Supporting information

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1. Methods and materials

1.1. Experimental Considerations

All manipulations were performed under a nitrogen atmosphere using standard Schlenk-line and glovebox methodology. All glassware was flame-dried before use.

Innovative Technologies anhydrous engineering solvent purification system was used to obtain dry THF, Et_2O, toluene and pentane. Solvents obtained in this way were subsequently degassed. DME was dried over Na and purified by distillation. Toluene-d_8, C_6D_6, THF-d_8 and $CDCl_3$ were dried over 3 Å molecular sieves.

Elemental red phosphorus (Sigma-Aldrich), Elemental grey arsenic (Alfa-Aesar), Naphthalene (Fluorochem), Me_3SiCl (Sigma-Aldrich), Me_3SnCl (Sigma-Aldrich), $^nBu_3SnCl$ (Sigma-Aldrich), Me_3GeCl (Alfa-Aesar), Et_3GeCl (Alfa-Aesar), PhNCO (Sigma-Aldrich), PhNCS (Sigma-Aldrich), *p*-toluenesulfonyl isocyanate (Fluorochem) were purchased from respective vendors and used without further purification. Elemental sodium (Scientific Laboratories Supplies) was cleaned by removal of the oxide layer and washed with toluene/hexane. $[Na(DME)_x]_3P_7$,[1] $(Me_3Ge)_3P_7$ and $(Me_3Si)_3As_7$ were synthesised using previously reported experimental procedures.[1-3]

1.2. Analytical Considerations

NMR spectroscopy – ^1H, $^{13}C\{^1H\}$, ^{29}Si DEPT90, ^{31}P, ^{119}Sn NMR spectra were recorded on a Bruker AVIII 400 spectrometer (operating frequencies: 399.78 MHz, 100.53 MHz, 79.48 MHz, 161.83 MHz and 149.14 MHz for ^1H, ^{13}C, ^{29}Si, ^{31}P and ^{119}Sn respectively). ^1H and ^{13}C chemical shifts were internally referenced to the residual solvent resonances (C_6D_6: ^1H δ = 7.16 ppm, $^{13}C\{^1H\}$ δ = 128.02 ppm, THF-d_8: ^1H δ = 3.58, 1.73 ppm, $^{13}C\{^1H\}$ δ = 67.57, 25.37 ppm, toluene-d_8 ^1H δ = 7.09, 7.00, 6.98, 2.09 ppm, $^{13}C\{^1H\}$ δ = 137.86, 129.24, 128.33, 125.49, 20.4 ppm, $CDCl_3$: ^1H δ = 7.26 ppm, $^{13}C\{^1H\}$ δ = 77.36 ppm). ^{29}Si, ^{31}P and ^{119}Sn chemical shifts were externally referenced to Me_4Si, H_3PO_4 and Me_4Sn respectively. NMR samples were prepared under an inert nitrogen atmosphere in a 5 mm J Young NMR tube.

Elemental analysis – Elemental analysis was carried out by the microanalysis service of the University of Manchester using a Flash 2000 elemental analyser.

Mass spectrometry – Mass spectrometry was carried out by the mass spectrometry service of the University of Manchester using an electrospray ionisation equipped Thermo Orbitrap

Executive Plus Extended Mass Range mass spectrometer. Mass spectrometry samples were prepared under an inert nitrogen atmosphere and injected directly into the ionisation source of the spectrometer.

Infrared spectroscopy - ATR-IR spectra were recorded as microcrystalline powders or oils using a Bruker Tensor 27 spectrometer under an inert nitrogen atmosphere.

1.3. X-ray diffraction Studies

Data collection: Data collection: X-ray diffraction data was collected for compounds **5**, **6**, **7**, **8** and **11** on a dual source Rigaku FR-X rotating anode at 100 K with Cu-Kα (1.54184 Å) radiation, equipped with a Hypix000HE detector and Oxford cryosystem. X-ray data was collected using CrysAlisPro software.

Crystal structure determination and refinements: X-ray data processed and reduced using CrysAlisPro. Absorption correction was performed using empirical methods (SCALE3 ABSPACK) based upon symmetry-equivalent reflections combined with measurements at different azimuthal angles. The crystal structure was solved and refined against all F^2 values using the SHELX and Olex2 suite of programmes.[4, 5]All atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions and refined using idealised geometries and assigned fixed isotropic displacement parameters.

Crystallographic data have been deposited with the CCDC (CCDC 2202018-2202022).

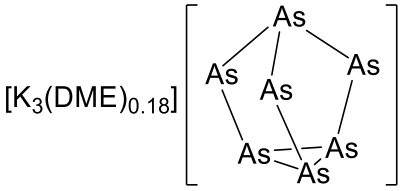
1.4. General computational considerations

Density Functional Theory (DFT) calculations were performed with the Gaussian09 program package3 (version g09, rev.d01).[6-8] Geometry optimisation and frequency calculations were performed at the BP86/SV(p) or PBE1PBE/6-311G(d,p) levels of theory. The SV(p) basis set was used for Sn atoms. No symmetry constraints were applied during optimisation. All minima were confirmed by the absence of imaginary frequencies. Initial geometries were prepared using X-ray diffraction coordinates where available and Facio V22.1.1.64 software. Gibbs free

energies and enthalpies were calculated at standard conditions (p = 1 atm, T = 298 K) and are unscaled.

2. Synthesis and Characterisation Data

2.1. Synthesis of $[K_3(DME)_x][As_7]$

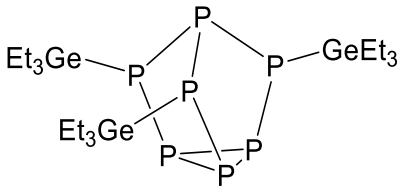


A Schlenk flask was loaded with grey arsenic (4.50 g, 60 mmol, 7 eq.), potassium (1.00 g, 25 mmol, 3 eq.) and naphthalene (109 mg, 0.85 mmol, 0.1 eq.). The powder mixture was cooled to 0 °C and suspended in THF (18 mL) and DME (18 mL). The reaction mixture was stirred while closely monitoring the temperature of the reaction, cooling if the temperature exceeded 50 °C, to prevent auto-acceleration. Once a stable temperature had been reached, the reaction was left to stir overnight to give a dark suspension. The headspace of the flask was removed under vacuum and the reaction mixture was slowly heated to 55 °C over the course of a day and left to stir over 7 days until a red suspension was observed. The suspension was cooled to room temperature and was washed with pentane (3 x 40 mL). The product was then dried under vacuum over the course of a day, yielding a red powder (4.98 g). Elemental analysis (Found: C 1.34, H 0.23) was used to determine the DME content as 0.18 equivalents. All characterization data was in line with literature precedence.[9, 10]

Mass spectrometry (ESI pos/neg): For K_3As_7+H ($[M+H]^+$): Calcd.: 642.3507; found: 642.3507.

2.2. Synthesis and Characterisation of $(R_3E)_3Pn_7$

2.2.1. Synthesis of $(Et_3Ge)_3P_7$, 2



A Schlenk flask was loaded with a stir bar and $[Na(DME)_x]_3[P_7]$ (2.0 g, 7.0 mmol), which were suspended in toluene (10 mL) to give a dark green suspension. The suspension was cooled to –80 °C and Et_3GeCl (3.5 mL, 21 mmol) was added dropwise with rapid stirring, affording a

yellow green solution with a brown suspension. The reaction was left to stir for 2 days, the reaction was then filtered and the residue washed with toluene (3 x 3 mL). Solvent was subsequently removed to give a yellow/green liquid. The crude product was then washed with toluene (3 mL) and dried under reduced pressure, and the product isolated as an oil.

Isolated yield: 2.97 g, 61%

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ = 1.17 (t, $^{3}J_{HH}$ = 7.4 Hz, 9H, C*H*$_3$), 1.08 (q, $^{3}J_{HH}$ = 7.9 Hz, 6H, C*H*$_2$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ = 9.9 (s, *C*H$_2$), 9.6 (s, *C*H$_3$) ppm.

^{31}P NMR (162 MHz, 298K, THF-d$_8$): δ = –4.4 - –13.1 (m, 3P, *bridging*), –103.6 (qq, $^{1}J_{PP}$ = 332.4 Hz, $^{2}J_{PP}$ = 48.1 Hz, 1P, *apical*), –163.6 - –170.0 (m, 3P, *basal*) ppm.

Mass spectrometry (ESI pos/neg): For $C_{18}H_{45}Ge_3P_7$+Li ([M+Li]$^+$): Calcd.: 706.9480; found: 706.9499.

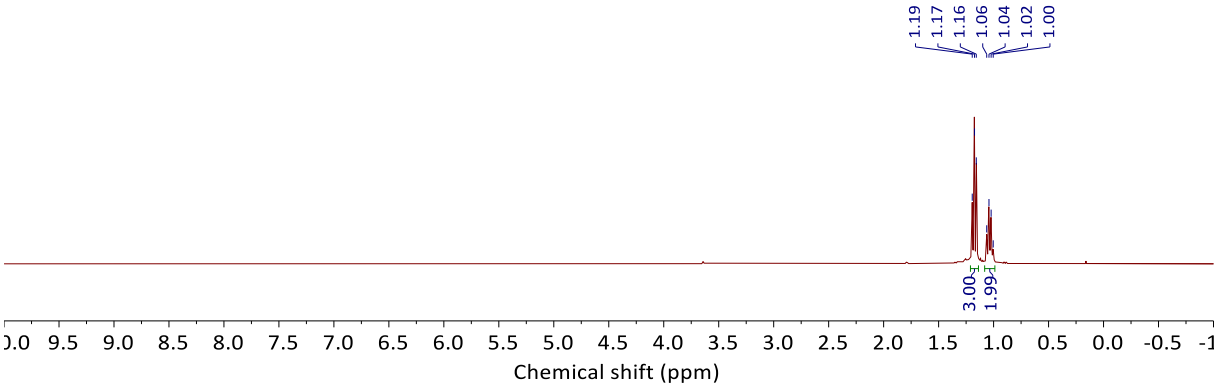


Figure S1. ^{1}H NMR spectrum (THF-d$_8$) of **2**.

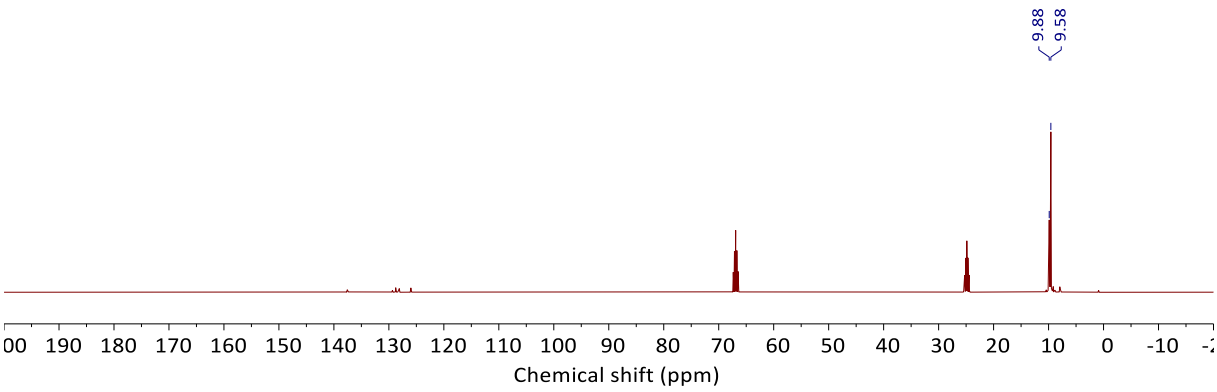


Figure S2. ^{13}C{^{1}H} NMR spectrum (THF-d$_8$) of **2**.

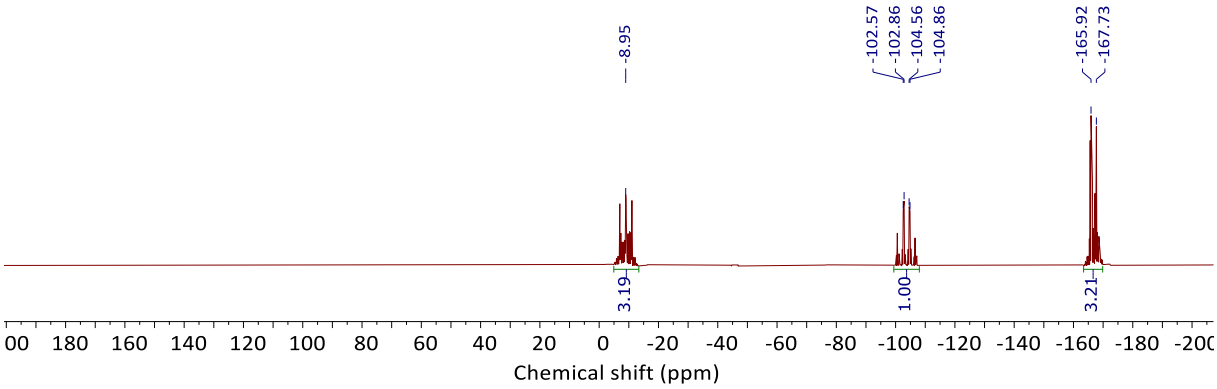
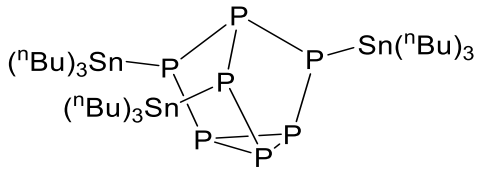


Figure S3. ^{31}P NMR spectrum (THF-d_8) of **2**.

2.2.2. Synthesis of (^{n}Bu$_3$Sn)$_3$P$_7$, 3



A Schlenk flask was loaded with a stir bar and [Na(DME)$_x$]$_3$[P$_7$] (500 mg, 1.75 mmol). Toluene (10 mL) was added to give a dark green suspension. The suspension was cooled, while stirring, to –80 °C. Once cooled, ^{n}Bu$_3$SnCl (1.40 mL, 5.25 mmol) was added dropwise with rapid stirring. The reaction was allowed to warm up to room temperature, by which point, a yellow/green solution with a black suspension was observed. The reaction was stirred for 5 days. The reaction was then filtered and solvent removed to give the product as a yellow oil. The crude product was washed with ether (3 mL) and dried at 50 °C under reduced pressure until traces of ^{n}Bu$_3$SnCl were removed.

Isolated yield: 980 mg, 52%

^{1}H NMR (400 MHz, 298 K, Toluene-d$_8$): δ = 1.53 - 1.41 (m, 6H, $CH_2CH_2CH_2CH_3$), 1.20 (tt, $^3J_{HH}$ = 7.4 Hz, (pseudo sextet), 6H, $CH_2CH_2CH_2CH_3$), 0.94 (t, $^3J_{HH}$ = 8.2 Hz, 6H, $CH_2CH_2CH_2CH_3$), 0.79 (t, $^3J_{HH}$ = 7.3 Hz, 9H, $CH_2CH_2CH_2CH_3$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, Toluene-d$_8$): δ = 29.7 (s, $CH_2CH_2CH_2CH_3$), 27.3 (s, $CH_2CH_2CH_2CH_3$), 14.9 (s, $CH_2CH_2CH_2CH_3$), 13.6 (s, $CH_2CH_2CH_2CH_3$) ppm.

^{31}P NMR (162 MHz, 298K, Toluene-d$_8$): δ = –13.3 - –24.0 (m, 3P, *bridging*), –88.3 (qq $^1J_{PP}$ = 306.8 Hz, $^2J_{PP}$ = 50.4 Hz, 1P, *apical*), –159.6 - –167.8 (m, 3P, *basal*) ppm.

^{119}Sn NMR (149 MHz, 298K, Toluene-d$_8$): δ = 20.4 (d, $^1J_{SnP}$ = 777.5 Hz, ^{n}Bu$_3$*Sn*) ppm.

Mass spectrometry (ESI pos/neg): For $C_{36}H_{81}Sn_3P_7$+Na ([M+Na]$^+$): Calcd.: 1113.1465; found: 1113.3469.

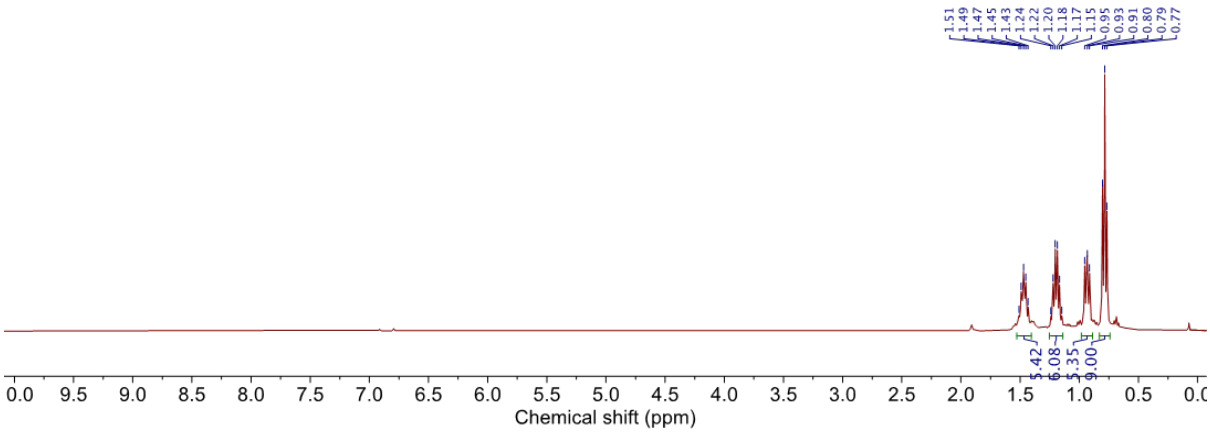


Figure S4. ^{1}H NMR spectrum (Toluene-d_8) of **3**.

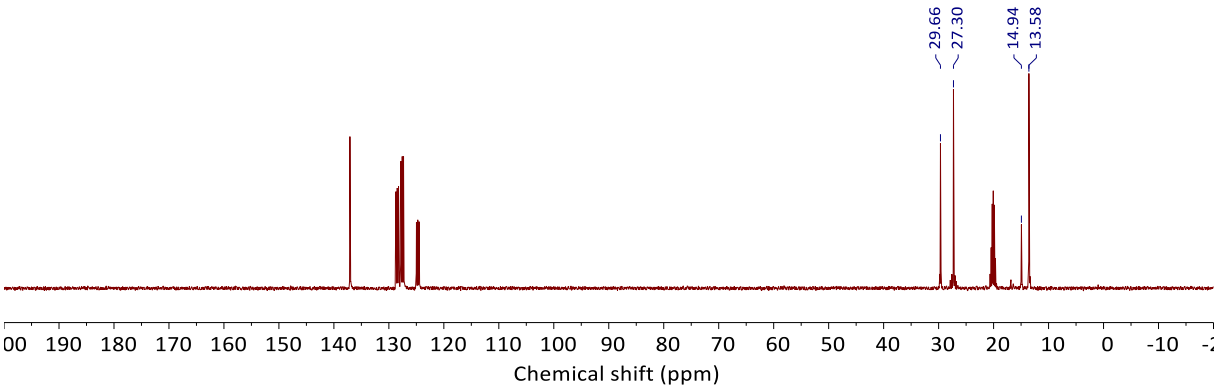


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum (Toluene-d_8) of **3**.

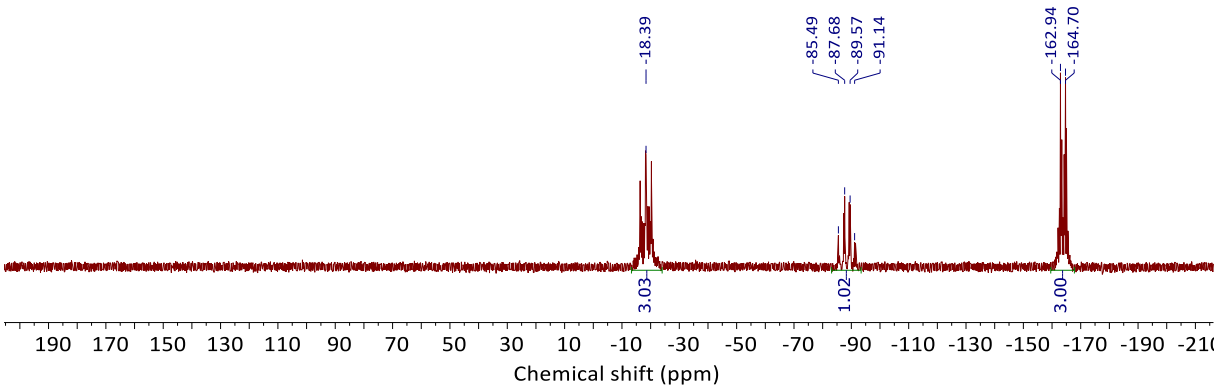


Figure S6. ^{31}P NMR spectrum (Toluene-d_8) of **3**.

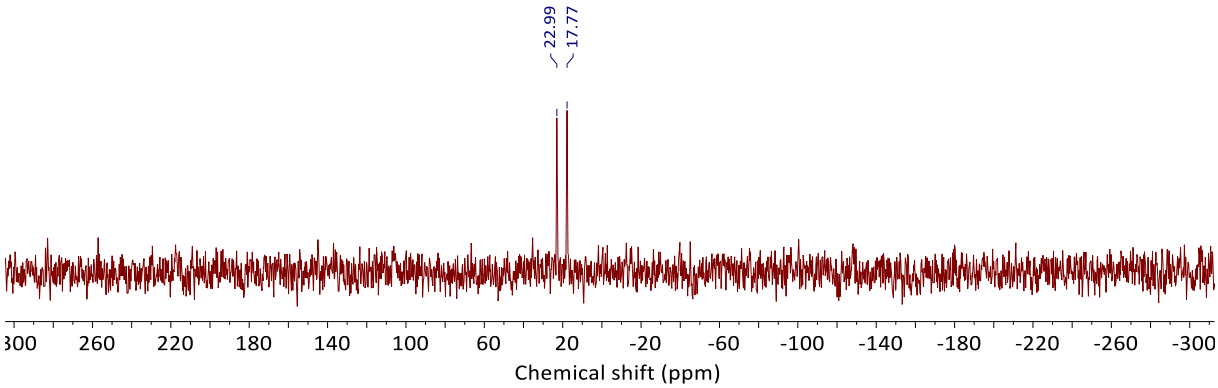
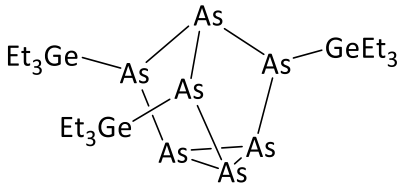


Figure S7. ^{119}Sn NMR spectrum (Toluene-d_8) of **3**.

2.2.3. Effort to Synthesis $(Et_3Ge)_3As_7$



A Schlenk flask was loaded with $[K_3(DME)_{0.18}][As_7]$ (500 mg, 0.78 mmol) and a stir bar. The contents were suspended in toluene (15 mL) and the suspension was cooled to –80 °C. Et_3GeCl (560 mg, 2.34 mmol) was added dropwise while stirring rapidly. The solution was allowed to warm to room temperature. Over the course of 2 hours at room temperature, the suspension turned dark purple, then black, with a red solution. The reaction was stirred for 7 days. After this, the reaction was filtered and the black residue was washed with toluene (3 x 5 mL). The solvent was removed under reduced pressure, yielding a dark red oil.

Yield: 233 mg, 30%

^{1}H NMR (400 MHz, 298 K, Toluene-d_8): δ = 1.13 – 1.09 (overlapping multiplets, 75H, CH_2CH_3) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, Toluene-d_8): δ = 11.4 (s, CH_2CH_3), 10.5 (s, CH_2CH_3) ppm.

Mass spectrometry (APCI): For $C_{18}H_{45}As_7Ge_3$ Calcd.: 1007.5668; found: 1007.5676.

