34041200
C	-4.80594600	2.16840600	-1.82285300
H	-3.66917900	3.97295700	-2.22689900
H	-5.61963300	0.23531600	-1.25643800
H	-5.77009000	2.58947200	-2.14373800
C	-3.56675000	-1.08360500	-0.35191300
C	-3.60814300	-2.21997800	-1.20548400
C	-3.78649800	-1.23550400	1.04486700
C	-3.80504400	-3.48960100	-0.63883500
C	-3.96452400	-2.52912100	1.57007100
C	-3.96637200	-3.67026900	0.74840500
H	-3.83276400	-4.36772400	-1.30362300
H	-4.11148200	-2.64411200	2.65637200
C	-1.23508500	3.37331600	-1.57427700
C	-1.10711000	4.40728900	-0.60507800
C	-0.37791700	3.35598800	-2.70596900
C	-0.10248100	5.37819700	-0.77045700
C	0.59804800	4.36074500	-2.83988400
C	0.75707000	5.38046200	-1.88473400
H	-0.00261300	6.17260500	-0.01142500
H	1.25141600	4.34942900	-3.72763600
C	1.23508500	-3.37331600	-1.57427700
C	1.10711000	-4.40728900	-0.60507800
C	0.37791700	-3.35598800	-2.70596900
C	0.10248100	-5.37819700	-0.77045700
C	-0.59804800	-4.36074500	-2.83988400
C	-0.75707000	-5.38046200	-1.88473400
H	0.00261300	-6.17260500	-0.01142500
H	-1.25141600	-4.34942900	-3.72763600
C	3.56675000	1.08360500	-0.35191300
C	3.78649800	1.23550400	1.04486700
C	3.60814300	2.21997800	-1.20548400
C	3.96452400	2.52912100	1.57007100
C	3.80504400	3.48960100	-0.63883500
C	3.96637200	3.67026900	0.74840500
H	4.11148200	2.64411200	2.65637200
H	3.83276400	4.36772400	-1.30362300
C	2.05646000	-4.50005000	0.56852400
H	1.66735500	-5.18639300	1.34610800
H	3.04994000	-4.88352800	0.25290900
H	2.24699400	-3.51328000	1.03567600
C	0.51913300	-2.28120300	-3.75616700
H	1.54614400	-2.25811000	-4.17552900
H	-0.19470400	-2.43066200	-4.58905500
H	0.33911700	-1.27400900	-3.32339700
C	-1.79215200	-6.46606100	-2.05403200
H	-2.42206300	-6.57173200	-1.14632800
H	-2.46221400	-6.26546100	-2.91279800
H	-1.31428400	-7.45392700	-2.22760200
C	3.44581400	2.06079800	-2.69614500
H	3.51553100	3.03546100	-3.21563800
H	4.21445500	1.38291600	-3.12041200
H	2.46193400	1.61061700	-2.94530700
C	3.88652900	0.02440400	1.94024100
H	2.96544400	-0.59323700	1.90331000
H	4.71577900	-0.63890100	1.61712500
H	4.06186200	0.31679700	2.99260800
C	4.11294300	5.05222600	1.33637500

H	3.11593700	5.50565600	1.52995200
H	4.65258300	5.03372400	2.30385200
H	4.65345400	5.73534800	0.65049300
C	1.79215200	6.46606100	-2.05403200
H	2.42206300	6.57173200	-1.14632800
H	2.46221400	6.26546100	-2.91279800
H	1.31428400	7.45392700	-2.22760200
C	-4.11294300	-5.05222600	1.33637500
H	-3.11593700	-5.50565600	1.52995200
H	-4.65258300	-5.03372400	2.30385200
H	-4.65345400	-5.73534800	0.65049300
C	-3.88652900	-0.02440400	1.94024100
H	-4.71577900	0.63890100	1.61712500
H	-4.06186200	-0.31679700	2.99260800
H	-2.96544400	0.59323700	1.90331000
C	-0.51913300	2.28120300	-3.75616700
H	-1.54614400	2.25811000	-4.17552900
H	0.19470400	2.43066200	-4.58905500
H	-0.33911700	1.27400900	-3.32339700
C	-2.05646000	4.50005000	0.56852400
H	-1.66735500	5.18639300	1.34610800
H	-3.04994000	4.88352800	0.25290900
H	-2.24699400	3.51328000	1.03567600
C	-3.44581400	-2.06079800	-2.69614500
H	-3.51553100	-3.03546100	-3.21563800
H	-4.21445500	-1.38291600	-3.12041200
H	-2.46193400	-1.61061700	-2.94530700
C	0.28591500	0.61993900	1.60153300
C	-0.28591500	-0.61993900	1.60153300
C	0.72265400	1.50041200	2.69718100
C	1.25518300	0.99717700	3.91240700
C	0.64583400	2.90799900	2.54446800
C	1.66650600	1.86350300	4.93240300
H	1.35755300	-0.08875000	4.04754700
C	1.03977800	3.77293000	3.57511400
H	0.27320100	3.32869500	1.59863100
C	1.55144500	3.25668400	4.77580500
H	2.08199500	1.44655800	5.86312900
H	0.95385800	4.86149300	3.43264200
H	1.86694300	3.93425900	5.58400400
C	-0.72265400	-1.50041200	2.69718100
C	-1.25518300	-0.99717700	3.91240700
C	-0.64583400	-2.90799900	2.54446800
C	-1.66650600	-1.86350300	4.93240300
H	-1.35755300	0.08875000	4.04754700
C	-1.03977800	-3.77293000	3.57511400
H	-0.27320100	-3.32869500	1.59863100
C	-1.55144500	-3.25668400	4.77580500
H	-2.08199500	-1.44655800	5.86312900
H	-0.95385800	-4.86149300	3.43264200
H	-1.86694300	-3.93425900	5.58400400

Optimized structure of **4As** (PBE/def2svp):

N	-1.10308500	0.50492100	-0.71755800
N	1.10308500	-0.50492100	-0.71755800
As	0.60297800	1.27918200	-0.20937800
As	-0.60297800	-1.27918200	-0.20937800
C	2.33849600	-1.05231300	-1.04710800
C	3.55019300	-0.28395100	-0.95911700

C	2.45347300	-2.40232200	-1.52808400
C	4.77391800	-0.83217100	-1.38815200
C	3.70409800	-2.90706200	-1.93342800
C	4.87048500	-2.13600400	-1.88658900
H	5.67542200	-0.20412000	-1.30381900
H	3.74171400	-3.94302600	-2.30682400
H	5.83533200	-2.54649300	-2.21863300
C	-2.33849600	1.05231300	-1.04710800
C	-2.45347300	2.40232200	-1.52808400
C	-3.55019300	0.28395100	-0.95911700
C	-3.70409800	2.90706200	-1.93342800
C	-4.77391800	0.83217100	-1.38815200
C	-4.87048500	2.13600400	-1.88658900
H	-3.74171400	3.94302600	-2.30682400
H	-5.67542200	0.20412000	-1.30381900
H	-5.83533200	2.54649300	-2.21863300
C	-3.61002300	-1.08783900	-0.36054300
C	-3.65690100	-2.24023000	-1.19189500
C	-3.78728200	-1.22034800	1.04659500
C	-3.82003100	-3.50379700	-0.59681300
C	-3.93134200	-2.50598900	1.59859300
C	-3.94055600	-3.66240400	0.79610900
H	-3.85035300	-4.39484600	-1.24386000
H	-4.04839300	-2.60366400	2.69024400
C	-1.29899400	3.34998400	-1.63130200
C	-1.14482300	4.37775900	-0.65938600
C	-0.44196100	3.31557600	-2.76398100
C	-0.12047400	5.32842100	-0.82502700
C	0.55379600	4.30089400	-2.89876000
C	0.73434700	5.31674500	-1.94268800
H	-0.00076000	6.11769900	-0.06374300
H	1.20632800	4.27640800	-3.78697200
C	1.29899400	-3.34998400	-1.63130200
C	1.14482300	-4.37775900	-0.65938600
C	0.44196100	-3.31557600	-2.76398100
C	0.12047400	-5.32842100	-0.82502700
C	-0.55379600	-4.30089400	-2.89876000
C	-0.73434700	-5.31674500	-1.94268800
H	0.00076000	-6.11769900	-0.06374300
H	-1.20632800	-4.27640800	-3.78697200
C	3.61002300	1.08783900	-0.36054300
C	3.78728200	1.22034800	1.04659500
C	3.65690100	2.24023000	-1.19189500
C	3.93134200	2.50598900	1.59859300
C	3.82003100	3.50379700	-0.59681300
C	3.94055600	3.66240400	0.79610900
H	4.04839300	2.60366400	2.69024400
H	3.85035300	4.39484600	-1.24386000
C	2.08535500	-4.48169600	0.51945400
H	1.69967700	-5.18839800	1.28029800
H	3.08646100	-4.84405600	0.20368600
H	2.26054800	-3.50157500	1.00690500
C	0.60297800	-2.24252700	-3.81318800
H	1.63043100	-2.23891800	-4.23170100
H	-0.11350100	-2.37819700	-4.64629900
H	0.44252600	-1.23279500	-3.37875100
C	-1.77824000	-6.39203500	-2.12638700
H	-2.30658700	-6.61452000	-1.17698500
H	-2.53495200	-6.10705800	-2.88355400
H	-1.31535900	-7.34367600	-2.46654600
C	3.52643400	2.10930600	-2.68997800