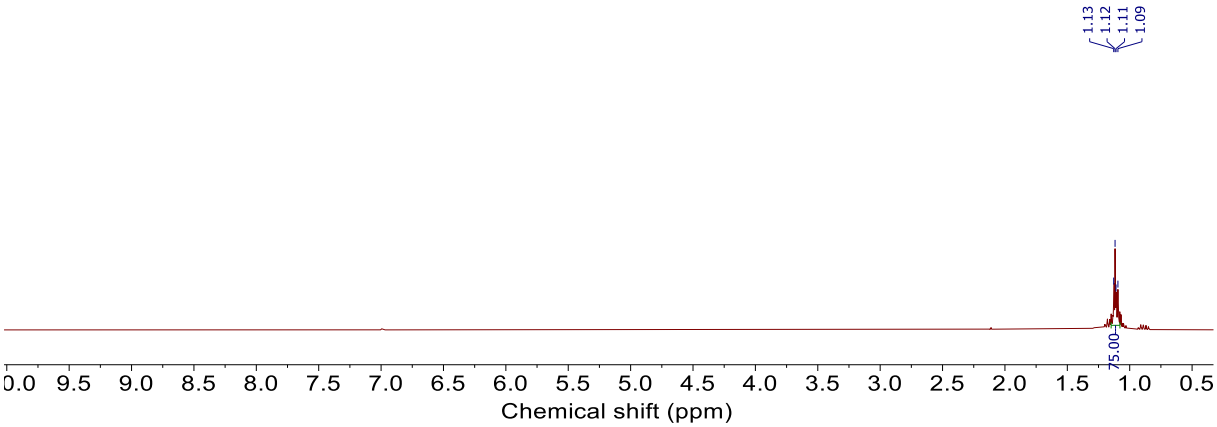


Figure S8: ^{1}H NMR spectrum (Toluene-d_8).

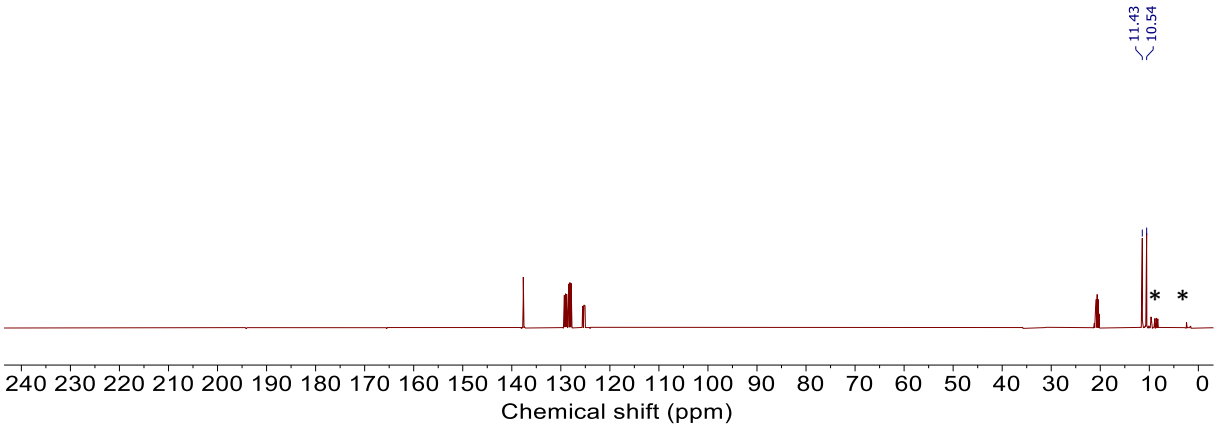


Figure S9. ^{31}C{^{1}H} NMR spectrum (Toluene-d_8) Unknown impurities labelled with a *.

2.2.4. Detection of $(Et_3Ge)_5As_{11}$, 5

If the batch of $[K_3(DME)_{0.18}][As_7]$ employed during the synthesis of $(Et_3Ge)_3As_7$ features the $[As_{11}]^{5-}$ impurity (detected by mass spectrometry), then crystals grew from the neat red oil isolated from section 2.2.4. XRD diffraction studies into these crystals confirmed the structure of **5**.

Yield of the Crystalline Material: 243 mg, 62%

Mass spectrometry (APCI): For $C_{30}H_{75}As_{11}Ge_5$ Calcd.: 1629.3303; found: 1629.3453. For $C_{18}H_{45}As_7Ge_3$ Calcd.: 1007.5668; found: 1007.5676.

*Note: Both $(Et_3Ge)_3As_7$ and **5** were present in the sample.*

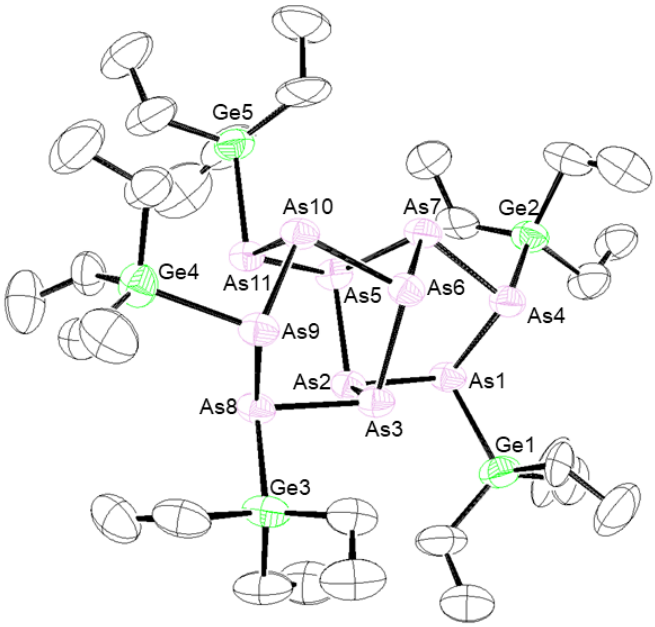
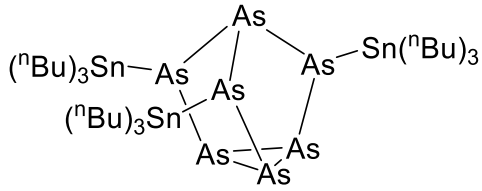


Figure S10. Molecular structure of **5.** Anisotropic displacement ellipsoids captured at 50% probability. Hydrogen atoms have been omitted for clarity. Arsenic: plum; Germanium: green; Carbon: white.

2.2.5. Effort to Synthesis (^{n}Bu$_3$Sn)$_3$As$_7$



A Schlenk flask was loaded with [K$_3$(DME)$_{0.18}$]As$_7$ (500 mg, 0.78 mmol) and a stir bar. The contents were suspended in toluene (10 mL). The suspension was cooled to –80 °C and ^{n}Bu$_3$SnCl (0.60 mL, 2.34 mmol) was added with strong stirring. The reaction was allowed to warm to room temperature, by which point a red solution with a black suspension was observed. The reaction was stirred for 4 days. The solvent was filtered off and residue washed with toluene (3 x 5 mL). The solvent was removed under reduced pressure to give a red oil. NMR analysis revealed the presence of unreacted ^{n}Bu$_3$SnCl, which was difficult to separate from **6** due to their similar solubility. Attempts were made at removing excess ^{n}Bu$_3$SnCl from the reaction mixture, including washing with the non-polar solvents pentane and ether, and by distillation under reduced pressure, but these proved to be unsuccessful and heating higher than 40 °C caused cluster decomposition.

^{119}Sn NMR yield: 62%

^{1}H NMR (400 MHz, 298 K, THF-d_8): δ = 1.75 - 1.61 (m, 6H, *^{n}Bu*), 1.46 - 1.36 (m, 6H, *^{n}Bu*), 1.29 - 1.10 (m, 6H, *^{n}Bu*), 0.99 - 0.94 (m, 9H, *^{n}Bu*) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d_8): δ = 31.7 (s, $CH_2CH_2CH_2CH_3$), 29.7 (s, $CH_2CH_2CH_2CH_3$, unreacted $^{n}Bu_3SnCl$), 29.1 (s, $CH_2CH_2CH_2CH_3$), 28.6 (s, $CH_2CH_2CH_2CH_3$), 19.4 (s, $CH_2CH_2CH_2CH_3$), 17.3 (s, $CH_2CH_2CH_2CH_3$, unreacted $^{n}Bu_3SnCl$), 15.0 (s, $CH_2CH_2CH_2CH_3$), 14.9 (s, $CH_2CH_2CH_2CH_3$, unreacted $^{n}Bu_3SnCl$) ppm.

^{119}Sn NMR (149 MHz, 298 K, THF-d_8): δ = 109.4 (s, $^{n}Bu_3SnCl$), 27.3 (s, $(^{n}Bu_3Sn)_3As_7$) ppm.

Mass spectrometry (APCI): For $C_{36}H_{81}Sn_3As_7$+H ($[M+H]^+$): Calcd.: 1394.7963; found: 1394.7997.

Note: ^{1}H NMR Integrations could not be definitively assigned due to overlapping signals of ***6*** *and $^{n}Bu_3SnCl$.*

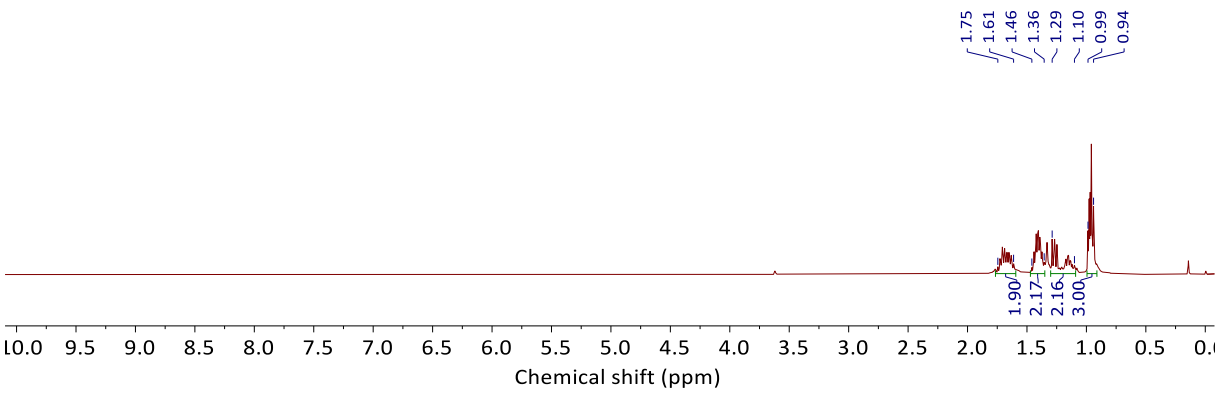


Figure S11. Crude ^{1}H NMR spectrum (THF-d_8) of $(^{n}Bu_3Sn)_3As_7$.

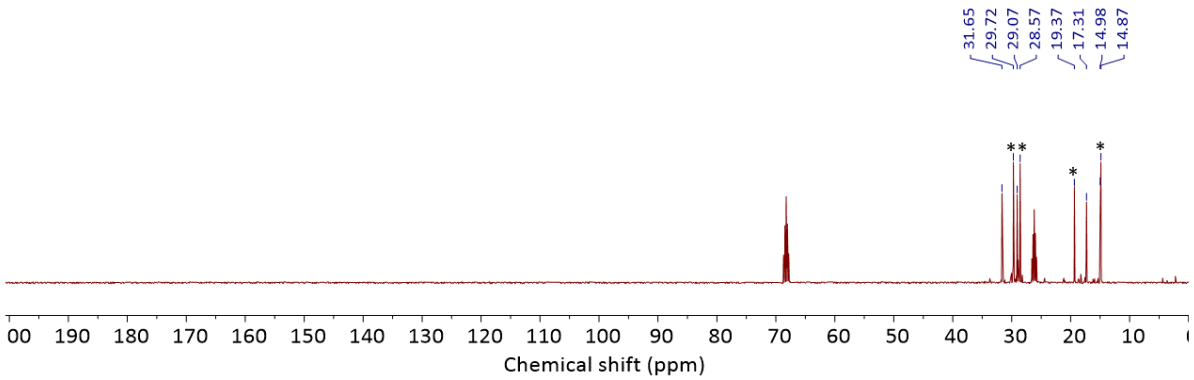


Figure S12. Crude ^{13}C{^{1}H} NMR spectrum (THF-d_8) of $(^{n}Bu_3Sn)_3As_7$, unreacted $^{n}Bu_3SnCl$ is marked with a *.

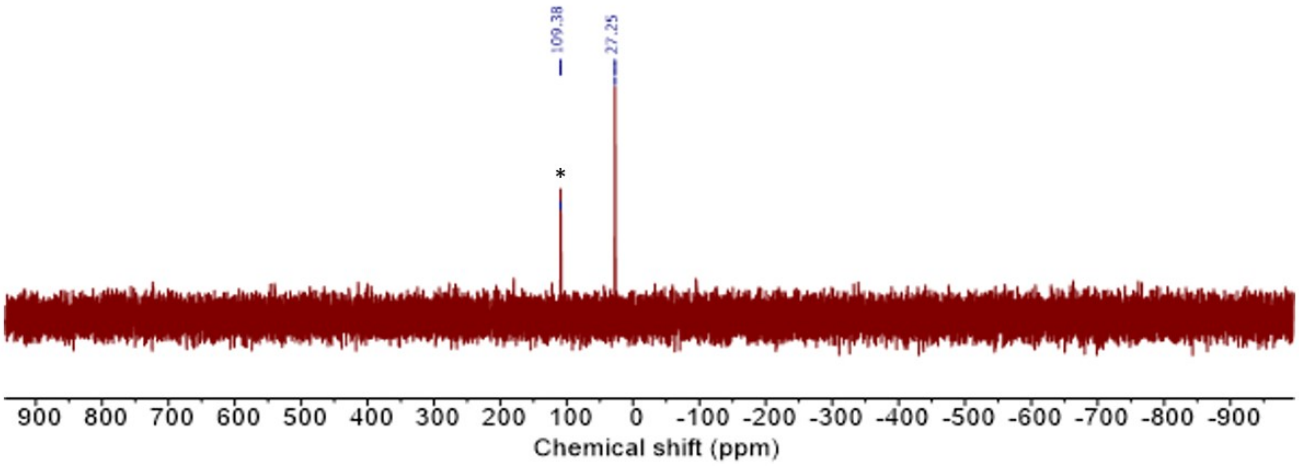


Figure S13. Crude ^{119}Sn NMR spectrum (THF-d_8) of (^{n}Bu$_3$Sn)$_3$As$_7$, unreacted ^{n}Bu$_3$SnCl is marked with a *.

3. Identifying Symmetric vs. Asymmetric Functionalized Clusters

The geometry at the bridging phosphorus atoms of the [P_7] core for functionalized clusters is pyramidal and introduces chirality. Further, there are two possible isomers a symmetric coordination mode (Figure S14, **A**) and an asymmetric coordination mode (Figure S14, **B**). In 2011, Hassler and co-workers studied the **A** and **B** isomers of ($Me_3Si)_3P_7$ using density functional theory (DFT) and ^{31}P NMR spectroscopy.[11] The symmetric coordination mode **A** gives three unique phosphorus magnetic environments (apical, bridging, and basal), while in the asymmetric coordination mode **B** all seven of the phosphorus atoms are magnetically inequivalent. The symmetric coordination mode **A** is expected to be the thermodynamic product, and has been selectively detected with [P_7] cages that feature bulky functional groups.[11, 12] The ^{31}P NMR spectrum of **6** and **7** showed three resonances corresponding to the apical, bridging, and basal phosphorus environments. Whereas, the ^{31}P NMR spectrum of **8-10**, display ten resonances, in line with both **A** and **B** isomers being present. These A and B isomers were identified with ^{31}P NMR COSY experiments.

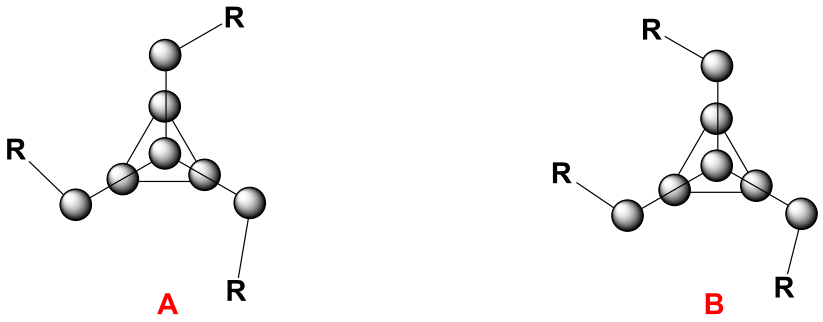
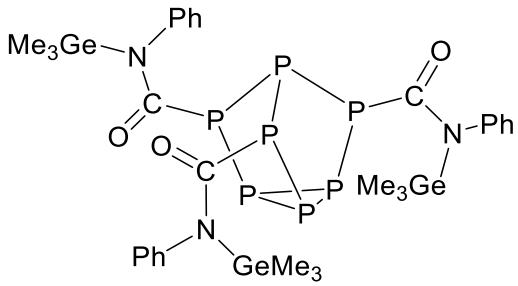


Figure S14. Symmetric (**A**) and Asymmetric (**B**) Isomers of Functionalised [P_7] Cages.

3.1. Synthesis and Characterization Data for $(R_3E)_3Pn_7$ Heteroallene Inserted Products

3.1.1. Synthesis of $(Me_3Ge\text{-}PhNCO)_3P_7$, 6



A Schlenk flask was loaded with a stir bar. $(Me_3Ge)_3P_7$ (100 mg, 0.18 mmol) was dissolved in pyridine (2 mL). To this solution, PhNCO (64 mg, 0.54 mmol) was added affording an intense orange solution which turned to a clear light yellow solution after an hour. The reaction was left to stir for 4 days, by which point, a light yellow solution was observed. Pyridine was removed under reduced pressure, affording a yellow glassy solid. The residue was dissolved in Et_2O (2 mL). Slow evaporation of this solution gave needle shaped crystals which were washed with pentane (2 mL) yielding a white powder. Crystals that were suitable for X-ray diffraction were grown through the slow evaporation of an Et_2O solution of the product. **Isolated yield:** 107 mg, 72%

^{1}H NMR (400 MHz, 298 K, THF-d_8): δ = 7.58 - 7.43 (m, 15H, *Ph*), 0.31 (s, 27H, *CH_3*) ppm.
^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d_8): δ = 144.3 (s, *Ph*), 130.5 (s, *Ph*), 129.8 (s, *Ph*), 128.8 (s, *Ph*), 1.8 (s, *C*H_3) ppm.

^{31}P NMR (162 MHz, 298 K, THF-d_8): δ = 133.2 - 127.3 (m, 3P, *bridging*), –123.5 - –131.7 (m, 1P, *apical*), –171.4 - –177.4 (m, 3P, *basal*) ppm.

Mass spectrometry (ESI neg/pos): For $C_{30}H_{42}Ge_3N_3O_3P_7$+Na ($[M+Na]^+$): Calcd.: 953.8923; found: 953.8936.

Elemental analysis: For $C_{30}H_{42}Ge_3N_3O_3P_7$: Calcd.: C 38.85, H 4.57, N 4.53; found: C 39.48, H 4.76, N 4.25.

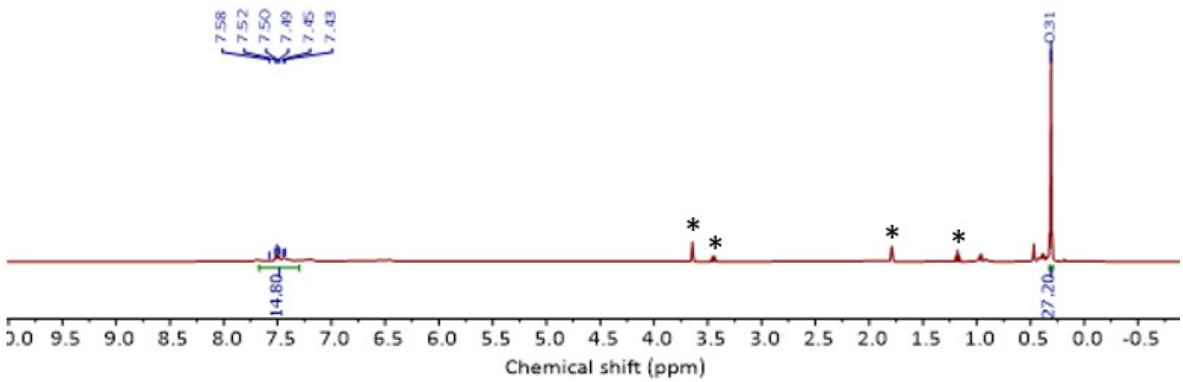


Figure S15. ^{1}H NMR spectrum (THF-d_8) of **6**. Residual THF and diethyl ether signals are marked with a *.

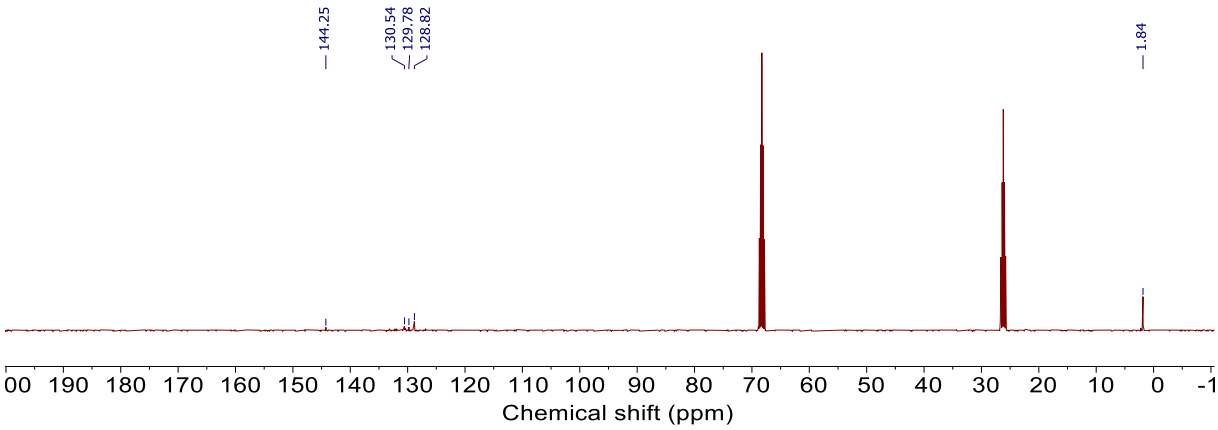


Figure S16. $^{13}C\{^1H\}$ NMR spectrum (THF-d_8) of **6**.

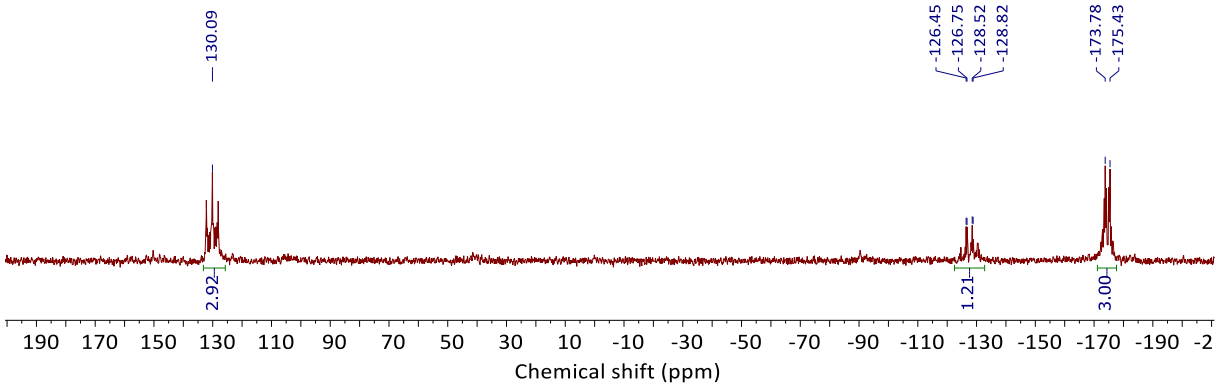


Figure S17. ^{31}P NMR spectrum (THF-d_8) of **6**.

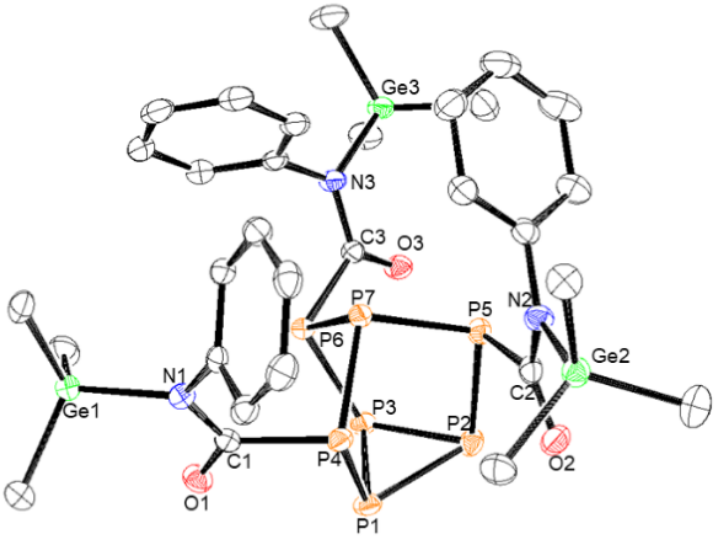


Figure S18. Molecular structure of **6**. Anisotropic displacement ellipsoids captured at 50% probability. Hydrogen atoms have been omitted for clarity. Phosphorus: orange; Nitrogen: blue; Oxygen: red; Germanium: green; Carbon: white.

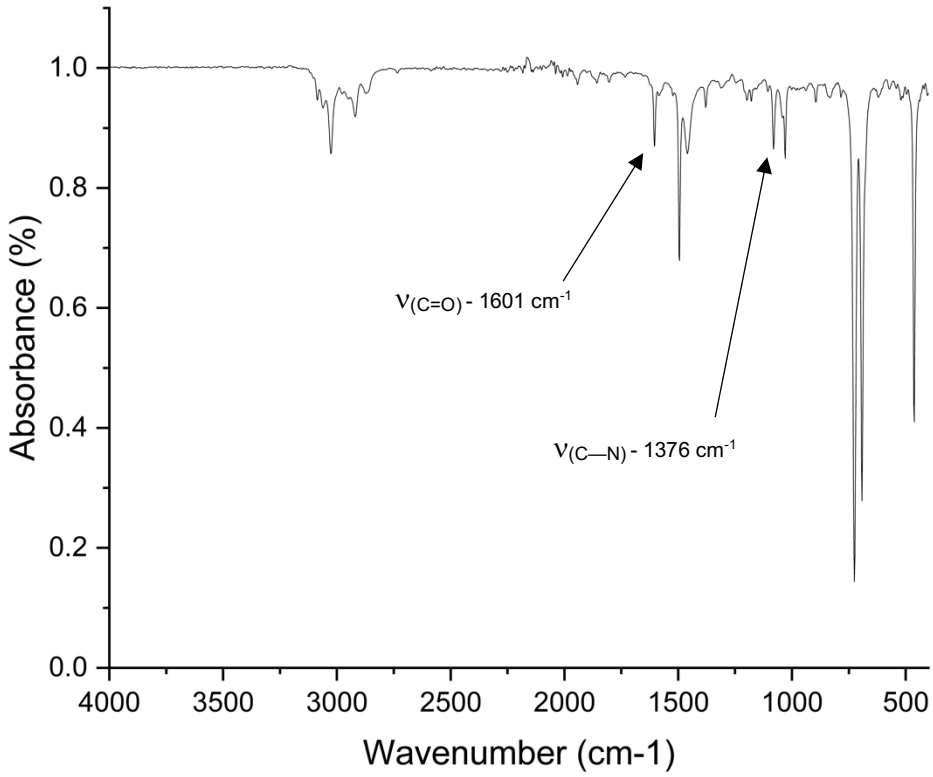
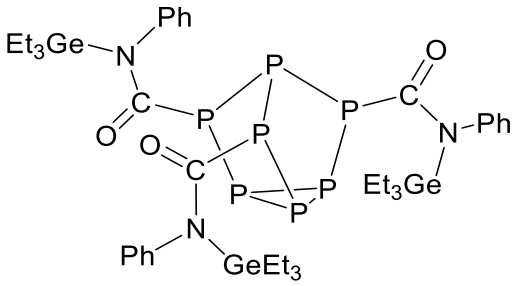


Figure S19. IR spectrum of **6**.

3.1.2. Synthesis of $(Et_3Ge\text{-}PhNCO)_3P_7$, 7



A Schlenk flask was loaded with a stir bar. $(Et_3Ge)_3P_7$ (500 mg, 0.72 mmol) was dissolved in pyridine (10 mL). To this solution, PhNCO (250 mg, 2.16 mmol) was added, yielding a yellow/green solution. Reaction was allowed to stir for 2 days. Solvent was removed under reduced pressure, to give a green waxy solid. The residue was dissolved in Et_2O (5 mL). Slow evaporation of Et_2O yielded block crystals. Crystals were washed with pentane (5 mL) affording a white crystalline solid. Crystals that were suitable for X-ray diffraction analysis were grown through the slow evaporation of an Et_2O solution of the product.
Isolated yield: 487 mg, 64%

^{1}H NMR (400 MHz, 298 K, THF-d_8): δ = 7.80 - 7.34 (m, 15 H, *Ph*), 1.29 - 0.79 (m, 45 H, C*H*$_2$C*H*$_3$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d_8): δ = 179.5 (d, $^1J_{CP}$ = 49 Hz (Et_3Ge-PhN*C*O)$_3P_7$) 144.1 (s, *Ph*), 133.2 (s, *Ph*), 132.1 (s, *Ph*), 128.6 (s, *Ph*), 9.4 (s, *C*H$_2$), 8.1 (s, *C*H$_3$) ppm.

^{31}P NMR (162 MHz, 298 K, THF-d_8): δ = 139.5 - 123.9 (m, 3P, *bridging*), –133.4 (qq, $^1J_{PP}$ = 339.7 Hz, $^2J_{PP}$ = 49.0 Hz, 1P, *apical*), –173.9 - –187.5 (m, 3P, *basal*) ppm.

Mass spectrometry (ESI neg/pos): $C_{39}H_{60}Ge_3N_3O_3P_7$+Na ([M+Na]$^+$): calcd.: 1076.0342; found: 1076.0365.

Elemental analysis: For $C_{39}H_{60}Ge_3N_3O_3P_7$: Calcd.: C 44.47, H, 5.74, N 3.99; found: C 44.51, H 5.83, N 4.07.

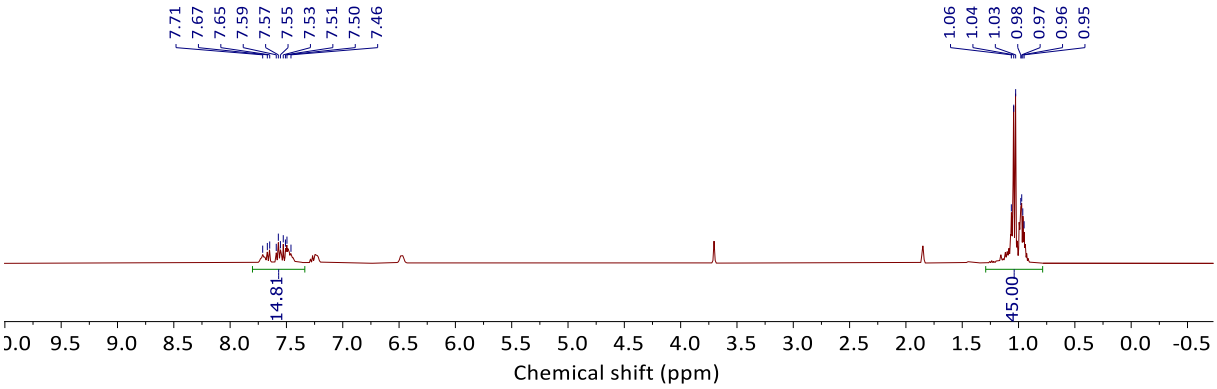


Figure S20. ^{1}H NMR spectrum (THF-d_8) of **7.**

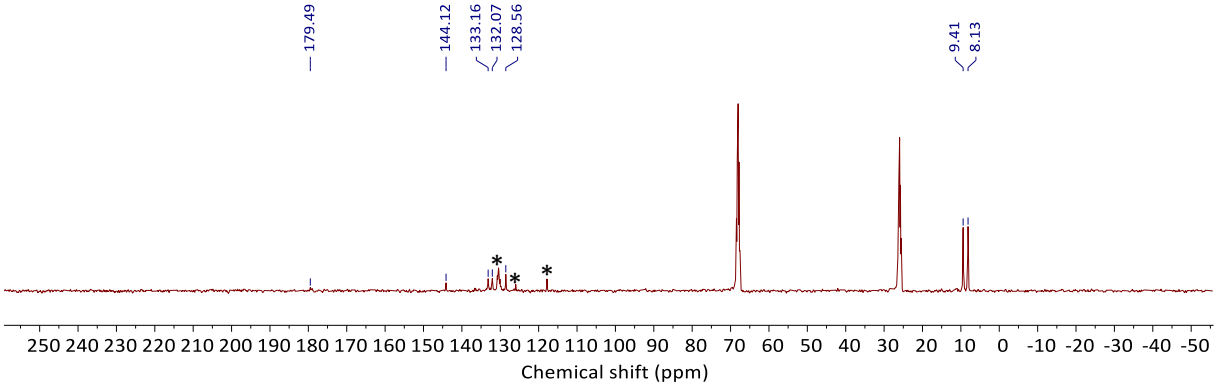


Figure S21. ^{31}C{^{1}H} NMR spectrum (THF-d_8) of **7**, residual pyridine signals are marked with a *.

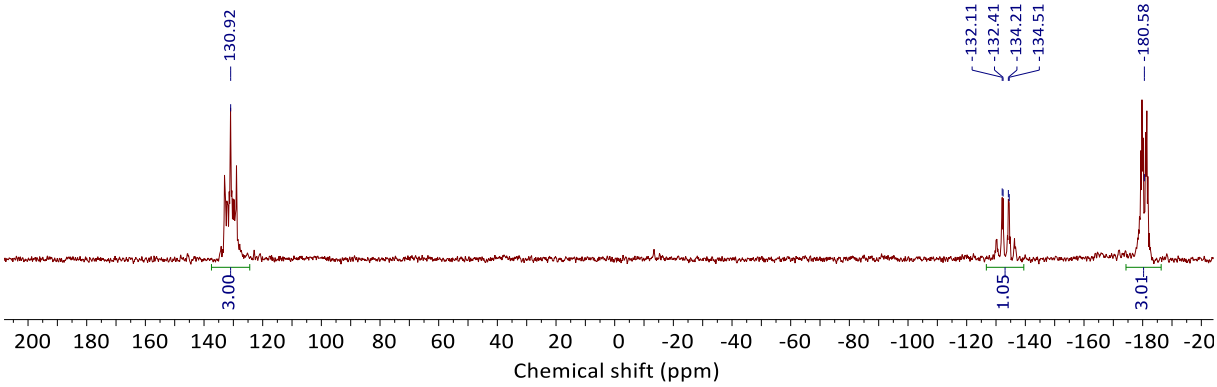


Figure S22. ^{31}P NMR spectrum (THF-d_8) of **7.**

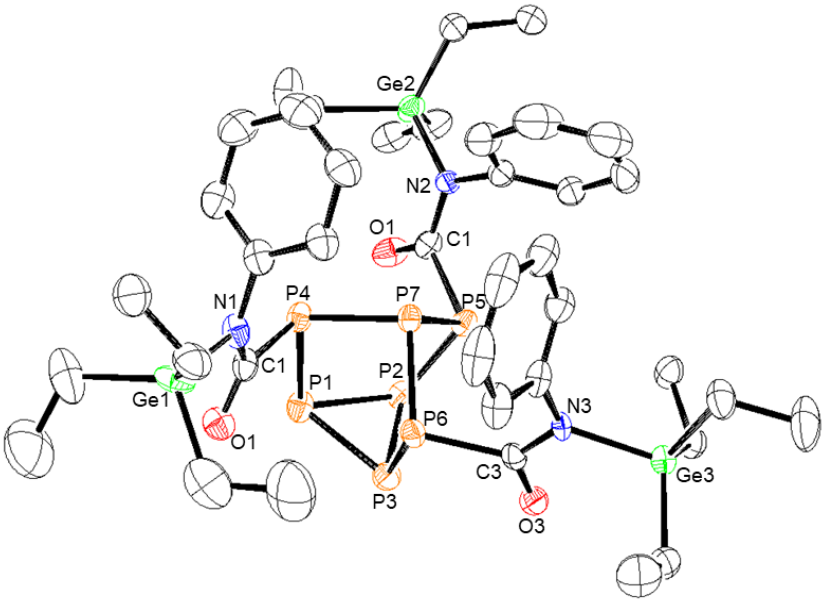


Figure S23. Molecular structure of **7**. Anisotropic displacement ellipsoids captured at 50% probability. Hydrogen atoms have been omitted for clarity. Phosphorus: orange; Nitrogen: blue; Oxygen: red; Germanium: green; Carbon: white.

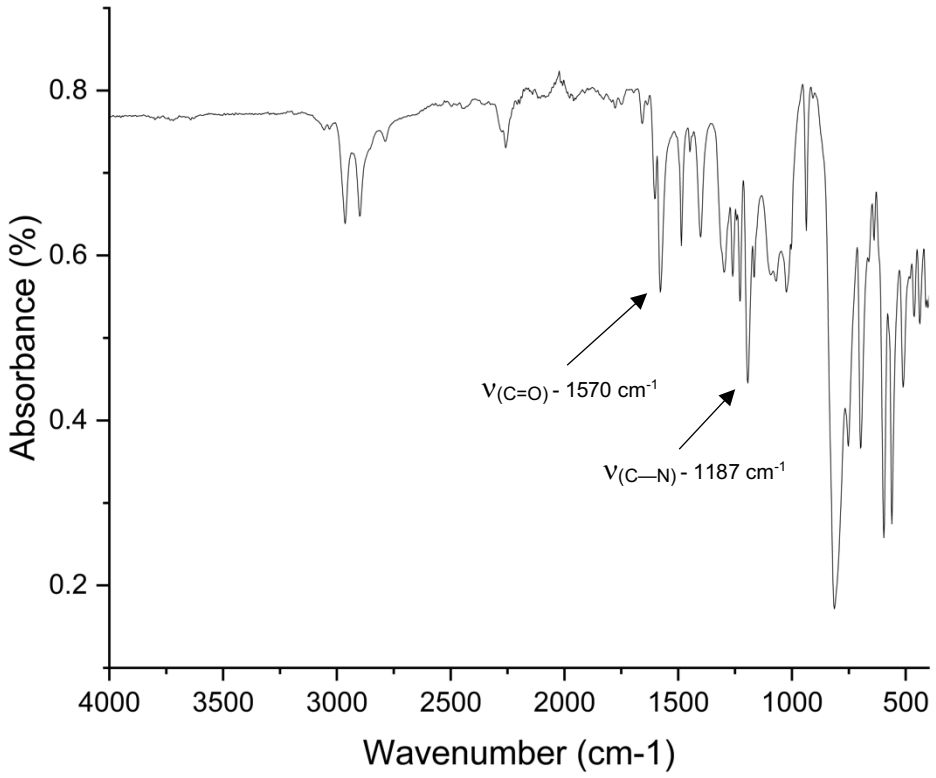
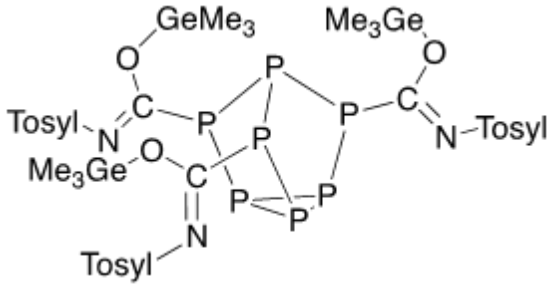


Figure S24. IR spectrum of **7**.

3.1.3. Synthesis of $(Me_3Ge\text{-}TsNCO)_3P_7$, 8



A Schlenk flask was loaded with a stir bar. $(Me_3Ge)_3P_7$ (150 mg, 0.26 mmol) and dissolved in toluene. To this solution, *p*-toluenesulfonyl isocyanate (155 mg, 0.79 mmol, 3 eq.) was added giving a yellow solution. The reaction was stirred for 4 days, no colour change was observed after this duration. The NMR spectrum of the reaction mixture revealed leftover starting material, however further consumption of starting material was not observed with prolonged reaction times and heating to 40 °C. Due to difficulties in separating the starting material from

the inserted product, the NMR spectra were assigned directly from the crude reaction mixture as washes with non-polar solvents did not affect the distribution of reaction components. Solvent was removed and the residue dissolved in pentane (2 mL). Crystals, suitable for X-ray diffraction analysis were growth through the slow evaporation of this solution.

^{31}P NMR Overall Conversion: 81%

^{31}P NMR Isomeric conversion: 44% symmetric (**A**), 37% asymmetric (**B**), 19% unreacted starting material.

Yield after crystallisation: 22 %

^{1}H NMR (400 MHz, 298 K, Toluene-d$_8$): δ = 8.14 (d, $^{3}J_{HH}$ = 8.2 Hz, 1H, *Ar*), 8.11 (d, $^{3}J_{HH}$ = 8.3 Hz, 2H, *Ar*), 8.02 (d, $^{3}J_{HH}$ = 6.5 Hz, 1H, *Ar*), 7.97 (d, $^{3}J_{HH}$ = 8.2 Hz, 1H, *Ar*), 7.71 (d, $^{3}J_{HH}$ = 8.4 Hz, 2H, *Ar* unreacted tosyl isocyanate), 7.24 (overlapping doublets, 2H, *Ar*), 7.12 (d, $^{3}J_{HH}$ = 7.7 Hz, 3H, *Ar*), 7.04 (d, $^{3}J_{HH}$ = 8.3 Hz, 2H, *Ar*), 6.93 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H, *Ar* unreacted tosyl isocyanate), 2.27 (s, 3H, *Me*-Ar), 2.15 (s, 2H,*Me*-Ar), 2.13 (overlapping singlets, 5H, *Me*-Ar), 2.10 (s, 4H, *Me*-Ar unreacted tosyl isocyanate), 0.64 (overlapping singlets, 9H, *Me$_3$*Ge), 0.61 (s, 8H, *Me$_3$*Ge), 0.50 (overlapping singlets, 11H, *Me$_3$*Ge) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, Toluene-d$_8$): δ = 146.8 (s, *Ar* unreacted tosyl isocyanate), 140.8 - 140.4 (3 overlapping singlets, *Ar*), 138.3 (s, *Ar* unreacted tosyl isocyanate), 138.2 (s, *Ar*), 131.2 (s, *Ar* unreacted tosyl isocyanate), 130.6 - 130.4 (3 overlapping singlets, *Ar*), 130.2 (s, *Ar*), 129.4 (s, *Ar*) 128.3 - 128.1 (3 overlapping singlets, *Ar*), 127.9 (s, *Ar* unreacted tosyl isocyanate), 126.5 (s, *Ar*), 22.3 (s, *Me*-Ar), 22.3 (s, *Me*-Ar), 22.2 (s, *Me*-Ar, unreacted tosyl isocyanate), 22.2 (s, *Me*-Ar), 22.1 (s, *Me*-Ar), 5.3 (overlapping singlets, *Me$_3$*Ge *B*), 5.0 (s, *Me$_3$*Ge *A*), 3.5 (s, *Me$_3$*Ge SM) ppm.

^{31}P NMR (162 MHz, 298 K, Toluene-d$_8$): δ = 120.2 (q, $^{1}J_{PP}$ = 383.5 Hz, 5P, *Bridging B*), 103.4 (pseudo quartet, 6P, *Bridging A*), 8.2 - 4.2 (m, 3P, (Me$_3$Ge)$_3$*P$_7$*), –11.9 (t, $^{1}J_{PP}$ = 311.6 Hz, 2P, *Bridging B*), –21.2 (t, $^{1}J_{PP}$ = 312.8 Hz, 2P, *Bridging B*), –91.7 - –97.7 (m, 1P, *Apical SM*), –104.9 (q, $^{1}J_{PP}$ = 323.2 Hz, 2P, *Apical B*), –115.1 (qq, $^{1}J_{PP}$ = 377.2 Hz, $^{2}J_{PP}$ = 42.9 Hz, 2P, *Apical A*), –147.2 - –153.7 (m, 5P, *Basal A*), –156.3 - –159.3 (m, 3P, *Basal SM*), –167.3 - –189.9 (overlapping multiplets, 9P, *Basal B*) ppm.

Mass spectrometry (ESI pos/neg): For $C_{33}H_{48}Ge_3N_3O_9S_3P_7$+Na ([M+Na]$^{+}$): Calcd.: 1187.8249; found: 1187.8259.

Note: Some ^{1}H NMR integrations could not be definitively assigned due to the reaction mixture being inseparable from starting material, resulting in overlapping signals of different

intensities. Starting material, along with both the symmetric and asymmetric isomers co-crystallised from the crude reaction mixture.

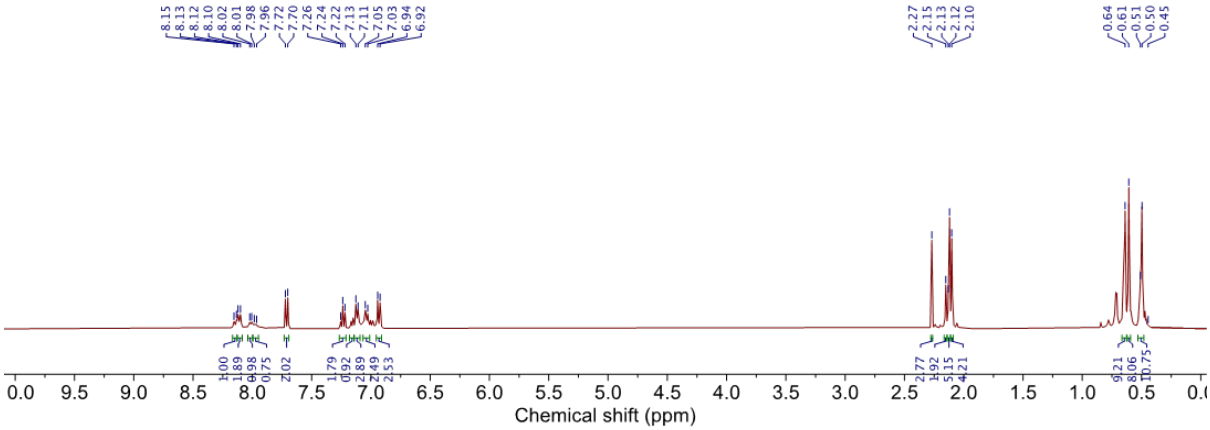


Figure S25. ^{1}H NMR spectrum (Toluene-d_8) of **8**.

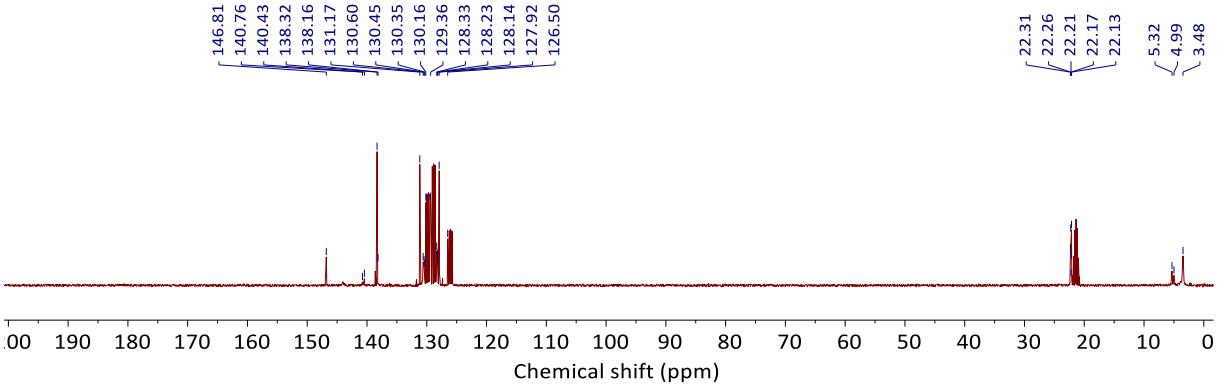


Figure S26. ^{13}C{^{1}H} NMR spectrum (Toluene-d_8) of **8.**

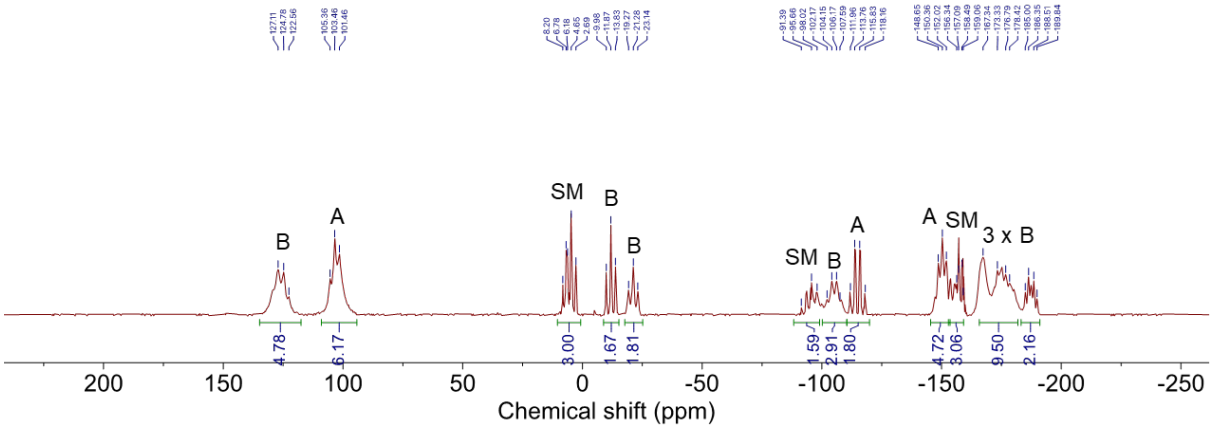


Figure S27. ^{31}P NMR spectrum (Toluene-d_8) of **8**.