H	3.59049900	3.09619300	-3.18682400
H	4.31355300	1.45257500	-3.11316100
H	2.55518700	1.64913500	-2.96961100
C	3.87371000	-0.00535100	1.92214700
H	2.94412400	-0.60953600	1.87409700
H	4.69464200	-0.67290600	1.58774300
H	4.05048800	0.26868800	2.97911500
C	4.06055100	5.03072900	1.41957200
H	3.09833300	5.33588400	1.88523200
H	4.82274500	5.04896500	2.22502000
H	4.33026000	5.80244900	0.67179600
C	1.77824000	6.39203500	-2.12638700
H	2.30658700	6.61452000	-1.17698500
H	2.53495200	6.10705800	-2.88355400
H	1.31535900	7.34367600	-2.46654600
C	-4.06055100	-5.03072900	1.41957200
H	-3.09833300	-5.33588400	1.88523200
H	-4.82274500	-5.04896500	2.22502000
H	-4.33026000	-5.80244900	0.67179600
C	-3.87371000	0.00535100	1.92214700
H	-4.69464200	0.67290600	1.58774300
H	-4.05048800	-0.26868800	2.97911500
H	-2.94412400	0.60953600	1.87409700
C	-0.60297800	2.24252700	-3.81318800
H	-1.63043100	2.23891800	-4.23170100
H	0.11350100	2.37819700	-4.64629900
H	-0.44252600	1.23279500	-3.37875100
C	-2.08535500	4.48169600	0.51945400
H	-1.69967700	5.18839800	1.28029800
H	-3.08646100	4.84405600	0.20368600
H	-2.26054800	3.50157500	1.00690500
C	-3.52643400	-2.10930600	-2.68997800
H	-3.59049900	-3.09619300	-3.18682400
H	-4.31355300	-1.45257500	-3.11316100
H	-2.55518700	-1.64913500	-2.96961100
C	0.27973300	0.62009900	1.72642500
C	-0.27973300	-0.62009900	1.72642500
C	0.71720400	1.48031800	2.83966800
C	1.30304900	0.94983200	4.01851000
C	0.59346500	2.88979400	2.74440000
C	1.72634800	1.79011500	5.05555200
H	1.43328100	-0.13769300	4.11095300
C	1.00172000	3.72841600	3.79158800
H	0.16766500	3.33533800	1.83245000
C	1.57144900	3.18426900	4.95336100
H	2.18293000	1.35160400	5.95668000
H	0.87767900	4.81837800	3.69457800
H	1.89864200	3.84147700	5.77356600
C	-0.71720400	-1.48031800	2.83966800
C	-1.30304900	-0.94983200	4.01851000
C	-0.59346500	-2.88979400	2.74440000
C	-1.72634800	-1.79011500	5.05555200
H	-1.43328100	0.13769300	4.11095300
C	-1.00172000	-3.72841600	3.79158800
H	-0.16766500	-3.33533800	1.83245000
C	-1.57144900	-3.18426900	4.95336100
H	-2.18293000	-1.35160400	5.95668000
H	-0.87767900	-4.81837800	3.69457800
H	-1.89864200	-3.84147700	5.77356600