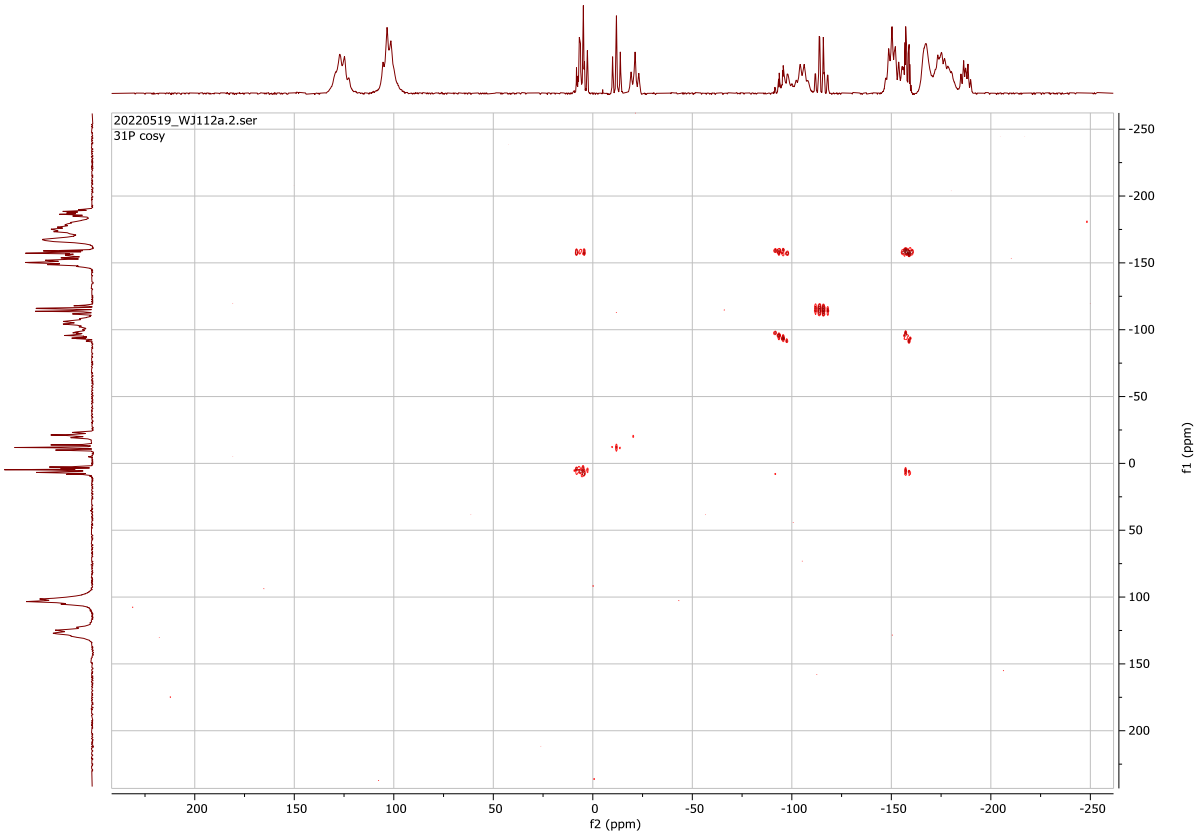


Figure S28. ^{31}P COSY NMR (Toluene-d_8) spectrum of **8.**

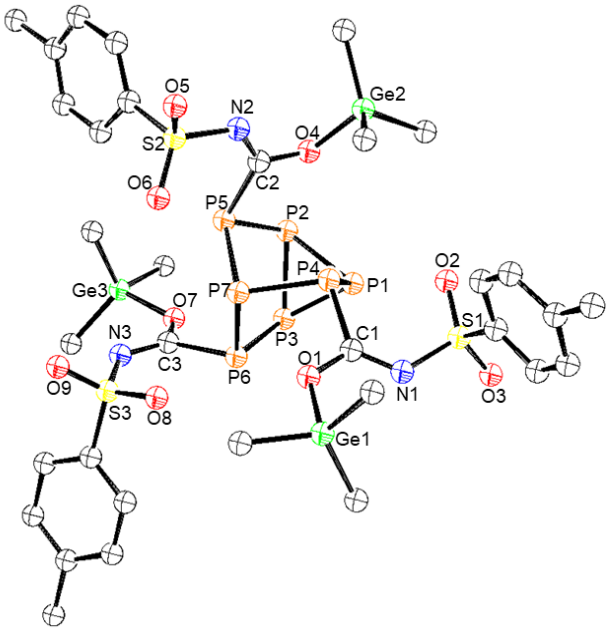


Figure S29. Molecular structure of **8**. Anisotropic displacement ellipsoids captured at 50% probability. Hydrogen atoms have been omitted for clarity. Phosphorus: orange; Nitrogen: blue; Oxygen: red; Germanium: green; Carbon: white.

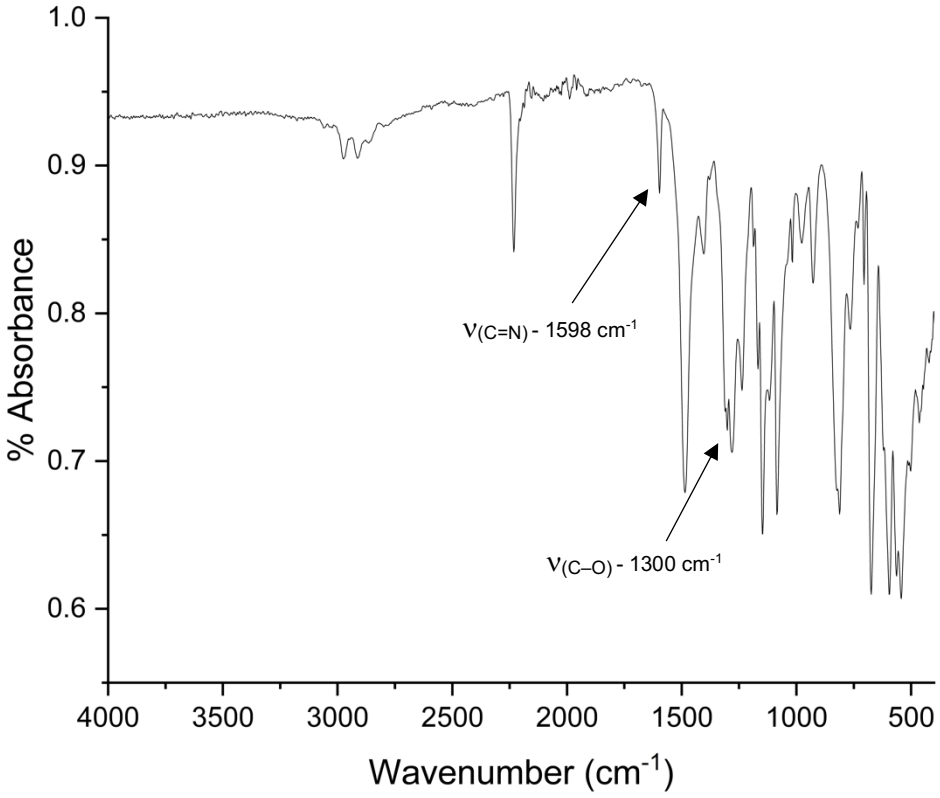
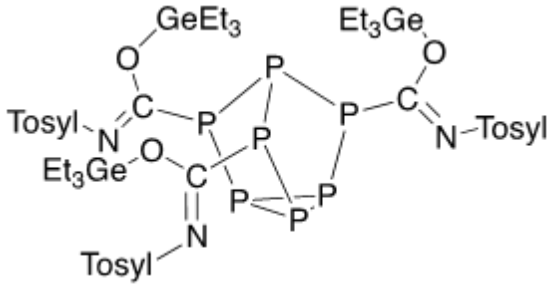


Figure S30. IR spectrum of **8.**

3.1.4. Synthesis of $(Et_3Ge\text{-}TsNCO)_3P_7$, 9



A flame dried Schlenk was loaded with a stir bar and $(Et_3Ge)_3P_7$ (200 mg, 0.29 mmol), dissolved in toluene (5 mL) was added. To this solution, *p*-toluenesulfonyl isocyanate (170 mg, 0.87 mmol) was added dropwise while stirring. This gave a light yellow/green solution which did not change appearance over the course of the reaction. The reaction was stirred for 4 days. Even after these long reaction times, NMR spectroscopy showed residual starting material. Therefore, conversions are quoted as *in situ* values determined from ^{31}P NMR spectroscopy. The solvent was removed to give a green waxy solid, which was dissolved in ether and left to slowly evaporate, yielding large block shaped crystals. Due to similarities in solubility, the inserted products were difficult to separate from the starting material and washes

with non-polar solvents such as ether and pentane did not affect the product to starting material distribution.

^{31}P NMR Overall Conversion: 55%

^{31}P NMR Isomeric conversion: Symmetric: 34% (**A**), asymmetric: 21% (**B**), 45% unreacted starting material.

Yield after crystallisation: 17%

^{1}H NMR (400 MHz, 298 K, Toluene-d$_8$): δ = 8.03 (d, $^{3}J_{HH}$ = 8.3 Hz, 6H, *Ar*), 8.00 (d, $^{3}J_{HH}$ = 8.3 Hz, 1H *Ar*), 7.92 (d, $^{3}J_{HH}$ = 8.3 Hz, 2H *Ar*), 7.87 (d, $^{3}J_{HH}$ = 8.4 Hz, 3H, *Ar*), 7.51 (d, $^{3}J_{HH}$ = 8.5 Hz, 8H *Ar* unreacted tosyl isocyanate), 7.08 - 7.03 (m, 1H *Ar*), 6.97-6.78 (m, 12H, *Ar*), 6.68 (d, $^{3}J_{HH}$ = 8.3 Hz, 8H *Ar* unreacted *tosyl* isocyanate), 2.12 (s, 2H, *Me*-Ar), 1.99 (s, 3 H, *Me*-Ar), 1.97 (s, 4H, *Me*-Ar *B*), 1.93 (s, 3H, *Me*-Ar), 1.92 (s, 13H, *Me*-Ar unreacted tosyl isocyanate), 1.17 - 0.88 (m, 146H, *Et$_3$Ge* of product A and B, and of $(Et_3Ge)_3P_7$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, Toluene-d$_8$): δ = 146.1 (s, *Ar* unreacted tosyl isocyanate), 143.3 (s, *Ar*), 143.1 (s, *Ar*), 140.7 (s, *Ar*), 140.5 (s, *Ar*), 140.2 (s, *Ar*), 140.1 (s, *Ar*) 137.9 (s, *Ar* unreacted tosyl isocyanate), 131.3 (s, *Ar*), 130.6 (s, *Ar*), 129.8 (s, *Ar*), 129.7 (s, *Ar B*), 128.9 (s, *Ar* unreacted tosyl isocyanate), 127.8 (s, *Ar*) 127.4 (s, *Ar* unreacted tosyl isocyanate), 127.0 (s, *Ar*), 126.0 (s, *Ar*), 22.8 (s, *Me*-Ar), 21.7 (s, *Me*-Ar unreacted tosyl isocyanate), 21.6 (s, *Me*-Ar), 21.6 (s, *Me*-Ar), 21.5 (s, *Me*-Ar), 10.4 (overlapping singlets, *Et$_3$Ge B*), 10.3 (overlapping singlets, *Et$_3$Ge*), 9.6 (s, *Et$_3$*Ge), 9.5 (overlapping singlets, *Et$_3$*Ge), 9.6 (s, *Et$_3$Ge*), 8.6 (overlapping singlets, *Et$_3$*Ge), 8.5 (overlapping singlets, *Et$_3$*Ge) ppm

^{31}P NMR (168 MHz, 298 K, Toluene-d$_8$): δ = 122.2 (q, 3P, *bridging A*), 100.3 (q, 1P, *bridging B*), –2.8 - –13.0 (m, 3P, *bridging SM*), –21.8 (t, 1P, *bridging B*), –30.0 (t, 1P, *bridging B*), –101.8 (qq, 1P, *apical SM*), –111.1 (qq, 1P, *apical A*), –119.2 (qq, 1P, *apical B*), –148.6 - –153.9 (m, 1P, *basal B*), –154.6 - –159.8 (m, 3P, *basal SM*), –162.1 - –166.3 (m, 1P, *basal B*), –174.7 - –183.2 (m, 3P, *basal A*), –188.3 - –195.7 (m, 1P, *basal B*) ppm.

Note: Multiple attempts at mass spectrometry were made but significant decomposition was seen upon ionisation. Starting material, along with both the symmetric and asymmetric isomers co-crystallised from the crude reaction mixture.

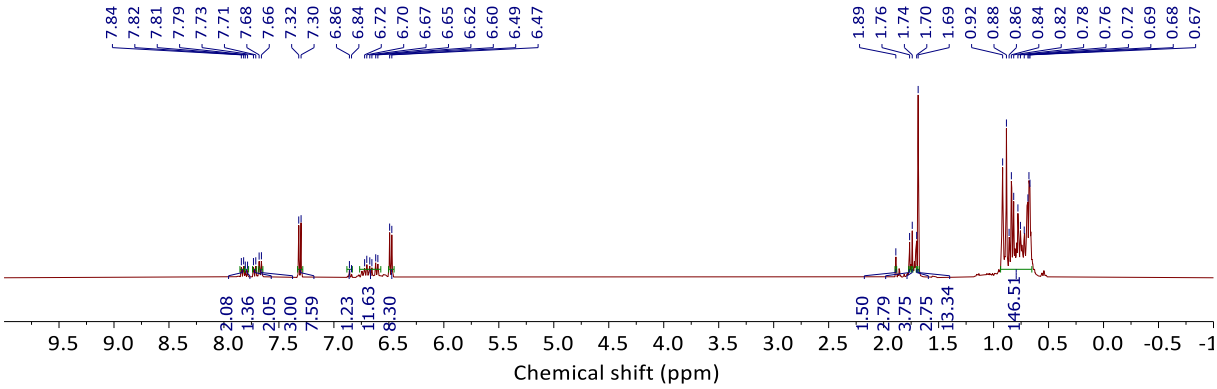


Figure S31. ^{1}H NMR spectrum (Toluene-d_8) of **9.**

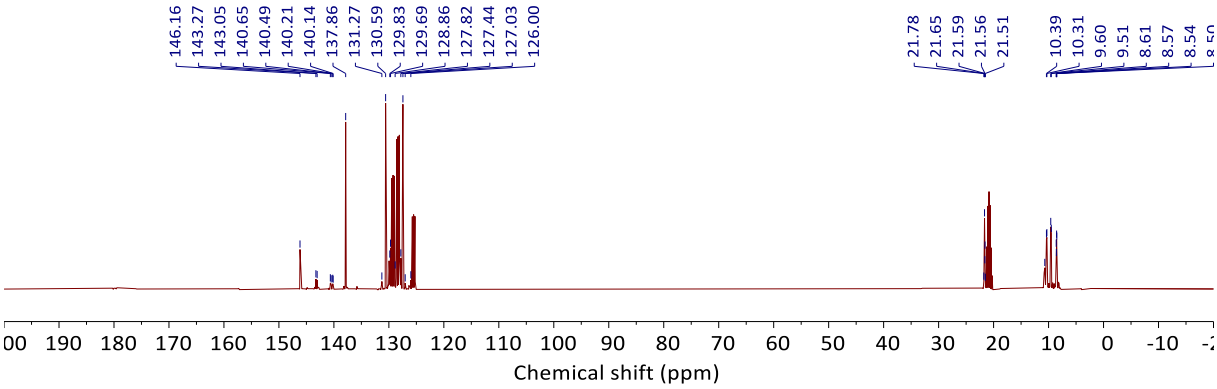


Figure S32. ^{13}C{^{1}H} NMR spectrum (Toluene-d_8) of **9.**

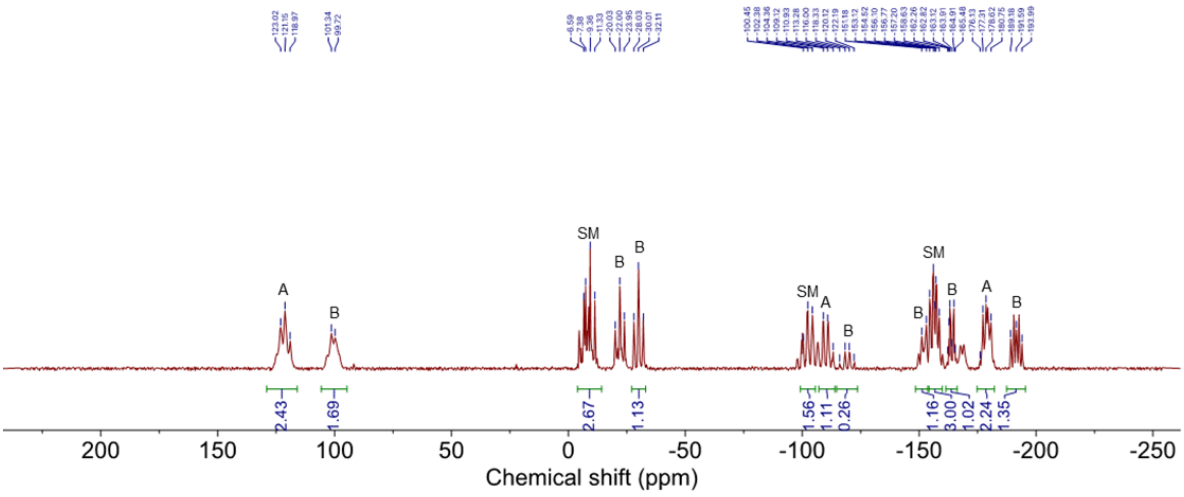


Figure S33. ^{31}P NMR spectrum (Toluene-d_8) of **9.**

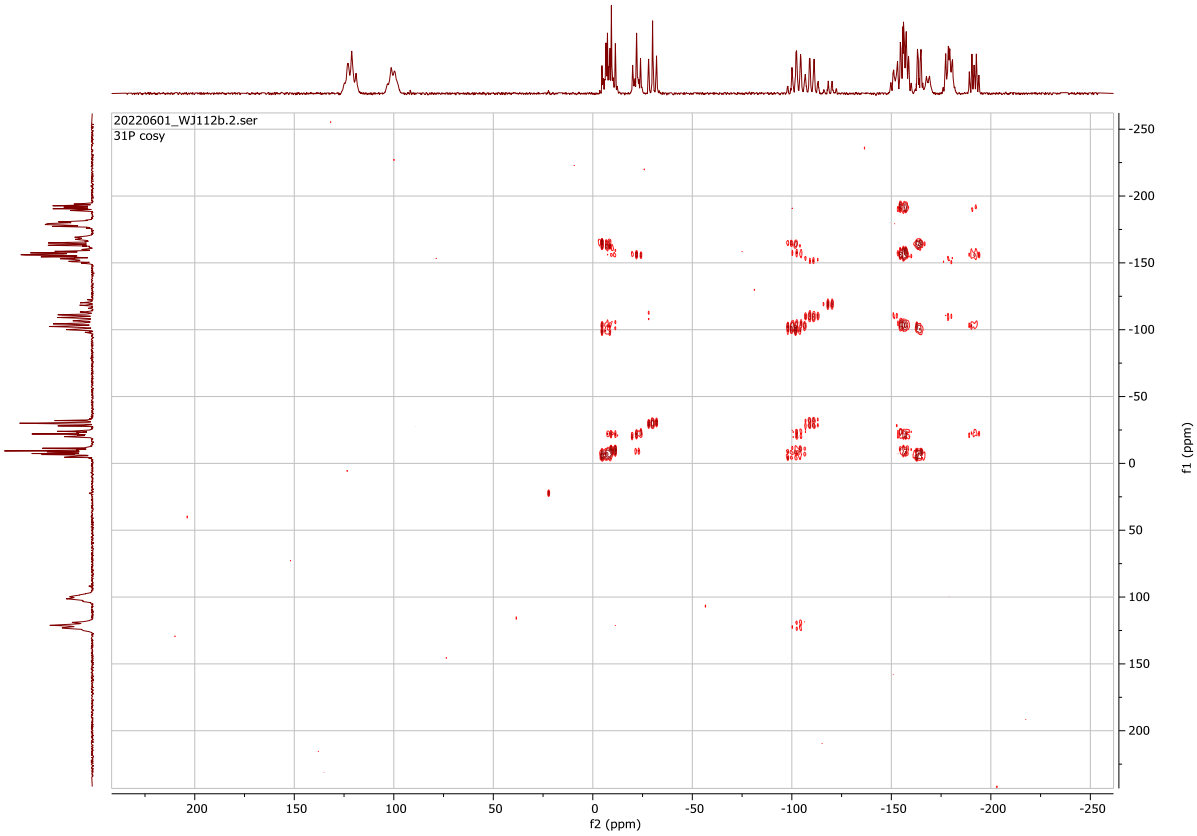


Figure S34. ^{31}P COSY NMR spectrum (Toluene-d_8) of **9.**

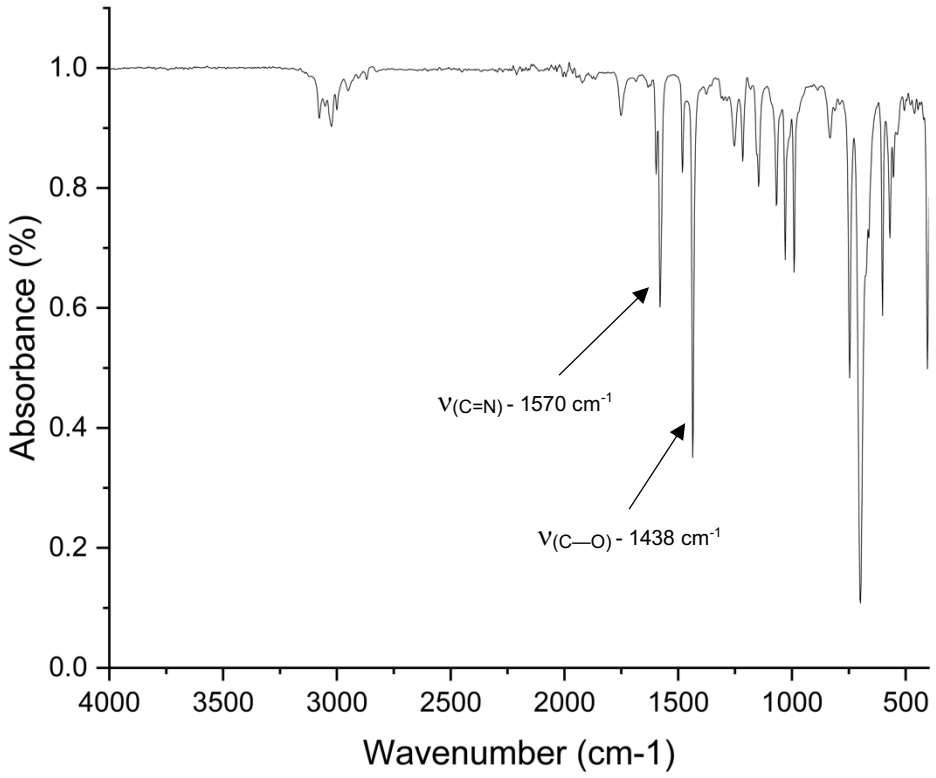
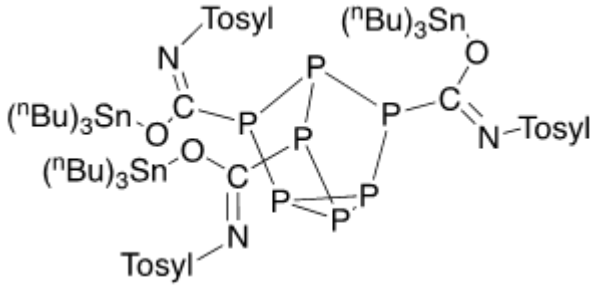


Figure S35. IR spectrum of **9**.

3.1.5. Synthesis of (^{n}Bu$_3$Sn-TsNCO)$_3$P$_7$, 10



A Schlenk flask was loaded with a stir bar. (^{n}Bu$_3$Sn)$_3$P$_7$ (100 mg, 0.092 mmol), was dissolved in toluene (3 mL) and added to the Schlenk. In a separate vial, *p*-toluenesulfonyl isocyanate (54 mg, 0.27 mmol) was dissolved in toluene (3 mL). The *p*-toluenesulfonyl isocyanate solution was added dropwise while stirring rapidly. Once addition was complete, a dark yellow solution was observed. The reaction was stirred for 4 days, by which point, no colour change was observed. NMR spectrum of the reaction mixture revealed left over starting material, however, complete consumption was not possible, even with prolonged reaction times and heating to

40 °C. Due to similarities in solubility, the inserted products were difficult to separate from the starting material. Therefore conversions are quoted as *in situ* values.

^{31}P NMR overall conversion: 45%

^{31}P NMR Isomeric conversion: 26% symmetric (**A**); 19% asymmetric (**B**); 55% unreacted starting material

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ = 7.49 (d, $^{3}J_{HH}$ = 8.3 Hz, 1H, *Ar*), 7.45 (d, $^{3}J_{HH}$ = 7.4 Hz, 2H, *Ar* unreacted tosyl isocyanate), 7.40 (d, $^{3}J_{HH}$ = 8.4 Hz, 1H, *Ar*), 7.35 (d, $^{3}J_{HH}$ = 8.3 Hz, 1H, *Ar*), 7.23 (d, $^{3}J_{HH}$ = 8.1 Hz, 2H, *Ar*), 7.01 (d, $^{3}J_{HH}$ = 8.3 Hz, 2H, *Ar* unreacted tosyl isocyanate), 6.90 - 6.78 (m, 5H, *Ar*), 2.00 (s, 3H, *Me*-Ar unreacted tosyl isocyanate), 1.98 - 1.88 (m, 8H, *Me*-Ar), 1.27 - 1.10 (m, 24H, ^{n}*Bu*), 0.92 - 0.87 (m, 26H, ^{n}*Bu*), 0.83 - 0.65 (m, 20H, ^{n}*Bu*), 0.60 - 0.56 (m, 11H, ^{n}*Bu*), 0.47 (t $^{3}J_{HH}$ = 7.3 Hz, 27H, ^{n}*Bu*) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ = 156.1 (s, *Ar* unreacted tosyl isocyanate), 147.9 (s, *Ar* unreacted tosyl isocyanate), 145.8 (s, *Ar*), 144.1 (s, *Ar*), 139.2 (s, *Ar*), 131.9 (s, *Ar* unreacted tosyl isocyanate), 131.3 (s, *Ar*), 130.9 (s, *Ar* unreacted tosyl isocyanate), 130.6 (s, *Ar*), 130.0 (s, *Ar*), 128.8 (s, *Ar*), 127.9 (s, *Ar*), 31.3 (s, *Me*-Ar), 29.7 (s, *Me*-Ar), 29.3 (s, *Me*-Ar), 29.0 (s, *Me*-Ar unreacted tosyl isocyanate), 28.7 (s, *Me*-Ar), 22.5 - 22.3 (overlapping singlets, ^{n}*Bu*) , 19.9 (s, ^{n}*Bu*), 19.4 (s, ^{n}*Bu*), 16.5 (s, ^{n}*Bu*), 15.0 - 14.8 (overlapping singlets, ^{n}*Bu*) ppm.

^{31}P NMR (168 MHz, 298 K, THF-d$_8$): δ = 132.4 (t, $^{1}J_{PP}$ = 340.8 Hz, 1P, *Bridging B*), 125.6 (t, $^{1}J_{PP}$ = 352.0 Hz, 3P, *Bridging A*), 105.47 (t, $^{1}J_{PP}$ = 339.6 Hz, 1P, *Bridging B*), –17.0 - –25.4 (m, 3P, *Bridging SM*), –46.2 (t, $^{1}J_{PP}$ = 312.8 Hz, 1P, *Bridging B*), –56.2 (t, $^{1}J_{PP}$ = 311.0 Hz, 1P, *Apical B*), –92.0 (qq, $^{1}J_{PP}$ = 303.2 Hz, $^{3}J_{PP}$ = 49.8 Hz, 1P, *Apical SM*), –95.6 - –102.9 (m, 1P, *Apical A*), –151.6 - –160.5 (m, 3P, *Basal A*), –163.8 - –170.1 (m, 3P, *Basal SM*), –175.2 - –204.7 (m, 3P, *Basal B*) ppm.

^{119}Sn NMR (149 MHz, 298 K, THF-d$_8$): δ = 106.8 (s, ^{n}Bu$_3$*Sn*), 72.9 (s, ^{n}Bu$_3$*Sn*), 18.9 (d, $^{1}J_{SnP}$ = 777.5 Hz, (^{n}Bu$_3$*Sn*)$_3$P$_7$) ppm.

Note: Multiple attempts at mass spectrometry were made but significant decomposition was seen upon ionisation.

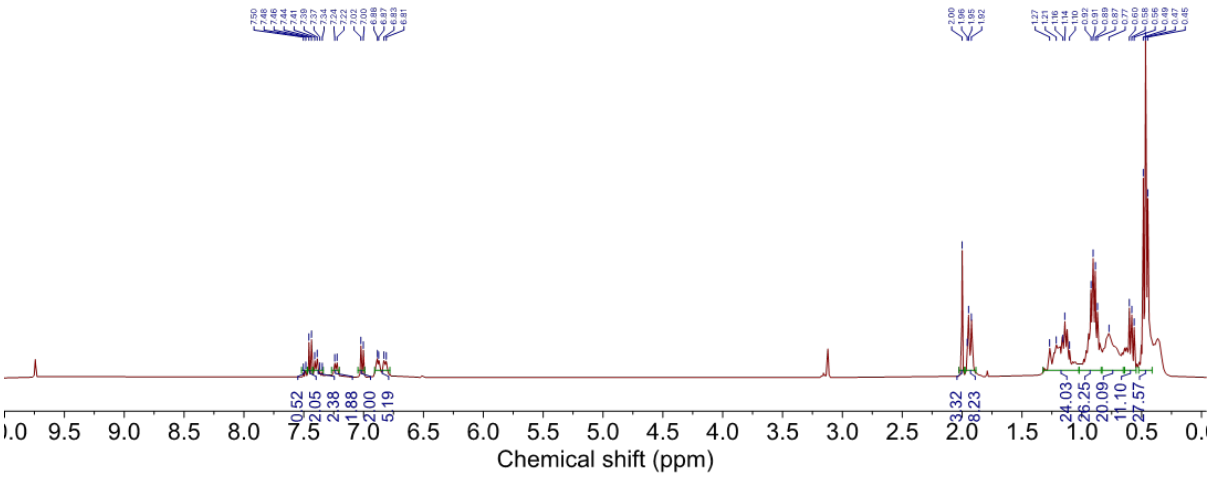


Figure S36. ^{1}H NMR spectrum (THF-d_8) of **10**.

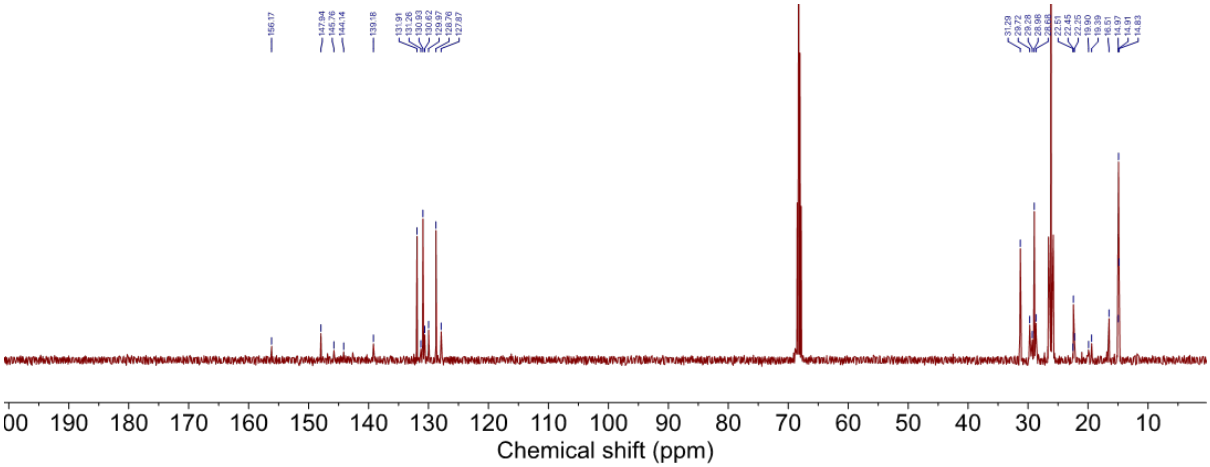


Figure S37. ^{13}C{^{1}H} NMR spectrum (THF-d_8) of **10.**

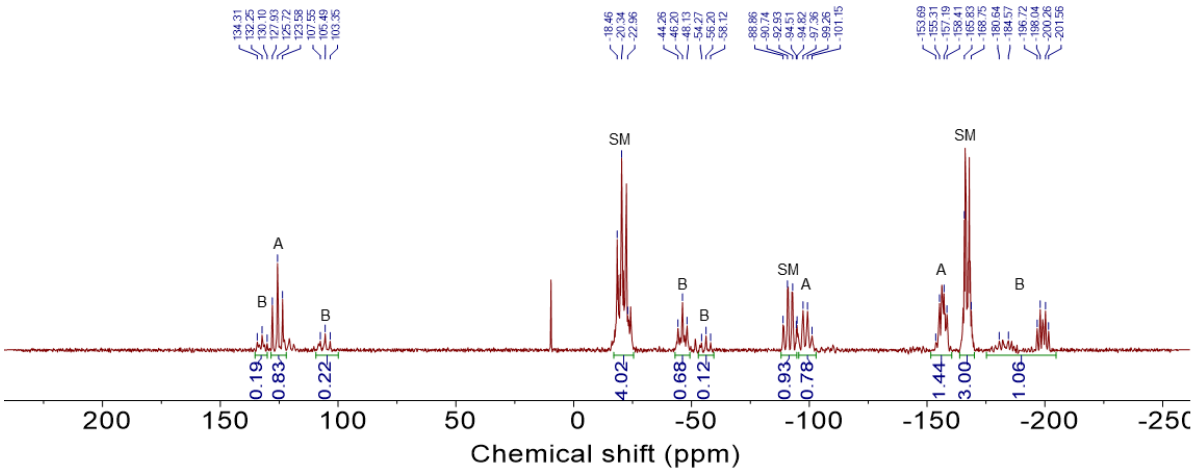


Figure S38. ^{31}P NMR spectrum (THF-d_8) of **10**.

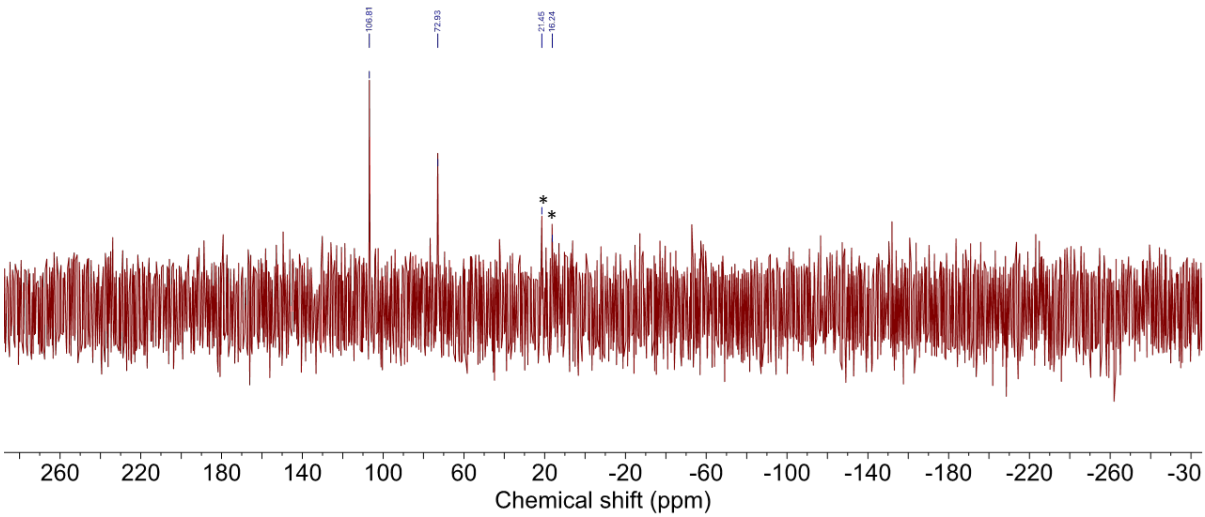


Figure S39. ^{119}Sn NMR spectrum (THF-d_8) of **10**. Unreacted ($^{n}Bu_3Sn)_3P_7$ is marked with a *.

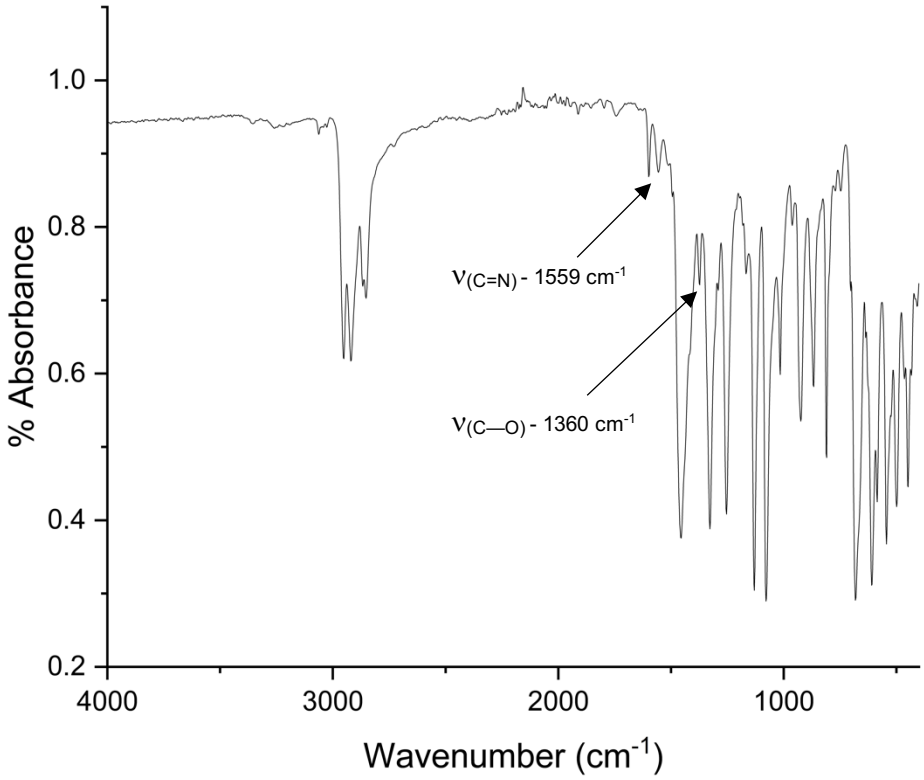
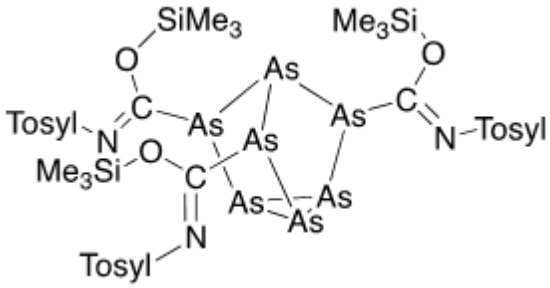


Figure S40. IR spectrum of **10**.

3.1.6. Synthesis of (TMS-TsNCO)$_3$As$_7$, 11



A Schlenk flask was loaded with a stir bar, $(Me_3Si)_3As_7$ (100 mg, 0.134 mmol) was dissolved in THF (3 mL). To this solution, *p*-toluenesulfonyl isocyanate (79 mg, 0.40 mmol) was added affording a deep red solution. The reaction was allowed to stir for 1 week, the solvent was then removed under reduced pressure to give a red oil. The residue was dissolved in Et_2O (2 mL). The resulting solution was left to slowly evaporate, yielding orange needle shaped crystals. The crystals were washed with pentane (3 x 1 mL), affording an orange powder. Crystals suitable for X-ray diffraction analysis were grown through the slow evaporation of an Et_2O solution of the product.

Isolated yield: 85 mg, 47%

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ = 7.75 (d, $^3J_{HH}$ = 8.3 Hz, 6H, *Ar*), 7.28 (d, $^3J_{HH}$ = 7.9 Hz , 6H, *Ar*), 2.33 (s, 9H, *Me*), 0.26 (s, 27H, (*Me*$_3$Si-TsNCO)$_3$As$_7$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ = 185.9 (s, (Me$_3$Si-TsN*C*O)$_3$As$_7$, 145.1 (s, *Ar*), 140.1 (s, *Ar*), 131.0 (s, *Ar*),128.6 (s, *Ar*), 22.1 (s, *Me*), 0.3 (s, (*Me*$_3$Si-TsNCO)$_3$As$_7$) ppm.

^{29}Si DEPT90 NMR (79 MHz, 298 K, THF-d$_8$): δ = 31.12 (s, Me$_3$*Si*–O) ppm.

Elemental analysis: For $C_{33}H_{48}As_7N_3O_9S_3Si_3$: Calcd.: C 29.68, H 3.62, N 3.15, S 7.20; found: C 29.73, H 3.66, N 3.25, S 7.11.

Note: Multiple attempts at mass spectrometry were made but significant decomposition was seen upon ionisation.

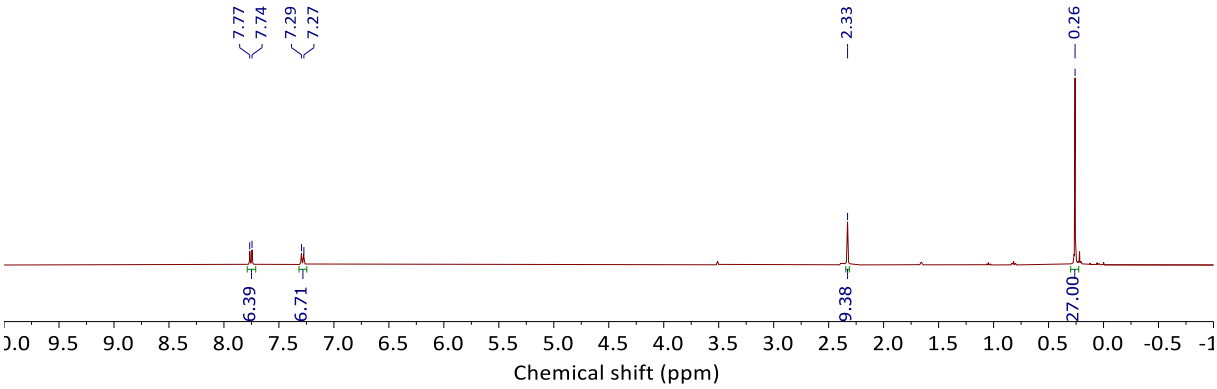


Figure S41. ^{1}H NMR spectrum (THF-d_8) of **11**.

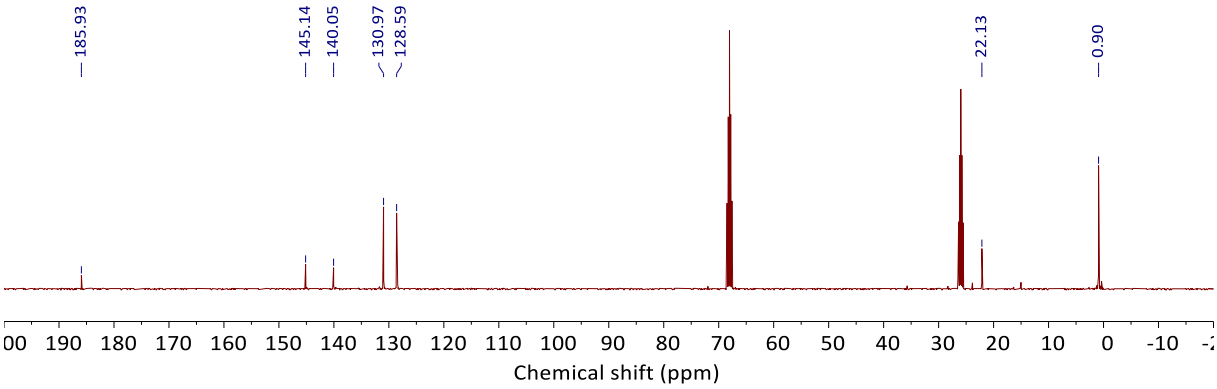


Figure S42. ^{13}C{^{1}H} NMR spectrum (THF-d_8) of **11.**

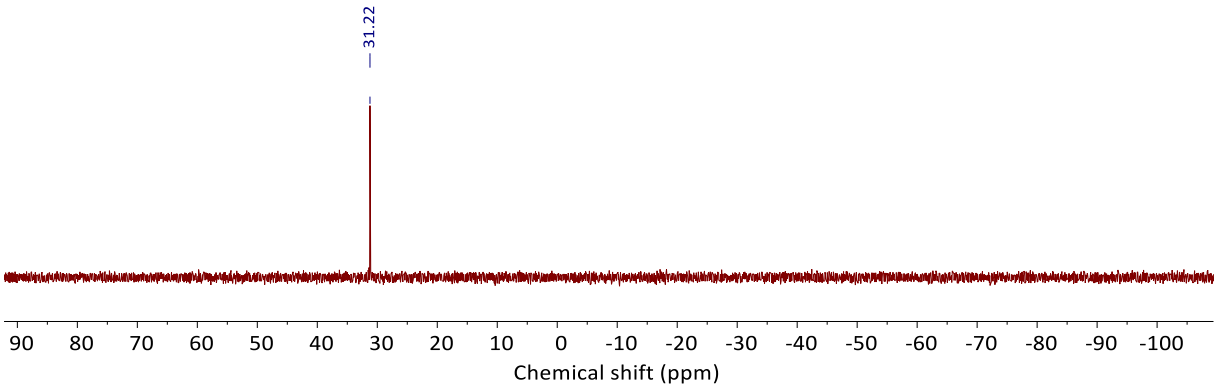


Figure S43. ^{29}Si DEPT90 NMR spectrum (THF-d_8) of **11.**

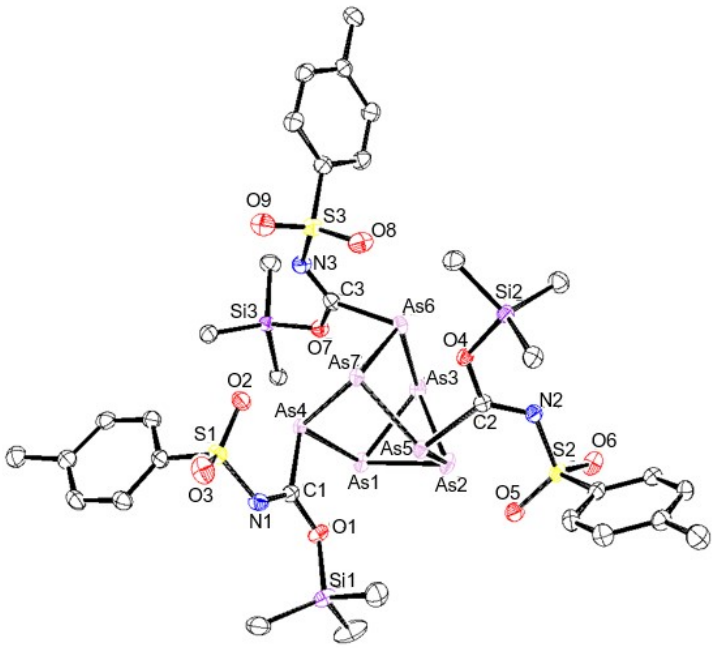


Figure S44. Molecular structure of **11**. Anisotropic displacement ellipsoids captured at 50% probability. Hydrogen atoms have been omitted for clarity. Arsenic: plum; Nitrogen: blue; Oxygen: red; Silicon: purple; Carbon: white.