Optimized structure of **4Sb** (PBE/def2svp):

N	1.31884000	0.13713200	-0.69797500
N	-1.31884000	-0.13713200	-0.69797500
Sb	0.14577100	-1.58419100	-0.15183700
Sb	-0.14577100	1.58419100	-0.15183700
C	-2.61531400	-0.30401700	-1.15057400
C	-3.28394100	-1.58212400	-1.10048700
C	-3.36838100	0.79010300	-1.70984800
C	-4.57577700	-1.73858900	-1.63622000
C	-4.66251900	0.58585300	-2.22261100
C	-5.27805200	-0.67187800	-2.20980900
H	-5.04438200	-2.73397800	-1.57047300
H	-5.19081800	1.45454100	-2.64824500
H	-6.28816300	-0.81342300	-2.62112900
C	2.61531400	0.30401700	-1.15057400
C	3.36838100	-0.79010300	-1.70984800
C	3.28394100	1.58212400	-1.10048700
C	4.66251900	-0.58585300	-2.22261100
C	4.57577700	1.73858900	-1.63622000
C	5.27805200	0.67187800	-2.20980900
H	5.19081800	-1.45454100	-2.64824500
H	5.04438200	2.73397800	-1.57047300
H	6.28816300	0.81342300	-2.62112900
C	2.68020400	2.77222700	-0.42544800
C	2.18233700	3.86964700	-1.18219600
C	2.72172800	2.85776500	0.99902200
C	1.68342200	4.99771600	-0.50380700
C	2.18836900	3.99491400	1.63288100
C	1.65643300	5.07430100	0.90033600
H	1.28866500	5.83993500	-1.09443100
H	2.20060400	4.04222700	2.73409600
C	2.83538400	-2.18733300	-1.76835600
C	3.21928800	-3.12727300	-0.77089300
C	2.03107300	-2.60806600	-2.86166400
C	2.78165400	-4.46058000	-0.88012400
C	1.62605600	-3.95445200	-2.93582500
C	1.99176900	-4.89922500	-1.95934500
H	3.07943300	-5.18331500	-0.10202600
H	1.00920500	-4.27598800	-3.79108900
C	-2.83538400	2.18733300	-1.76835600
C	-3.21928800	3.12727300	-0.77089300
C	-2.03107300	2.60806600	-2.86166400
C	-2.78165400	4.46058000	-0.88012400
C	-1.62605600	3.95445200	-2.93582500
C	-1.99176900	4.89922500	-1.95934500
H	-3.07943300	5.18331500	-0.10202600
H	-1.00920500	4.27598800	-3.79108900
C	-2.68020400	-2.77222700	-0.42544800
C	-2.72172800	-2.85776500	0.99902200
C	-2.18233700	-3.86964700	-1.18219600
C	-2.18836900	-3.99491400	1.63288100
C	-1.68342200	-4.99771600	-0.50380700
C	-1.65643300	-5.07430100	0.90033600
H	-2.20060400	-4.04222700	2.73409600
H	-1.28866500	-5.83993500	-1.09443100
C	-4.10313400	2.70947600	0.38415000
H	-4.17865200	3.51034600	1.14552100
H	-5.13035200	2.47169800	0.03703900
H	-3.73369800	1.78723100	0.87740200
C	-1.62834400	1.62369900	-3.93007800

H	-2.51662600	1.19181600	-4.43537600
H	-0.98724700	2.09888700	-4.69772900
H	-1.07450200	0.76610900	-3.49338300
C	-1.59141200	6.34908400	-2.08159400
H	-1.29276300	6.77544700	-1.10245400
H	-0.74913300	6.48391600	-2.78837400
H	-2.43645000	6.96629900	-2.45656500
C	-2.17266800	-3.82325400	-2.68986900
H	-1.66504400	-4.71092900	-3.11412300
H	-3.19992300	-3.78198600	-3.10633900
H	-1.65476300	-2.91546300	-3.06349200
C	-3.36838100	-1.76189100	1.81033000
H	-2.82031800	-0.80231500	1.70597100
H	-4.40326300	-1.57298900	1.45805900
H	-3.40141200	-2.02412800	2.88433700
C	-1.08939900	-6.27740900	1.61470300
H	-0.28780000	-5.97897400	2.32236200
H	-1.86738700	-6.79451100	2.21536200
H	-0.66632200	-7.01515000	0.90503300
C	1.59141200	-6.34908400	-2.08159400
H	1.29276300	-6.77544700	-1.10245400
H	0.74913300	-6.48391600	-2.78837400
H	2.43645000	-6.96629900	-2.45656500
C	1.08939900	6.27740900	1.61470300
H	0.28780000	5.97897400	2.32236200
H	1.86738700	6.79451100	2.21536200
H	0.66632200	7.01515000	0.90503300
C	3.36838100	1.76189100	1.81033000
H	4.40326300	1.57298900	1.45805900
H	3.40141200	2.02412800	2.88433700
H	2.82031800	0.80231500	1.70597100
C	1.62834400	-1.62369900	-3.93007800
H	2.51662600	-1.19181600	-4.43537600
H	0.98724700	-2.09888700	-4.69772900
H	1.07450200	-0.76610900	-3.49338300
C	4.10313400	-2.70947600	0.38415000
H	4.17865200	-3.51034600	1.14552100
H	5.13035200	-2.47169800	0.03703900
H	3.73369800	-1.78723100	0.87740200
C	2.17266800	3.82325400	-2.68986900
H	1.66504400	4.71092900	-3.11412300
H	3.19992300	3.78198600	-3.10633900
H	1.65476300	2.91546300	-3.06349200
C	0.07944600	-0.67425800	1.93338000
C	-0.07944600	0.67425800	1.93338000
C	0.13003600	-1.60104400	3.08114000
C	-0.74386300	-1.46763000	4.19146700
C	1.03532400	-2.69235400	3.08680000
C	-0.70682700	-2.37940600	5.25435100
H	-1.46406400	-0.63697200	4.20711800
C	1.08173000	-3.59614000	4.15859100
H	1.72420500	-2.82597200	2.23752200
C	0.20807900	-3.44724000	5.24785700
H	-1.40056600	-2.25450600	6.10059600
H	1.80613000	-4.42554600	4.14025300
H	0.23743900	-4.15964500	6.08648800
C	-0.13003600	1.60104400	3.08114000
C	0.74386300	1.46763000	4.19146700
C	-1.03532400	2.69235400	3.08680000
C	0.70682700	2.37940600	5.25435100
H	1.46406400	0.63697200	4.20711800

C	-1.08173000	3.59614000	4.15859100
H	-1.72420500	2.82597200	2.23752200
C	-0.20807900	3.44724000	5.24785700
H	1.40056600	2.25450600	6.10059600
H	-1.80613000	4.42554600	4.14025300
H	-0.23743900	4.15964500	6.08648800

Optimized structure of **4Bi** (PBE/def2svp):