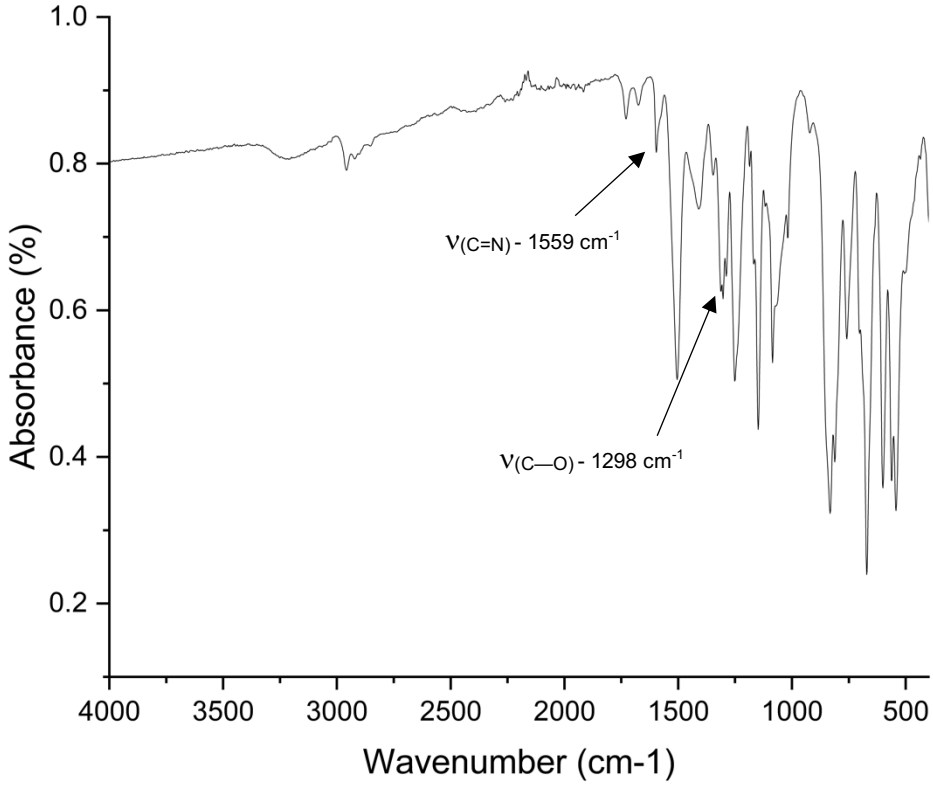


Figure S45. IR spectrum of **11**.

4. IR data

Table S1. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **6**.

$(Me_3Ge\text{-}PhNCO)_3P_7$ - OOO binding		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1710	-
C—O	1342	-
$(Me_3Ge\text{-}PhNCO)_3P_7$ - NNN binding (expected)		
C—N	1366	1376
C=O	1709	1601

Table S2. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **7.**

$(Et_3Ge\text{-}PhNCO)_3P_7$ - OOO binding		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1704	-
C—O	1328	-
$(Et_3Ge\text{-}PhNCO)_3P_7$ - NNN binding (expected)		
C—N	1228	1187
C=O	1705	1570

Table S3. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **8**.

$(Me_3Ge\text{-}TsNCO)_3P_7$ - OOO binding (expected)		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1580	1598
C—O	1343	1300
$(Me_3Ge\text{-}TsNCO)_3P_7$ - NNN binding		
C—N	1202	-
C=O	1736	-

Table S4. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **9**.

$(Et_3Ge\text{-}TsNCO)_3P_7$ - OOO binding (expected)		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1569	1570
C—O	1438	1340
$(Et_3Ge\text{-}TsNCO)_3P_7$ - NNN binding		
C—N	1221	**-**
C=O	1736	-

Table S5. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **10**.

$(^nBu_3Sn\text{-}TsNCO)_3P_7$ - OOO binding (expected)		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1540	1559
C—O	1343	1360
$(^nBu_3Sn\text{-}TsNCO)_3P_7$ - NNN binding		
C—N	1258	-
C=O	1658	-

Table S6. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **11**.

$(Me_3Si\text{-}TsNCO)_3P_7$ - OOO binding (expected)		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=N	1587	1587
C—O	1293	1298
$(Me_3Si\text{-}TsNCO)_3P_7$ - NNN binding		
C—N	1174	-
C=O	1717	-

Table S7. Comparison of observed IR wavenumber against computationally calculated wavenumber, calculated at the pbe1pbe 6-311G(d,p) level of theory for compound **12**.

$(Me_3Si\text{-}CO_2)_3P_7$		
Bond vibration	**Calculated wavenumber / cm^{-1}**	**Observed wavenumber / cm^{-1}**
C=O	1785	1623
C—O	1219	1122

5. CO_2 Reactivity

A J Young NMR tube was loaded with functionalised heptapnictide clusters **1**-**4** (50 mg) and dissolved in $CDCl_3$ (1 mL). The solution was subsequently degassed by removing the headspace of the J Young NMR tube and placing it in a sonicator. This process was repeated until no bubbles were seen upon sonication. The J Young NMR tube was then pressurised with CO_2 (1 atm.) and rotated to ensure dissolution of CO_2. The reaction mixture was then investigated by NMR and IR spectroscopy.

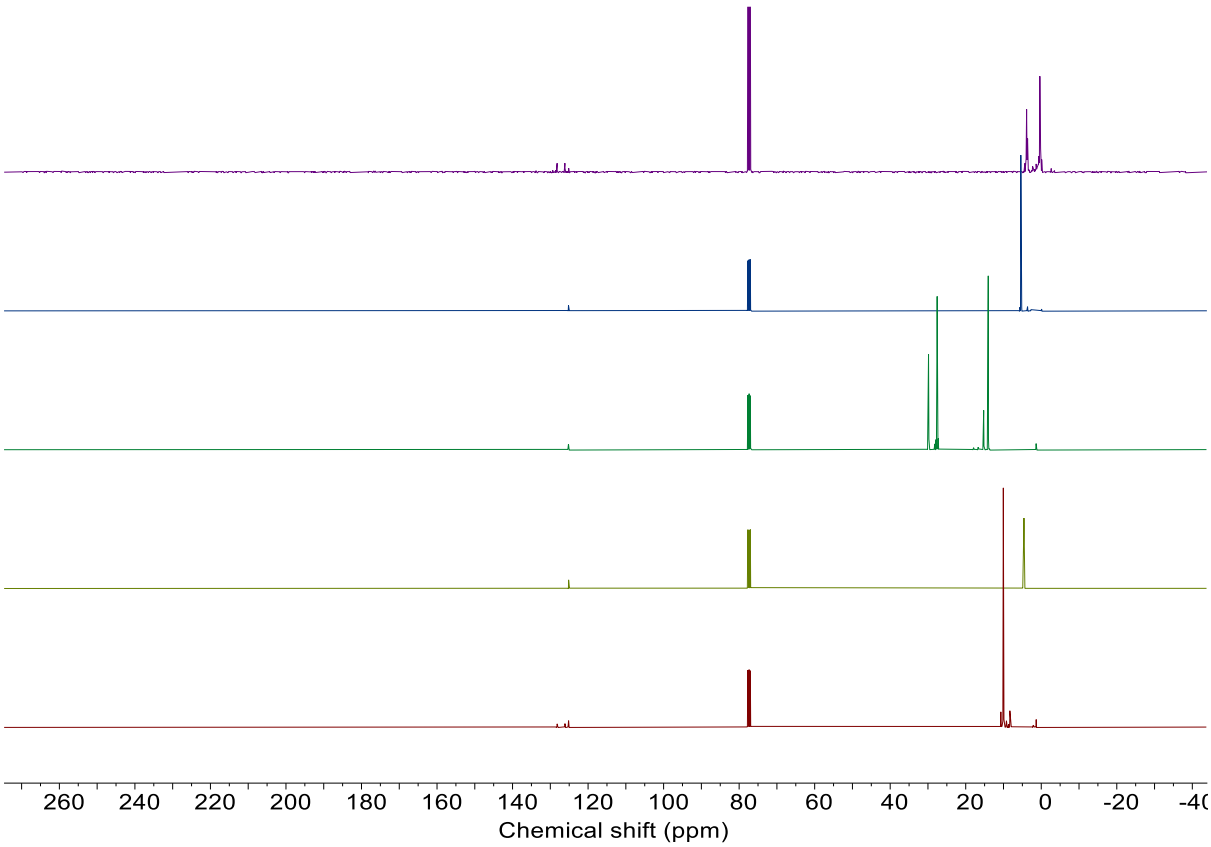


Figure S46. Stacked $^{13}C\{H\}$ NMR spectra ($CDCl_3$) of reactivity of selected clusters towards CO_2. Top – bottom; $(Me_3Si)_3P_7$, $(Me_3Si)_3As_7$, $(^nBu_3Sn)_3P_7$, $(Me_3Ge)_3P_7$, $(Et_3Ge)_3P_7$.

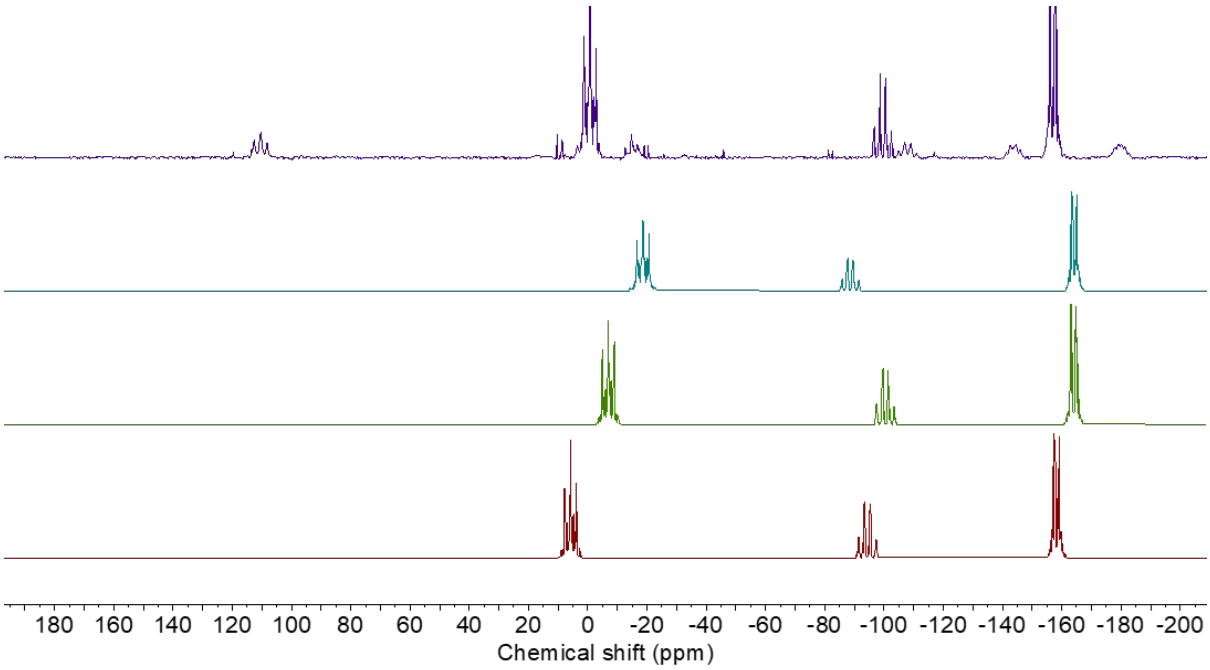


Figure S47. Stacked ^{31}P NMR spectra ($CDCl_3$) of reactivity of selected clusters towards CO_2. Top - bottom; $(Me_3Si)_3P_7$, $(^nBu_3Sn)_3P_7$, $(Me_3Ge)_3P_7$, $(Et_3Ge)_3P_7$.

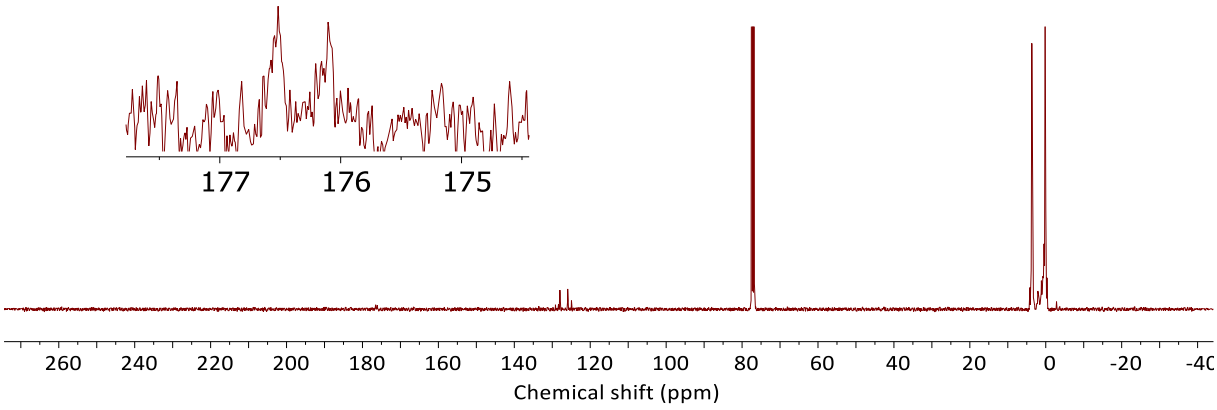


Figure S48. $^{13}C\{^1H\}$ NMR spectrum ($CDCl_3$) $(Me_3Si)_3P_7$ reactivity towards CO_2.

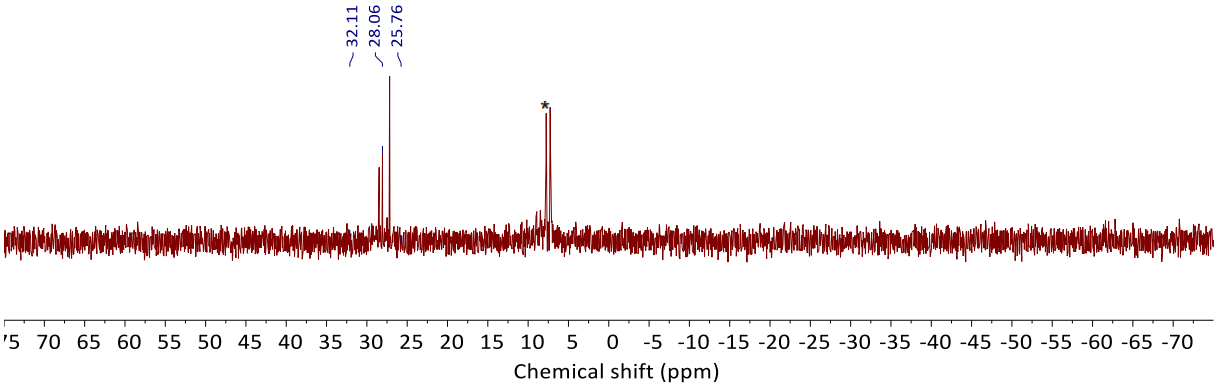


Figure S49. ^{29}Si DEPT90 NMR spectrum ($CDCl_3$) of reactivity $(Me_3Si)_3P_7$ towards CO_2. $(Me_3Si)_3P_7$ marked by *.

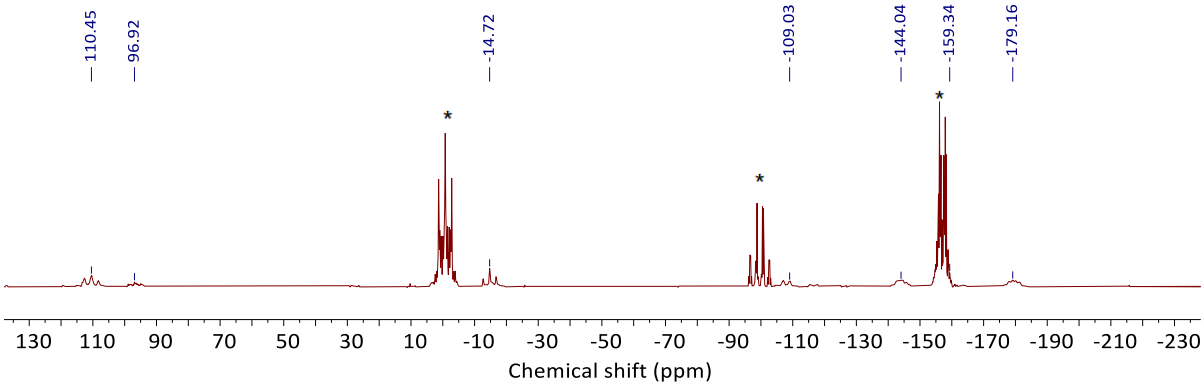


Figure S50. ^{31}P NMR spectrum ($CDCl_3$) of reactivity $(Me_3Si)_3P_7$ towards CO_2. $(Me_3Si)_3P_7$ marked by *.

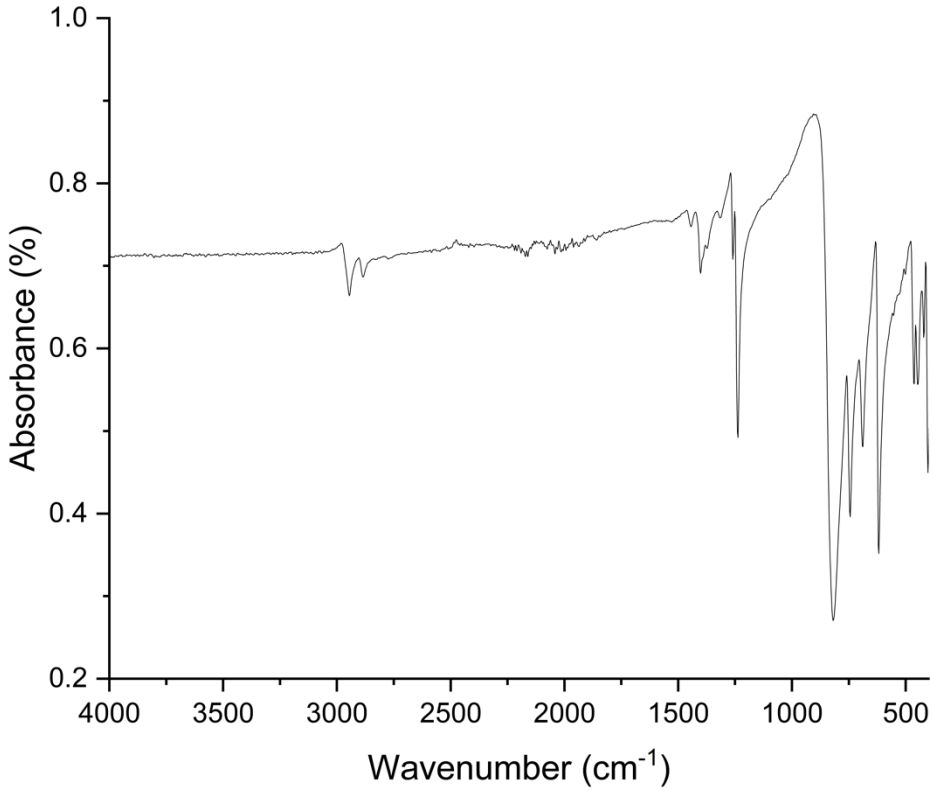


Figure S51. IR spectrum of $(Me_3Si)_3P_7$

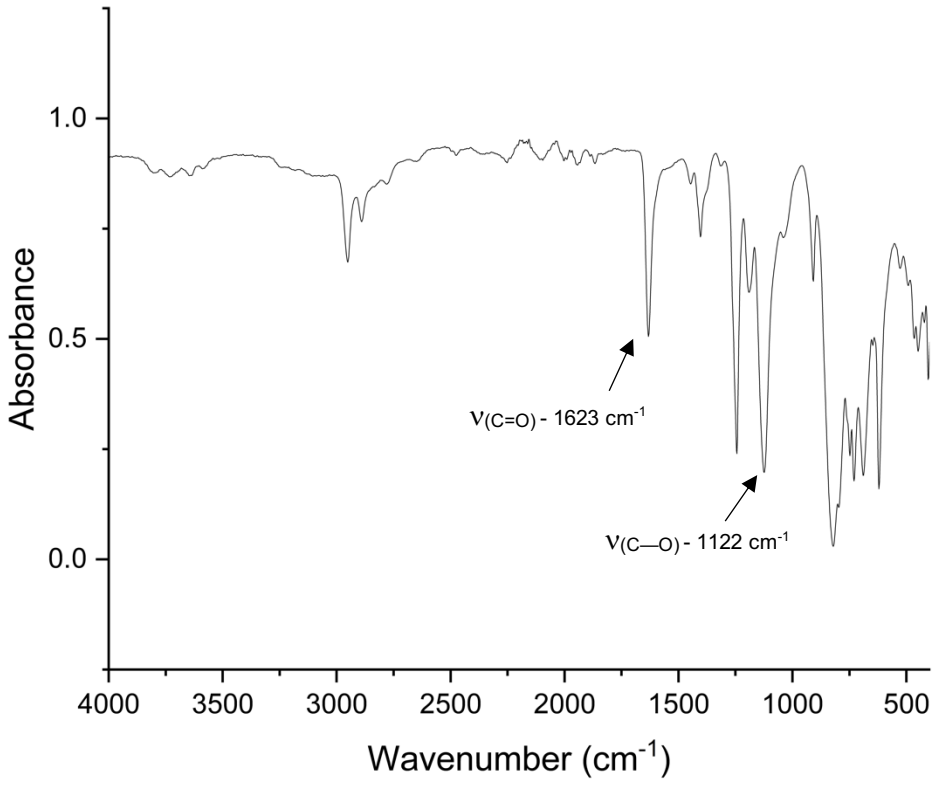
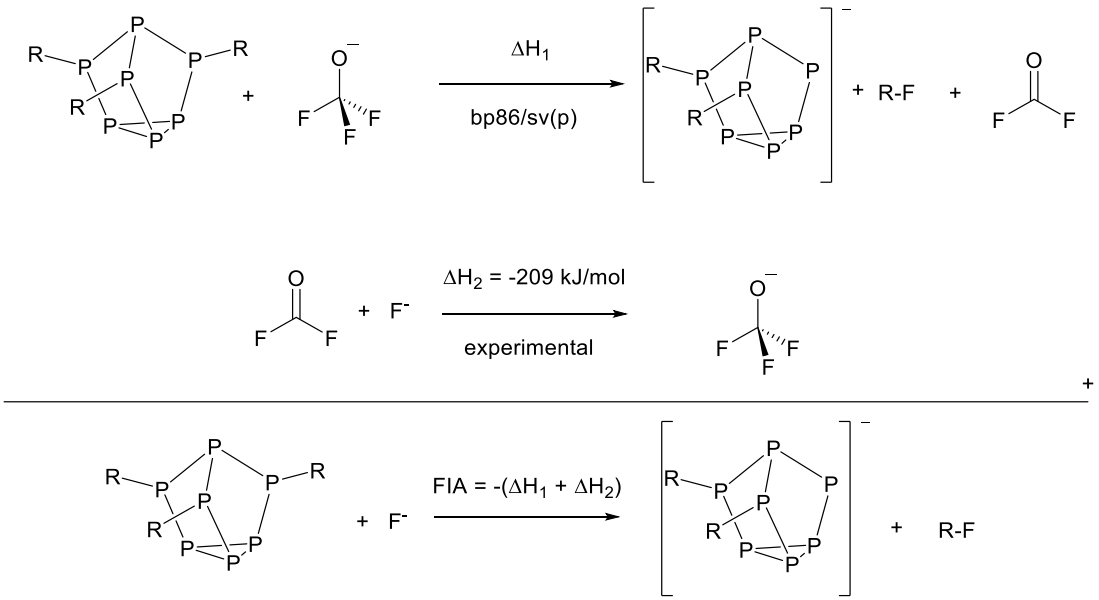


Figure S52. IR spectrum of **12**.

6. Computational Studies

6.1. Fluoride ion Affinity of $(R_3E)_3Pn_7$ Clusters

Lewis acidity was assessed through the calculation of Fluoride Ion Affinity (FIA) using the $CF_2O \rightarrow CF_3O$ reaction as a reference (Christe's method).[13] This method was carried out using the BP86/SV(p) level of theory. The FIA of three benchmarks were calculated, $B(C_6F_5)_3$, SbF_5 and Me_3Si^+ and are consistent with literature calculated values.[14]



Scheme S1. FIA protocol used for compounds in **Table S10**.

Table S10. FIA values for reference Lewis acids and selected functionalised clusters, calculated at the BP86/SV(P) level of theory.

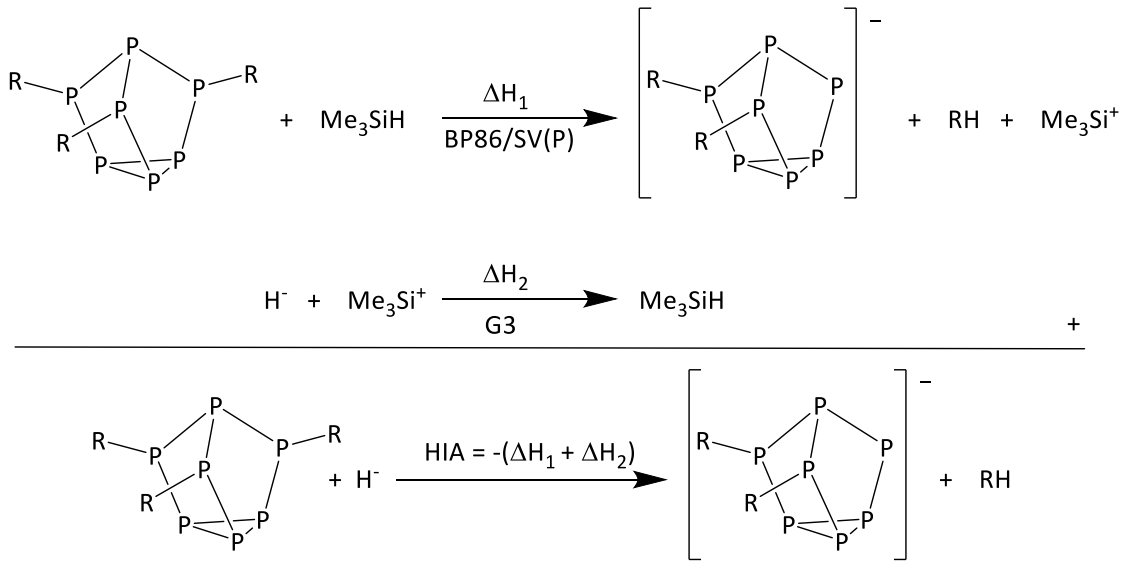
Compound	FIA (kJ mol^{-1})	
$B(C_6F_5)_3$	444	
SbF_5	489	
$[Me_3Si]^+$	948	
	Pn = P	**Pn = As**
$(Me_3Si)_3Pn_7$	324	332
$(Me_3Ge)_3Pn_7$	265	-
$(Et_3Ge)_3Pn_7$	277	281
$(^nBu_3Sn)_3Pn_7$	266	269

Table S11. Computed energies of reference Lewis acids Selected functionalised clusters, relating to FIA calculations, calculated at the BP86/SV(P) level of theory.

Compound	E / a.u.	G / a.u.
CF_2O	–312.7854163	–312.76742
$[CF_3O]^-$	–412.6141114	–412.594474
$B(C_6F_5)_3$	–2206.628214	–2206.448141
$[FB(C_6F_5)_3]^-$	–2306.547159	–2306.364788
SbF_5	–6814.717684	–6814.698435
$[SbF_6]^-$	–6914.652886	–6914.631992
$[Me_3Si]^+$	–408.8174622	–408.70319
Me_3SiF	–508.931154136	–508.81189
$^nBu_3SnF$	–6598.24693198	–6597.868217
$(^nBu_3Sn)_3P_7$	–21884.4993751	–21883.346266
$[(^nBu_3Sn)_2P_7]^-$	–15386.1007131	–15385.326736
$(^nBu_3Sn)_3As_7$	–35146.7341606	–35145.583690
$[(^nBu_3Sn)_2As_7]^-$	–28648.3367946	–28647.565194
Me_3GeF	–2296.47761263	–2296.359209
$(Me_3Ge)_3P_7$	–8979.17062838	–8978.799105
$[(Me_3Ge)_2P_7]^-$	–6782.54195196	–6782.288315
Et_3GeF	–2414.31649080	–2414.110062
$(Et_3Ge)_3P_7$	–9332.67980335	–9332.044779
$[(Et_3Ge)_2P_7]^-$	–7018.21645801	–7017.787540
$(Et_3Ge)_3As_7$	–22594.9112847	–22594.278756
$[(Et_3Ge)_2As_7]^-$	–20280.4501365	–20280.023356
$(Me_3Si)_3P_7$	–3616.46134639	–3616.088086
$[(Me_3Si)_2P_7]^-$	–3207.40214107	–3207.147222
$(Me_3Si)_3As_7$	–16878.6873263	–16878.317909
$[(Me_3Si)_2As_7]^-$	–16469.6322647	–16469.379865

6.2. Hydride ion affinity for the $(R_3E)_3Pn_7$ clusters.

Lewis acidity was assessed through the calculation of Hydride Ion Affinity (HIA) using the Me_3Si^+ → Me_3SiH reaction as a reference.[15] This method was carried out using the BP86/SV(p) level of theory.



Scheme S2. HIA protocol used for compounds in **Table S13.**

Table S13. HIA values for reference Lewis acids and selected functionalised clusters, calculated at the BP86/SV(P) level of theory.

Compound	**HIA (kJ mol^{-1})**	
$B(C_6F_5)_3$	487	
SbF_5	545	
$[Me_3Si]^+$	819	
	Pn = P	**Pn = As**
$(Me_3Ge)_3Pn_7$	331	-
$(Et_3Ge)_3Pn_7$	340	344
$(^nBu_3Sn)_3Pn_7$	333	335
$(Me_3Si)_3Pn_7$	-	-

Note: Entries for $(Me_3Si)_3Pn_7$ have not been included as Me_3Si^+ is used in the HIA protocol reference reaction (Scheme S2).

Table S14. Computed energies of reference Lewis acids Selected functionalised clusters, relating to HIA calculations, calculated at the BP86/SV(P) level of theory.

Compound	E / a.u.	G / a.u.
$B(C_6F_5)_3$	-2206.628234	-2206.44815
$[HB(C_6F_5)_3]^-$	-2207.3285042	-2207.14043
SbF_5	-6814.71771307	-6814.698459
$[HSbF_5]^-$	-6815.43952664	-6815.412861
H^-	-0.488737487818	-0.486377
Me_3Si^+	-408.817035912	-408.703695
Me_3SiH	-409.699318773	-409.575699
Me_3GeH	-2197.26657258	-2197.143811
$(Me_3Ge)_3P_7$	-8979.17062394	-8978.799096
$[(Me_3Ge)_2P_7]^-$	-6782.54195195	-6782.288315
Et_3GeH	-2315.10390822	-2314.893338
$(Et_3Ge)_3P_7$	-9332.67980334	-9332.044779
$[(Et_3Ge)_2P_7]^-$	-7018.21645801	-7017.78754
$(Et_3Ge)_3As_7$	-22594.9110235	-22594.278624
$[(Et_3Ge)_2As_7]^-$	-20280.449888	-20280.023073
$^nBu_3SnH$	-6499.03533519	-6498.653163
$(^nBu_3Sn)_3P_7$	-21884.4993749	-21883.346266
$[(^nBu_3Sn)_2P_7]^-$	-15386.1006414	-15385.326765
$(^nBu_3Sn)_3As_7$	-35146.7341605999	-35145.5836899999
$[(^nBu_3Sn)_2As_7]^-$	-28648.3367946	-28647.565194

6.3. Lewis acid binding affinity for PhNCO and TsNCO inserted products of $(R_3E)_3Pn_7$ clusters

Experimental observations suggest that the Lewis acidic tetrel moiety binds preferentially to either the oxygen or the nitrogen atom of the corresponding isocyanate on all three arms of the cluster (O,O,O vs N,N,N). These binding affinities were calculated computationally by taking the difference in energy between the [O,O,O]–[N,N,N] binding modes, calculated at the pbe1pbe/6-311G(d,p) level of theory.

Table S15. Computed difference in energies between O,O,O and N,N,N tetrel binding modes of the Lewis acidic moieties for compounds **6-11** and $(Me_3Sn\text{-}TsNCO)_3P_7$, calculated at the PBE1PBE/6-311G(d,p) level of theory.

Compound	ΔE / kJ mol^{-1}	ΔG / kJ mol^{-1}
$(Me_3Ge\text{-}PhNCO)_3P_7$	61.3	54.4
$(Et_3Ge\text{-}PhNCO)_3P_7$	41.7	31.4
$(Me_3Ge\text{-}TsNCO)_3P_7$	2.4	-1.1
$(Et_3Ge\text{-}TsNCO)_3P_7$	1.5	-18.9
$(^nBu_3Sn\text{-}TsNCO)_3P_7$	19.3	7.2
$(Me_3Si\text{-}TsNCO)_3As_7$	-35.5	-48.2

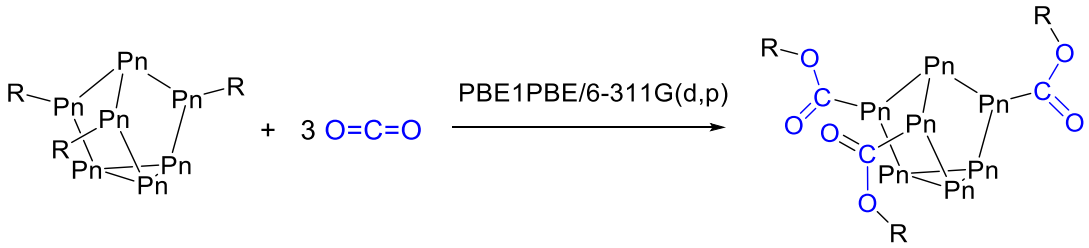
*Note: All listed energies in **Table S15** are calculated by taking the free energy of the O,O,O mode and subtracting the free energy of the N,N,N mode. Thus, a positive number suggests*

that tetrel N,N,N is preferred and a negative number that O,O,O coordination is more favourable.

Table S16. Computed energies of inserted products **6-11** and $(Me_3Sn\text{-}TsNCO)_3P_7$.

	N,N,N		O,O,O	
Compound	**E / a.u.**	**G / a.u.**	**E / a.u.**	**G / a.u.**
$(Me_3Ge\text{-}PhNCO)_3P_7$	-10175.9510773	-10175.385603	-10175.9281277	-10175.364978
$(Et_3Ge\text{-}PhNCO)_3P_7$	-10529.3813067	-10528.570457	-10529.3654242	-10528.558509
$(Me_3Ge\text{-}TsNCO)_3P_7$	-11938.7702743	-11938.11447	-11938.769376	-11938.114894
$(Et_3Ge\text{-}TsNCO)_3P_7$	-12292.2042706	-12291.299041	-12292.2037186	-12291.306242
$(^nBu_3Sn\text{-}TsNCO)_3P_7$	-24842.1321144	-24840.765447	-24842.124764	-24840.762713
$(Me_3Si\text{-}TsNCO)_3As_7$	-19837.3253321	-19836.676104	-19837.3388398	-19836.694453

6.2. CO_2 Capture with $(R_3E)_3Pn_7$ Clusters.



Scheme S2. Capture of CO_2 at group 14 functionalised [Pn] clusters.

Table S17. Computed energies for the capture of CO_2 at group 14 functionalised [Pn] clusters. Performed at the PBE1PBE/6-311G(d,p) level of theory. [a] Calculated using SV(p) basis set for Sn atoms.

Compound	ΔG (kJ/mol)
$(Me_3Si)_3P_7$	–27.1
$(Me_3Ge)_3P_7$	93.2
$(Et_3Ge)_3P_7$	91.9
$(^nBu_3Sn)_3P_7$[a]	100.2
$(Me_3Si)_3As_7$	–32.2
$(Et_3Ge)_3As_7$	94.5
$(^nBu_3Sn)_3As_7$[a]	136.5

Table S18. Computed energies for the capture of CO_2 at group 14 functionalised [Pn] clusters. Performed at the PBE1PBE/6-311G(d,p) level of theory. [a] Calculated using SV(p) basis set for Sn atoms.

Compound	E / a.u.	G / a.u.
CO_2	–188.437815	–188.423625
$(Me_3Si)_3P_7$	–3615.871612	–3615.486748
$(Me_3Si–CO_2)_3P_7$	–4181.202418	–4180.767937
$(Me_3Ge)_3P_7$	–8977.813650	–8977.430293
$(Me_3Ge–CO_2)_3P_7$	–9543.098316	–9542.665690
$(Et_3Ge)_3P_7$	–9331.248783	–9330.592955
$(Et_3Ge–CO_2)_3P_7$	–9896.534228	–9895.828833
$(^nBu_3Sn)_3P_7$[a]	–21881.168602	–21879.978911
$(^nBu_3Sn–CO_2)_3P_7$[a]	–22446.450550	–22445.211615
$(Me_3Si)_3As_7$	–16876.337472	–16875.955770
$(Me_3Si–CO_2)_3As_7$	–17441.669937	–17441.238918
$(Et_3Ge)_3As_7$	–22591.715636	–22591.063174
$(Et_3Ge–CO_2)_3As_7$	–23157.000037	–23156.298067
$(^nBu_3Sn)_3As_7$[a]	–35141.644033	–35140.457269
$(^nBu_3Sn–CO_2)_3As_7$[a]	–35706.911783	–35705.676149

6.3. Optimised Structures BP86/SV(p) Level of Theory for FIA calculations

CF2O

Charge = 0 Multiplicity = 1

O	-0.0466230000	-0.7269130000	0.7078620000
C	-0.0198320000	0.4570640000	0.6604760000
F	-1.0755860000	1.2641720000	0.6177690000
F	1.0710410000	1.2166780000	0.6398920000

[CF3O]-

Charge = -1 Multiplicity = 1

O	-0.0024660000	-0.0727380000	0.7919310000
C	-0.0077480000	-1.2197580000	1.2200720000
F	-0.0372870000	-1.3904350000	2.6566080000
F	1.1166540000	-2.0616680000	0.8724600000
F	-1.1111530000	-2.0694010000	0.8259280000

$B(C_6F_5)_3$

Charge = 0 Multiplicity = 1

B	-0.1527200000	0.4557970000	-0.1605200000

C	-0.5860590000	1.3581700000	-1.3766080000
C	-0.1083040000	-1.1107320000	-0.3176840000
C	0.2355380000	1.1209860000	1.2133700000
C	-0.0238350000	-3.9535890000	-0.6022600000
C	0.3991710000	-3.1282370000	-1.6617220000
C	0.3396250000	-1.7339100000	-1.5065250000
C	-0.5130710000	-1.9823330000	0.7209530000
C	-0.4887670000	-3.3807870000	0.5971040000
F	0.0160700000	-5.2789060000	-0.7349120000
F	0.8493990000	-3.6771200000	-2.7944170000
F	0.7672890000	-0.9904480000	-2.5413400000
F	-0.9782470000	-1.4844150000	1.8795460000
F	-0.8990550000	-4.1686170000	1.5960760000
C	0.9379580000	2.3272340000	3.7079460000
C	1.6577230000	1.2114750000	3.2392850000
C	1.2910990000	0.6273090000	2.0161560000
C	-0.4498370000	2.2498640000	1.7217490000
C	-0.1271350000	2.8499490000	2.9495890000
F	1.2651870000	2.8894560000	4.8708630000
F	2.6748620000	0.7255680000	3.9577470000
F	2.0184480000	-0.4257380000	1.6056550000
F	-1.4829100000	2.7773710000	1.0427140000
F	-0.8136720000	3.9032240000	3.4036760000
C	-1.3737740000	2.9974720000	-3.5815760000
C	-2.0361030000	1.7786450000	-3.3397880000
C	-1.6274720000	0.9825950000	-2.2575660000
C	0.0416280000	2.5951620000	-1.6551120000
C	-0.3235410000	3.4096670000	-2.7390890000
F	-1.7413530000	3.7617730000	-4.6093870000
F	-3.0391770000	1.3964250000	-4.1365090000
F	-2.3001260000	-0.1641980000	-2.0603520000
F	1.0588850000	3.0253600000	-0.8892410000
F	0.3092550000	4.5625400000	-2.9788190000

$[FB(C_6F_5)_2]^-$

Charge = -1 Multiplicity = 1

B	-1.0312930000	0.2232650000	0.0282600000
C	-0.9890050000	1.2531340000	-1.2823180000
C	-0.3707440000	-1.2773630000	-0.2797500000
C	-0.2759520000	1.0317420000	1.2858070000
C	0.5070170000	-3.9914620000	-0.6547500000
C	0.4773630000	-3.0981990000	-1.7352940000
C	0.0361790000	-1.7742170000	-1.5287690000
C	-0.3270790000	-2.2166340000	0.7693280000
C	0.1011300000	-3.5465250000	0.6148250000
F	0.9186910000	-5.2624450000	-0.8310130000
F	0.8572570000	-3.5187830000	-2.9597680000
F	0.0221920000	-0.9984240000	-2.6379190000
F	-0.6982780000	-1.8584350000	2.0180080000
F	0.1283960000	-4.3989990000	1.6599830000
C	0.8329230000	2.5318650000	3.4745310000
C	1.5555730000	1.4758250000	2.8979060000
C	0.9954700000	0.7624780000	1.8202290000
C	-0.9522780000	2.1116220000	1.8861300000
C	-0.4358920000	2.8532150000	2.9663140000
F	1.3509140000	3.2296770000	4.5048280000
F	2.7781100000	1.1653470000	3.3773000000
F	1.7704130000	-0.2248360000	1.3162040000
F	-2.1605890000	2.5039580000	1.4302660000
F	-1.1318830000	3.8755200000	3.5062330000
C	-0.8508750000	3.1531150000	-3.4367820000
C	-2.0824890000	2.6064350000	-3.0465420000
C	-2.1310160000	1.6724020000	-1.9899130000
C	0.2195170000	1.8229440000	-1.7215220000
C	0.3193290000	2.7532990000	-2.7702760000
F	-0.7891280000	4.0449120000	-4.4458020000
F	-3.2081690000	2.9781200000	-3.6917710000
F	-3.3572600000	1.1913170000	-1.7056160000
F	1.3867140000	1.4601540000	-1.1373620000
F	1.5113150000	3.2615440000	-3.1462110000
F	-2.3785710000	-0.0295660000	0.4192040000

SbF_5

Charge = 0 Multiplicity = 1

F	-1.9354430000	0.7880830000	0.0118850000
F	0.1865520000	1.0762600000	-1.6358360000
F	-1.0232240000	-1.7224270000	-0.3860040000
F	0.2213570000	0.5881340000	1.6245680000
F	1.5235260000	-0.8318660000	-0.2673920000
Sb	-0.2057670000	-0.0211940000	-0.1292210000

$[SbF_6]^-$

Charge = -1 Multiplicity = 1

F	0.6934610000	1.8491390000	0.2844740000
F	0.2883260000	-0.4182980000	1.7840280000
F	-1.8501630000	0.8765200000	0.6436940000
F	-0.6454980000	0.6963010000	-1.8202990000
F	1.4930270000	-0.5985220000	-0.6799630000
F	-1.0505750000	-1.5711420000	-0.3207950000
Sb	-0.1785690000	0.1390010000	-0.0181390000

$(Me_3Si)_3P_7$

Charge = 0 Multiplicity = 1

P	-0.4531200000	0.0273000000	-0.3213600000
P	0.5239630000	0.2945230000	-2.3048660000
P	0.5912810000	-1.8422420000	0.2898830000
P	-2.3536600000	-0.8906030000	-1.0342170000
P	0.2145770000	-3.2067080000	-1.4476510000
P	-1.6369940000	-2.4250850000	-2.5008900000
P	0.4233020000	-1.7631900000	-3.1850560000
Si	2.7932550000	0.5756030000	-1.8827070000
Si	-0.6831780000	-2.8014950000	1.9817350000
Si	-3.3674480000	0.6933460000	-2.4059720000
C	-3.1718340000	2.3701160000	-1.5427920000
C	-5.1926350000	0.1711030000	-2.4241120000
C	-2.7088550000	0.7554940000	-4.1794280000
C	-1.1547630000	-1.4012860000	3.1710980000
C	0.5269180000	-3.9966870000	2.8253900000

C	-2.2137600000	-3.7464690000	1.3947690000
C	2.9268090000	1.7491280000	-0.3987760000
C	3.4410450000	1.4247780000	-3.4523500000
C	3.7627560000	-1.0213040000	-1.5793210000
H	2.3400790000	2.6773750000	-0.5579190000
H	3.9892070000	2.0376150000	-0.2434130000
H	2.5620310000	1.2653650000	0.5305650000
H	3.3889130000	-1.5510410000	-0.6797870000
H	4.8370210000	-0.7771560000	-1.4267490000
H	3.6880050000	-1.7114100000	-2.4451850000
H	2.9042890000	2.3751110000	-3.6521910000
H	3.3229930000	0.7717400000	-4.3422770000
H	4.5232630000	1.6550150000	-3.3426420000
H	0.0341280000	-4.4926970000	3.6898350000
H	1.4259060000	-3.4645560000	3.1993170000
H	0.8648950000	-4.7905970000	2.1270070000
H	-1.9405850000	-4.5551670000	0.6856300000
H	-2.9294030000	-3.0686290000	0.8867220000
H	-2.7210160000	-4.2111280000	2.2685580000
H	-1.6317540000	-1.8273650000	4.0805470000
H	-1.8747100000	-0.6985020000	2.7037130000
H	-0.2645590000	-0.8217530000	3.4920140000
H	-5.7885580000	0.8899810000	-3.0276750000
H	-5.6186910000	0.1442990000	-1.3999100000
H	-5.3203790000	-0.8356770000	-2.8740320000
H	-3.7553890000	3.1431940000	-2.0885240000
H	-2.1095470000	2.6890280000	-1.5250010000
H	-3.5411550000	2.3369040000	-0.4970530000
H	-1.6345440000	1.0296740000	-4.1980530000
H	-3.2792830000	1.5146430000	-4.7583970000
H	-2.8268180000	-0.2235860000	-4.6884810000

$[(Me_3Si)_2P_7]^-$

Charge = -1 Multiplicity = 1

P	-0.4059540000	-0.0554550000	-0.0693580000
P	0.4140040000	0.2763240000	-2.1612650000

P	0.4510290000	-1.9305040000	0.6251970000
P	-2.3647230000	-0.9015210000	-0.8051280000
P	0.2024040000	-3.1553780000	-1.1596670000
P	-1.6914680000	-2.4654260000	-2.2560010000
P	0.3558760000	-1.7795870000	-3.0066370000
Si	2.6753490000	0.5032530000	-1.8126800000
Si	-3.3211350000	0.6467400000	-2.2172180000
C	-3.0449240000	2.3851230000	-1.4848780000
C	-5.1972200000	0.2748920000	-2.1695290000
C	-2.7904780000	0.6385210000	-4.0441990000
C	2.9190610000	1.7654290000	-0.4053910000
C	3.3842820000	1.2567560000	-3.4207430000
C	3.6335810000	-1.0848000000	-1.4144180000
H	2.3602560000	2.7040980000	-0.6038040000
H	3.9958020000	2.0189910000	-0.2861550000
H	2.5485400000	1.3451580000	0.5526000000
H	3.1756700000	-1.5752110000	-0.5285970000
H	4.7022010000	-0.8549930000	-1.2044360000
H	3.5855800000	-1.8019590000	-2.2602150000
H	2.8844930000	2.2169480000	-3.6688890000
H	3.2318410000	0.5665500000	-4.2774280000
H	4.4765150000	1.4471310000	-3.3235390000
H	-5.7669940000	1.0054730000	-2.7862820000
H	-5.5864270000	0.3180800000	-1.1304050000
H	-5.4061670000	-0.7426610000	-2.5630510000
H	-3.6145130000	3.1507640000	-2.0572390000
H	-1.9674530000	2.6484240000	-1.5184540000
H	-3.3705500000	2.4284610000	-0.4244240000
H	-1.7016430000	0.8314240000	-4.1331150000
H	-3.3439610000	1.4227280000	-4.6078720000
H	-3.0018760000	-0.3457740000	-4.5117770000