N	-1.25504000	0.57831400	-0.71634200
N	1.25504000	-0.57831400	-0.71634200
Bi	0.72161900	1.51314200	-0.13638400
Bi	-0.72161900	-1.51314200	-0.13638400
C	2.45406100	-1.09259400	-1.14948400
C	3.68421400	-0.33219400	-1.10886500
C	2.55482400	-2.42962400	-1.68676200
C	4.87906300	-0.86450900	-1.62615500
C	3.77578700	-2.92272400	-2.17974500
C	4.94622300	-2.15233800	-2.17317000
H	5.78861300	-0.24442900	-1.56783300
H	3.79271000	-3.94765600	-2.58547500
H	5.89114000	-2.55217700	-2.56890500
C	-2.45406100	1.09259400	-1.14948400
C	-2.55482400	2.42962400	-1.68676200
C	-3.68421400	0.33219400	-1.10886500
C	-3.77578700	2.92272400	-2.17974500
C	-4.87906300	0.86450900	-1.62615500
C	-4.94622300	2.15233800	-2.17317000
H	-3.79271000	3.94765600	-2.58547500
H	-5.78861300	0.24442900	-1.56783300
H	-5.89114000	2.55217700	-2.56890500
C	-3.76077200	-1.01226900	-0.45732800
C	-3.87686000	-2.19925900	-1.23428600
C	-3.83043900	-1.09385900	0.96722500
C	-4.01003300	-3.43889800	-0.57709800
C	-3.93811400	-2.35675000	1.57907000
C	-4.02495400	-3.54456200	0.82524000
H	-4.09331600	-4.35411900	-1.18492300
H	-3.96883800	-2.41109000	2.67957400
C	-1.37777800	3.35124500	-1.73802400
C	-1.19781800	4.32954400	-0.71954500
C	-0.48382700	3.31360500	-2.84342500
C	-0.13162500	5.24379800	-0.82539500
C	0.55998900	4.25693200	-2.91510000
C	0.75183100	5.23498900	-1.92142800
H	0.00127300	5.99893400	-0.03247200
H	1.24111000	4.22929300	-3.78166600
C	1.37777800	-3.35124500	-1.73802400
C	1.19781800	-4.32954400	-0.71954500
C	0.48382700	-3.31360500	-2.84342500
C	0.13162500	-5.24379800	-0.82539500
C	-0.55998900	-4.25693200	-2.91510000
C	-0.75183100	-5.23498900	-1.92142800
H	-0.00127300	-5.99893400	-0.03247200
H	-1.24111000	-4.22929300	-3.78166600
C	3.76077200	1.01226900	-0.45732800
C	3.83043900	1.09385900	0.96722500
C	3.87686000	2.19925900	-1.23428600
C	3.93811400	2.35675000	1.57907000
C	4.01003300	3.43889800	-0.57709800

C	4.02495400	3.54456200	0.82524000
H	3.96883800	2.41109000	2.67957400
H	4.09331600	4.35411900	-1.18492300
C	2.14986100	-4.40353000	0.45198500
H	1.78430500	-5.10800000	1.22458000
H	3.15675300	-4.74233900	0.13040200
H	2.30423800	-3.41089200	0.92210000
C	0.66281700	-2.28066000	-3.92888600
H	1.64991700	-2.38695300	-4.42392400
H	-0.12627800	-2.36123900	-4.70155500
H	0.63787600	-1.25444400	-3.50558800
C	-1.84026800	-6.27361100	-2.04230000
H	-2.34045400	-6.45686800	-1.06978300
H	-2.61323100	-5.97666800	-2.77804000
H	-1.42420400	-7.24799000	-2.37833100
C	3.85349900	2.13938600	-2.74325000
H	3.78936600	3.15323700	-3.18381200
H	4.76408000	1.64820600	-3.14454600
H	2.99675800	1.54052600	-3.11504400
C	3.83043900	-0.16394600	1.79957700
H	2.87764600	-0.72259400	1.68839500
H	4.63795700	-0.85008000	1.47120000
H	3.97162300	0.06597700	2.87214800
C	4.14289100	4.88102300	1.51636700
H	3.28816900	5.05148800	2.20411600
H	5.06307900	4.93485400	2.13559000
H	4.17542200	5.71786700	0.79149200
C	1.84026800	6.27361100	-2.04230000
H	2.34045400	6.45686800	-1.06978300
H	2.61323100	5.97666800	-2.77804000
H	1.42420400	7.24799000	-2.37833100
C	-4.14289100	-4.88102300	1.51636700
H	-3.28816900	-5.05148800	2.20411600
H	-5.06307900	-4.93485400	2.13559000
H	-4.17542200	-5.71786700	0.79149200
C	-3.83043900	0.16394600	1.79957700
H	-4.63795700	0.85008000	1.47120000
H	-3.97162300	-0.06597700	2.87214800
H	-2.87764600	0.72259400	1.68839500
C	-0.66281700	2.28066000	-3.92888600
H	-1.64991700	2.38695300	-4.42392400
H	0.12627800	2.36123900	-4.70155500
H	-0.63787600	1.25444400	-3.50558800
C	-2.14986100	4.40353000	0.45198500
H	-1.78430500	5.10800000	1.22458000
H	-3.15675300	4.74233900	0.13040200
H	-2.30423800	3.41089200	0.92210000
C	-3.85349900	-2.13938600	-2.74325000
H	-3.78936600	-3.15323700	-3.18381200
H	-4.76408000	-1.64820600	-3.14454600
H	-2.99675800	-1.54052600	-3.11504400
C	0.27737200	0.61702800	2.03041400
C	-0.27737200	-0.61702800	2.03041400
C	0.73081000	1.43120600	3.17362800
C	1.43780800	0.85749200	4.26333400
C	0.52162600	2.83425100	3.19690800
C	1.90958100	1.64936100	5.31825500
H	1.62060800	-0.22689300	4.26762400
C	0.98114200	3.62405900	4.26129700
H	-0.02552400	3.31144600	2.36740300
C	1.68290900	3.03711300	5.32691000

H	2.46034200	1.17705500	6.14696700
H	0.79041300	4.70887300	4.25620800
H	2.05221400	3.65640400	6.15859500
C	-0.73081000	-1.43120600	3.17362800
C	-1.43780800	-0.85749200	4.26333400
C	-0.52162600	-2.83425100	3.19690800
C	-1.90958100	-1.64936100	5.31825500
H	-1.62060800	0.22689300	4.26762400
C	-0.98114200	-3.62405900	4.26129700
H	0.02552400	-3.31144600	2.36740300
C	-1.68290900	-3.03711300	5.32691000
H	-2.46034200	-1.17705500	6.14696700
H	-0.79041300	-4.70887300	4.25620800
H	-2.05221400	-3.65640400	6.15859500

Optimized structure of **2P**H (CAS(6,4)/def2svp):

H	0.00000000	0.00000000	2.08806600
H	0.00000000	0.00000000	-2.08806600
N	0.00000000	0.00000000	1.08833100
N	0.00000000	0.00000000	-1.08833100
P	0.00000000	1.30736400	0.00000000
P	0.00000000	-1.30736400	0.00000000

Optimized structure of **2As**H (CAS(6,4)/def2svp):

H	0.00000000	0.00000000	2.14739800
H	0.00000000	0.00000000	-2.14739800
N	0.00000000	0.00000000	1.14702300
N	0.00000000	0.00000000	-1.14702300
As	0.00000000	1.41451400	0.00000000
As	0.00000000	-1.41451400	0.00000000

Optimized structure of **2Sb**H (CAS(6,4)/def2svp):

H	0.00000000	0.00000000	2.24935200
H	0.00000000	0.00000000	-2.24935200
N	0.00000000	0.00000000	1.24695400
N	0.00000000	0.00000000	-1.24695400
Sb	0.00000000	1.59656600	0.00000000
Sb	0.00000000	-1.59656600	0.00000000

Optimized structure of **2Bi**H (CAS(6,4)/def2svp):

H	0.00000000	0.00000000	2.29709800
H	0.00000000	0.00000000	-2.29709800
N	0.00000000	0.00000000	1.29252000
N	0.00000000	0.00000000	-1.29252000
Bi	0.00000000	1.68555800	0.00000000
Bi	0.00000000	-1.68555800	0.00000000

Optimized structure of **2P**H (CCSD/def2svp):

H	0.00000000	0.00000000	2.09380800
H	0.00000000	0.00000000	-2.09380800
N	0.00000000	0.00000000	1.08778400
N	0.00000000	0.00000000	-1.08778400

P	0.00000000	1.30538800	0.00000000
P	0.00000000	-1.30538800	0.00000000

Optimized structure of **2As**H (CCSD/def2svp):

H	0.00000000	0.00000000	2.15448600
H	0.00000000	0.00000000	-2.15448600
N	0.00000000	0.00000000	1.14698700
N	0.00000000	0.00000000	-1.14698700
As	0.00000000	1.41845700	0.00000000
As	0.00000000	-1.41845700	0.00000000

Optimized structure of **2Sb**H (CCSD/def2svp):

H	0.00000000	0.00000000	2.24499900
H	0.00000000	0.00000000	-2.24499900
N	0.00000000	0.00000000	1.23509700
N	0.00000000	0.00000000	-1.23509700
Sb	0.00000000	1.58082800	0.00000000
Sb	0.00000000	-1.58082800	0.00000000

Optimized structure of **2Bi**H (CCSD/def2svp):

H	0.00000000	0.00000000	2.29077500
H	0.00000000	0.00000000	-2.29077500
N	0.00000000	0.00000000	1.27882000
N	0.00000000	0.00000000	-1.27882000
Bi	0.00000000	1.66626000	0.00000000
Bi	0.00000000	-1.66626000	0.00000000

4. References

[1] S. Demeshko, C. Godemann, R. Kuzora, A. Schulz, A. Villinger, *Angew. Chem. Int. Ed.* **2013**, *52*, 2105–2108.

[2] D. Michalik, A. Schulz, A. Villinger, *Angew. Chem. Int. Ed.* **2010**, *49*, 7575–7577.

[3] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw, K. I. Goldberg, *Organometallics* **2010**, *29*, 2176–2179.

[4] G. M. Sheldrick, *SHELXS-2013: Program for the Solution of Crystal Structures*, University of Göttingen, Germany, **2013**.

[5] G. M. Sheldrick, *SHELXL-2013: Program for the Refinement of Crystal Structures*, University of Göttingen, Germany, **2013**.

[6] G. M. Sheldrick, *SADABS Version 2*, University of Göttingen, Germany, **2004**.

[7] *Gaussian 09, Revision C.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Peterson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Know, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrezewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.

[8] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, F. Weinhold, *NBO 6.0*, Theoretical Chemistry Institute, University of Wisconsin, Madison, **2013**.

[9] J. E. Carpenter, F. Weinhold, *J. Mol. Struct.: THEOCHEM* **1988**, *169*, 41–62.

[10] F. Weinhold, J. E. Carpenter, *The Structure of Small Molecules and Ions*, Plenum Press, **1988**.

[11] F. Weinhold, C. R. Landis, *Valency and Bonding. A Natural Bond Orbital Donor-Acceptor Perspective*, Cambridge University Press, **2005**.

[12] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.

[13] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1997**, *78*, 1396–1396.

[14] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–305.

[15] B. Metz, H. Stoll, M. Dolg, *J. Chem. Phys.* **2000**, *113*, 2563–2569.

[16] C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158–6170.

[17] D. H. Ess, E. R. Johnson, X. Hu, W. Yang, *J. Phys. Chem. A* **2011**, *115*, 76–83.

[18] D. Hegarty, M. A. Robb, *Mol. Phys.* **1979**, *38*, 1795–1812.

[19] R. H. A. Eade, M. A. Robb, *Chem. Phys. Lett.* **1981**, *83*, 362–368.

[20] H. B. Schlegel, M. A. Robb, *Chem. Phys. Lett.* **1982**, *93*, 43–46.

[21] F. Bernardi, A. Bottoni, J. J. W. McDouall, M. A. Robb, H. B. Schlegel, *Faraday Symp. Chem. Soc.* **1984**, *19*, 137.

[22] P. E. M. Siegbahn, *Chem. Phys. Lett.* **1984**, *109*, 417–423.

[23] M. A. Robb, U. Niazi, in *Reports Mol. Theory, Vol. 1* (Eds.: H. Weinstein, G. Náray-Szabó), CRC Press, Boca Raton, FL, **1990**, pp. 23–55.

[24] M. Frisch, I. N. Ragazos, M. A. Robb, H. B. Schlegel, *Chem. Phys. Lett.* **1992**, *189*, 524–528.

[25] N. Yamamoto, T. Vreven, M. A. Robb, M. J. Frisch, H. B. Schlegel, *Chem. Phys. Lett.* **1996**, *250*, 373–378.

[26] M. Klene, M. A. Robb, M. J. Frisch, P. Celani, *J. Chem. Phys.* **2000**, *113*, 5653–5665.

[27] E. Miliordos, K. Ruedenberg, S. S. Xantheas, *Angew. Chem. Int. Ed.* **2013**, *52*, 5736–5739.