Me_3SiF

Charge = 0 Multiplicity = 1

Si	-0.0002000000	-0.0001130000	-0.0000860000
C	-1.8306730000	-0.2180430000	-0.0001470000

C	1.1043370000	-1.4757570000	0.0000570000
C	0.7265010000	1.6938980000	0.0000840000
H	1.7763700000	-1.4347240000	-0.8884030000
H	0.5543200000	-2.4369350000	0.0008830000
H	1.7777070000	-1.4337300000	0.8874080000
H	-2.1314140000	-0.8264600000	-0.8843510000
H	-2.3870780000	0.7394000000	-0.0054770000
H	-2.1314250000	-0.8157220000	0.8914840000
H	0.3534440000	2.2567190000	0.8870480000
H	0.3559000000	2.2553790000	-0.8888160000
H	1.8339950000	1.6970620000	0.0014590000

$(Me_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	1.1191830000	3.4482640000	0.2274760000
Ge	2.5418900000	-2.6219060000	-0.2670780000
P	-1.1916270000	-1.4975700000	-0.0543670000
P	1.9586240000	-0.3720160000	0.3179220000
P	-0.6150770000	1.7988540000	0.3212000000
P	0.1394670000	0.0841540000	-0.8832170000
P	-1.0719000000	-1.1250680000	2.1542860000
P	1.1251010000	-0.6127620000	2.3872490000
P	-0.4336550000	1.0338900000	2.4221110000
C	2.5586440000	3.2011400000	1.5557290000
H	3.2838380000	4.0364860000	1.4597180000
H	2.1468820000	3.2036720000	2.5845940000
C	0.1739840000	5.1519260000	0.5776270000
H	-0.2733900000	5.1513790000	1.5919220000
H	0.8917900000	5.9960840000	0.5110310000
C	1.5839410000	-4.0087920000	0.7601790000
H	1.9546180000	-5.0079760000	0.4484170000
H	1.7645400000	-3.8850080000	1.8465350000
C	1.8401660000	3.4455500000	-1.6132790000
H	2.3775000000	2.4986510000	-1.8185360000
H	1.0263230000	3.5628530000	-2.3562190000
C	2.2313230000	-2.8271060000	-2.2089900000

H	2.6189130000	-3.8138710000	-2.5382730000
H	1.1479850000	-2.7750460000	-2.4355300000
H	4.8614920000	-3.7312160000	-0.1651720000
H	5.0371680000	-1.9601950000	-0.4536960000
C	-3.3887350000	-0.0429690000	-2.4060160000
H	-2.9342440000	-0.7630310000	-3.1152050000
H	-3.5949050000	1.4366690000	0.7151350000
C	4.4803180000	-2.7281960000	0.1194630000
Ge	-3.4191880000	-0.7864680000	-0.5744140000
C	-4.1902440000	0.5025470000	0.7063470000
H	-4.2057830000	0.0758500000	1.7289360000
C	-4.4719510000	-2.4628810000	-0.5473600000
H	-4.4590770000	-2.9177170000	0.4634680000
H	-5.5255920000	-2.2449280000	-0.8210690000
H	-2.8085360000	0.9007490000	-2.4338110000
H	0.4951720000	-3.9462770000	0.5667670000
H	2.7545480000	-2.0333570000	-2.7782880000
H	4.6744930000	-2.5725060000	1.1996530000
H	-4.0615050000	-3.1958080000	-1.2702200000
H	-4.4289010000	0.1672860000	-2.7313360000
H	-5.2321750000	0.7345240000	0.4009280000
H	-0.6334360000	5.3123100000	-0.1642740000
H	2.5501920000	4.2910390000	-1.7282820000
H	3.0818260000	2.2407950000	1.3799390000

$[(Me_3Ge)_2P_7]^-$

Charge = -1 Multiplicity = 1

Ge	2.4984510000	-2.6063610000	-0.0843120000
P	-1.0796940000	-1.5223150000	-0.0051670000
P	1.9505810000	-0.4805580000	0.8184670000
P	-0.4397050000	1.8086660000	1.0604240000
P	0.2096780000	0.3105210000	-0.3753550000
P	-1.2028830000	-1.5513210000	2.2159010000
P	0.9693820000	-1.0836300000	2.7428290000
P	-0.6011420000	0.5807520000	2.8565020000
C	1.5306420000	-4.1932030000	0.6107290000

H	1.8957010000	-5.1087370000	0.0970580000
H	1.6995820000	-4.2974610000	1.7013770000
C	2.3137800000	-2.5461790000	-2.0625840000
H	2.6995970000	-3.4852410000	-2.5143330000
H	1.2461900000	-2.4239890000	-2.3331400000
H	4.7923190000	-3.8359070000	-0.1222880000
H	5.0374580000	-2.0479940000	-0.0948050000
C	-3.1750210000	0.2825570000	-2.2182140000
H	-2.6957040000	-0.3302660000	-3.0083530000
H	-3.4346360000	1.2653270000	1.0993380000
C	4.4333910000	-2.8811650000	0.3191610000
Ge	-3.2505400000	-0.7173250000	-0.5027590000
C	-4.1077220000	0.4119540000	0.8772750000
H	-4.2620060000	-0.1683340000	1.8090390000
C	-4.3935240000	-2.3250790000	-0.7973830000
H	-4.4539880000	-2.9294900000	0.1308120000
H	-5.4222030000	-2.0226910000	-1.0896830000
H	-2.5803910000	1.2076050000	-2.0816420000
H	0.4435800000	-4.0761420000	0.4309860000
H	2.8804910000	-1.6886610000	-2.4786010000
H	4.5975360000	-2.9156550000	1.4158070000
H	-3.9684370000	-2.9627980000	-1.5994170000
H	-4.2005390000	0.5548310000	-2.5479120000
H	-5.0892260000	0.7822880000	0.5102430000

Me_3GeF

Charge = 0 Multiplicity = 1

Ge	3.0398140000	-3.3191960000	-0.6484650000
C	1.6003720000	-4.5662200000	-1.1248160000
H	2.0211770000	-5.5446120000	-1.4359860000
H	0.9306850000	-4.7303300000	-0.2569640000
C	4.1835670000	-2.8498380000	-2.1733670000
H	4.7293360000	-3.7441520000	-2.5388910000
H	3.5703640000	-2.4470270000	-3.0042090000
H	4.6035560000	-4.8337420000	0.7193960000
H	4.7979860000	-3.1125830000	1.2110990000

C	4.0596010000	-3.8896440000	0.9291340000
H	1.0001770000	-4.1580280000	-1.9624400000
H	4.9248560000	-2.0812870000	-1.8762080000
H	3.3784440000	-4.0581790000	1.7870690000
F	2.2280660000	-1.8081630000	-0.1743520000

$(Et_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	1.0610860000	3.4195100000	-0.0358480000
Ge	2.6547150000	-2.6345920000	-0.4241120000
P	-1.3053010000	-1.5330400000	0.1705010000
P	1.8953280000	-0.4384280000	0.1802550000
P	-0.6353510000	1.7538110000	0.2973680000
P	-0.0199770000	-0.0377550000	-0.8753610000
P	-0.9610280000	-1.0501120000	2.3291670000
P	1.2552400000	-0.5753600000	2.3224990000
P	-0.2669720000	1.1076490000	2.4095720000
C	2.6059400000	3.3631520000	1.2343210000
H	2.7161580000	4.4081730000	1.6003220000
H	2.2843170000	2.7629910000	2.1123790000
C	0.0593800000	5.1142130000	0.3003050000
H	-0.2550980000	5.0965910000	1.3668400000
H	0.8048770000	5.9368600000	0.2155990000
C	1.2771310000	-3.9756750000	-0.9381590000
H	1.7975380000	-4.9585970000	-0.8751020000
H	0.4926160000	-3.9758940000	-0.1527820000
C	1.5989480000	3.3126540000	-1.9539540000
H	2.2116970000	2.3941540000	-2.0730010000
H	0.6721000000	3.1436330000	-2.5427920000
C	3.8570090000	-2.2739170000	-1.9760540000
H	4.1584620000	-3.2715360000	-2.3688660000
H	3.2439420000	-1.8018030000	-2.7739780000
H	4.4303910000	-4.0761080000	0.6331810000
H	4.4002680000	-2.4981470000	1.4510920000
C	-3.6343040000	-0.1966140000	-2.0892670000
H	-3.1843900000	-1.0125280000	-2.6948780000

H	-4.5212570000	-3.3036760000	-1.9001580000
C	3.9338380000	2.8371710000	0.6747840000
H	4.7265330000	2.8424670000	1.4541430000
H	3.8326160000	1.7930090000	0.3120800000
H	4.3050150000	3.4532020000	-0.1711330000
C	0.6545150000	-3.7754670000	-2.3255470000
H	-0.0807540000	-4.5759290000	-2.5579460000
H	0.1134150000	-2.8078540000	-2.3904370000
H	1.4164760000	-3.7855260000	-3.1331730000
C	-1.1418410000	5.3616290000	-0.6208900000
H	-1.6703070000	6.3054470000	-0.3643150000
H	-0.8382810000	5.4377760000	-1.6867160000
H	-1.8837400000	4.5380600000	-0.5510280000
C	5.0887270000	-1.4164130000	-1.6554720000
H	5.7063180000	-1.2312550000	-2.5609390000
H	4.7985400000	-0.4259040000	-1.2455430000
H	5.7479410000	-1.9012520000	-0.9047590000
C	2.3492840000	4.5532940000	-2.4635820000
H	2.6268420000	4.4469990000	-3.5349390000
H	1.7355280000	5.4748520000	-2.3774620000
H	3.2904090000	4.7345930000	-1.9023900000
C	-5.0456740000	0.1429620000	-2.5943310000
H	-5.0339670000	0.4228350000	-3.6703250000
H	-5.7452920000	-0.7136220000	-2.4900920000
H	-5.4897520000	0.9988980000	-2.0438130000
C	2.9649260000	-3.9466110000	2.2574970000
H	3.6470160000	-4.3368890000	3.0436180000
H	2.2984610000	-3.2033580000	2.7458110000
H	2.3284890000	-4.7939140000	1.9257560000
H	-3.7271620000	1.6255750000	0.6724540000
C	-5.6516680000	0.7619430000	1.3045400000
H	-5.9036890000	1.5981510000	1.9924810000
H	-6.2122660000	0.9386550000	0.3623410000
H	-6.0601020000	-0.1645410000	1.7601290000
C	3.7494360000	-3.3248730000	1.0945840000
Ge	-3.5533300000	-0.7650500000	-0.1783360000

C	-4.1342610000	0.6746730000	1.0763370000
H	-3.6042000000	0.5029560000	2.0376780000
C	-4.6538840000	-2.4047340000	0.1087380000
H	-4.5172750000	-2.7065180000	1.1701420000
H	-5.7178150000	-2.0937260000	0.0135930000
C	-4.3392430000	-3.5712250000	-0.8375770000
H	-4.9664690000	-4.4613230000	-0.6139330000
H	-3.2773840000	-3.8860780000	-0.7574410000
H	-2.9544490000	0.6758880000	-2.1938790000

$[(Et_3Ge)_2P_7]^-$

Charge = -1 Multiplicty = 1

Ge	2.9837360000	0.7807880000	0.1454530000
P	-1.8362630000	-1.4875220000	-0.7233740000
P	1.2083830000	-2.6713150000	-1.3406670000
P	0.6421800000	0.4217930000	0.3051790000
P	0.1438130000	-0.7888720000	-1.5482870000
P	-1.2565960000	-2.2872910000	1.2897970000
P	0.8091030000	-3.1214690000	0.7543590000
P	0.6149510000	-1.1243280000	1.8979330000
C	4.2284480000	-0.7036720000	0.6602500000
H	5.0218600000	-0.2281440000	1.2809640000
H	3.6515190000	-1.3701670000	1.3366610000
C	3.3544370000	2.2765680000	1.4364960000
H	3.1832670000	1.8613610000	2.4542820000
H	4.4440080000	2.5018970000	1.3742720000
C	3.3567890000	1.4443190000	-1.7067550000
H	3.2657100000	0.5651800000	-2.3795500000
H	2.5224680000	2.1244500000	-1.9825790000
C	-2.7522640000	1.8414040000	-1.5196070000
H	-2.9496460000	1.3508150000	-2.4973130000
H	-5.3473880000	0.1005150000	-2.3279330000
C	4.8341790000	-1.5145500000	-0.4919920000
H	5.5171000000	-2.3084140000	-0.1133820000
H	4.0314440000	-2.0150820000	-1.0761930000
H	5.4249190000	-0.8812510000	-1.1894880000

C	2.5161900000	3.5434370000	1.2240990000
H	2.7261210000	4.3242730000	1.9901000000
H	2.7061030000	4.0031050000	0.2297450000
H	1.4304580000	3.3127280000	1.2683740000
C	4.7125460000	2.1432740000	-1.8843380000
H	4.8734680000	2.4804720000	-2.9336130000
H	4.8050940000	3.0428870000	-1.2380900000
H	5.5623090000	1.4745870000	-1.6275660000
C	-3.5866300000	3.1215160000	-1.3711500000
H	-3.4016720000	3.8387580000	-2.2031390000
H	-4.6784230000	2.9108740000	-1.3633710000
H	-3.3535600000	3.6603560000	-0.4274860000
H	-1.8307260000	1.9325020000	1.5884970000
C	-3.8737490000	1.9108480000	2.4050000000
H	-3.5888200000	2.3236960000	3.3993800000
H	-4.2817970000	2.7568160000	1.8103850000
H	-4.7136510000	1.2046350000	2.5795820000
Ge	-3.0484360000	0.4597080000	-0.0984730000
C	-2.6818290000	1.2306430000	1.7155990000
H	-2.2900150000	0.3979600000	2.3380570000
C	-4.9818810000	-0.0877270000	-0.1627030000
H	-5.1287210000	-0.8406090000	0.6429270000
H	-5.5968100000	0.7955080000	0.1227390000
C	-5.4342180000	-0.6534630000	-1.5156040000
H	-6.4950750000	-0.9920900000	-1.4980360000
H	-4.8097780000	-1.5224600000	-1.8144260000
H	-1.6650470000	2.0684740000	-1.5070390000

Et_3GeF

Charge = 0 Multiplicity = 1

Ge	2.8272640000	-2.9281440000	-0.5301420000
C	1.3842440000	-4.1622890000	-1.0791380000
H	1.8607730000	-5.1354510000	-1.3447260000
H	0.7683750000	-4.3570330000	-0.1788900000
C	4.0264320000	-2.3957020000	-2.0089590000
H	4.5580410000	-3.3077830000	-2.3496780000

H	3.3879460000	-2.0845430000	-2.8461680000
H	4.3656030000	-4.4317720000	0.8229310000
H	4.5501860000	-2.7353330000	1.3182400000
C	0.5115210000	-3.6375660000	-2.2321910000
H	-0.3084180000	-4.3494780000	-2.4831620000
H	0.0406580000	-2.6641220000	-1.9702700000
H	1.1044250000	-3.4782540000	-3.1656520000
C	5.0168100000	-1.2829830000	-1.6381040000
H	5.6345220000	-0.9783640000	-2.5081680000
H	4.4843320000	-0.3741000000	-1.2694940000
H	5.7135380000	-1.6015430000	-0.8406010000
C	2.8891590000	-3.7649950000	2.3065290000
H	3.4772270000	-4.0392440000	3.2031180000
H	2.2993420000	-2.8651780000	2.5602630000
H	2.1721260000	-4.5868780000	2.1251460000
C	3.7934770000	-3.5158520000	1.0915390000
F	1.9884170000	-1.4223930000	-0.0534220000

$(^{n}Bu_3Sn)_3P_7$

Charge = 0 Multiplicity = 1

Sn	-3.3519210000	-1.2302530000	-0.0464330000
Sn	3.0396010000	-2.0688080000	-0.2331650000
P	1.5093910000	1.4970410000	-0.6508570000
P	0.4756020000	-1.7136630000	-0.5512090000
P	-1.7828910000	0.7877890000	-0.5582200000
P	0.0958340000	0.2162130000	0.4947600000
P	0.8874150000	1.1214650000	-2.7696950000
P	0.4280250000	-1.1021850000	-2.7057280000
P	-1.2676550000	0.4059900000	-2.7030400000
Sn	0.5792070000	3.8974110000	-0.2261570000
C	5.9343340000	-6.8817560000	1.0018690000
H	5.9413400000	-7.9907070000	1.0472930000
H	6.1487080000	-6.5048610000	2.0250560000
C	4.5971040000	-6.3440360000	0.4768220000
H	6.7803200000	-6.5697710000	0.3522270000
H	4.3911750000	-6.7667120000	-0.5329990000

C	4.5378570000	-4.8066490000	0.3964570000
H	3.7660860000	-6.7035310000	1.1258130000
H	5.3719360000	-4.4518520000	-0.2526310000
H	4.7525120000	-4.3876680000	1.4069800000
C	3.1931700000	-4.2694940000	-0.1229750000
H	2.9784620000	-4.6628000000	-1.1412120000
H	2.3572020000	-4.6158270000	0.5236460000
C	2.5543200000	-1.5271100000	5.4621630000
H	2.9402130000	-1.0777120000	6.4008740000
H	2.5959700000	-2.6314130000	5.5802210000
C	3.3571720000	-1.0635560000	4.2401480000
H	1.4831690000	-1.2454280000	5.3732450000
H	3.3263770000	0.0475580000	4.1698410000
C	2.8586350000	-1.6606770000	2.9109540000
H	4.4317920000	-1.3251590000	4.3754430000
H	1.7839990000	-1.3971980000	2.7783390000
H	2.8873550000	-2.7727620000	2.9833930000
C	3.6603170000	-1.1879470000	1.6885150000
H	3.5963900000	-0.0848180000	1.5700740000
H	4.7403600000	-1.4326390000	1.8056690000
C	8.0386420000	-0.7487930000	-2.7197810000
H	8.5692580000	-0.3254170000	-3.5978970000
H	8.4120260000	-1.7852780000	-2.5733310000
C	6.5171430000	-0.7231090000	-2.9120490000
H	8.3456030000	-0.1591910000	-1.8291560000
H	6.1777050000	0.3217150000	-3.0948810000
C	5.7328380000	-1.2996680000	-1.7178010000
H	6.2443190000	-1.2906010000	-3.8308390000
H	6.0065710000	-0.7287880000	-0.8005840000
H	6.0805560000	-2.3427660000	-1.5335530000
C	4.2087530000	-1.2714060000	-1.9224490000
H	3.8522860000	-0.2324880000	-2.0890070000
H	3.9176350000	-1.8544350000	-2.8234270000
C	-5.2059010000	-5.9962570000	-2.6716540000
H	-5.0056180000	-6.7963130000	-3.4144470000
H	-6.1373010000	-5.4771120000	-2.9849490000

C	-4.0290430000	-5.0185050000	-2.5616300000
H	-5.4157780000	-6.4905570000	-1.6986100000
H	-3.1032640000	-5.5730180000	-2.2860610000
C	-4.2573360000	-3.8883760000	-1.5399210000
H	-3.8204090000	-4.5662580000	-3.5577930000
H	-4.4679730000	-4.3433980000	-0.5444010000
H	-5.1859560000	-3.3386020000	-1.8187460000
C	-3.0705050000	-2.9152550000	-1.4406510000
H	-2.1426080000	-3.4366560000	-1.1222880000
H	-2.8465730000	-2.4643580000	-2.4323830000
C	-3.6479550000	-4.9138950000	4.3496930000
H	-3.4352720000	-5.1228400000	5.4188100000
H	-3.1384100000	-5.6979150000	3.7491930000
C	-3.1843930000	-3.5090330000	3.9442610000
H	-4.7413850000	-5.0405130000	4.1968640000
H	-3.6839110000	-2.7481600000	4.5865310000
C	-3.4555930000	-3.1719620000	2.4656050000
H	-2.0941810000	-3.3998030000	4.1446450000
H	-4.5467320000	-3.2846330000	2.2678440000
H	-2.9565330000	-3.9370600000	1.8275550000
C	-2.9836060000	-1.7644920000	2.0638140000
H	-3.4837110000	-0.9868960000	2.6824570000
H	-1.8921660000	-1.6506610000	2.2393950000
C	-8.9535210000	-1.1008690000	1.2412070000
H	-9.9393470000	-0.6091220000	1.1061890000
H	-8.7152850000	-1.0765260000	2.3264600000
C	-7.8600050000	-0.4153420000	0.4122880000
H	-9.0716820000	-2.1679040000	0.9539670000
H	-8.1444490000	-0.4216880000	-0.6646660000
C	-6.4701900000	-1.0622710000	0.5661420000
H	-7.7904380000	0.6595600000	0.6962560000
H	-6.5437700000	-2.1379920000	0.2838920000
H	-6.1927340000	-1.0581550000	1.6457410000
C	-5.3748690000	-0.3681070000	-0.2616570000
H	-5.6281770000	-0.3864090000	-1.3447660000
H	-5.2943100000	0.7046430000	0.0202300000

C	-4.1488300000	5.0874420000	-3.2978750000
H	-4.5871450000	5.5781350000	-4.1918250000
H	-4.6395520000	5.5263910000	-2.4024320000
C	-2.6258920000	5.2624580000	-3.2446950000
H	-4.4306570000	4.0133700000	-3.3346510000
H	-2.1680860000	4.8445760000	-4.1700010000
C	-1.9729870000	4.5956920000	-2.0197130000
H	-2.3716920000	6.3474520000	-3.2484680000
H	-2.2274810000	3.5115020000	-2.0162280000
H	-2.4382020000	5.0086100000	-1.0947290000
C	-0.4483790000	4.7740800000	-1.9702890000
H	0.0292550000	4.3470750000	-2.8790080000
H	-0.1760550000	5.8538850000	-1.9545970000
C	5.5000040000	4.7094110000	2.6119070000
H	6.4194770000	5.3147040000	2.7539860000
H	5.8174860000	3.6704510000	2.3782080000
C	4.6079210000	5.2838990000	1.5041880000
H	4.9670740000	4.6790080000	3.5866800000
H	4.3370770000	6.3367720000	1.7480010000
C	3.3184200000	4.4755140000	1.2677620000
H	5.1808220000	5.3367030000	0.5501530000
H	2.7496100000	4.4193600000	2.2251210000
H	3.5915010000	3.4224640000	1.0248220000
C	2.4235830000	5.0481490000	0.1580010000
H	2.1079650000	6.0880460000	0.4018690000
H	2.9794790000	5.1098660000	-0.8036760000
C	-2.0513640000	6.6988380000	4.0100410000
H	-2.6883850000	6.6578160000	4.9180140000
H	-2.5607310000	7.3591030000	3.2754270000
C	-1.8025130000	5.3013220000	3.4288910000
H	-1.0985770000	7.1957060000	4.2937330000
H	-1.3266710000	4.6523280000	4.1989950000
C	-0.9193760000	5.3061280000	2.1661940000
H	-2.7747820000	4.8148920000	3.1872260000
H	0.0493360000	5.8010040000	2.4097590000
H	-1.3992500000	5.9569530000	1.3984290000

C	-0.6686600000	3.9019000000	1.5913000000
H	-0.1665960000	3.2507510000	2.3394820000
H	-1.6225280000	3.3971120000	1.3273320000

$[(^{n}Bu_3Sn)_2P_7]^-$

Charge = -1 Multiplicity = 1

Sn	-2.7199890000	-0.2010410000	-0.0436550000
P	2.3602420000	1.8297170000	0.1728590000
P	-0.7132210000	3.1363400000	-0.0060590000
P	-0.1632660000	-0.3252920000	0.3030480000
P	0.4087430000	1.4987080000	-0.9038610000
P	1.7147120000	1.7989090000	2.3162250000
P	-0.3529610000	2.7558700000	2.1091290000
P	-0.1503000000	0.4708090000	2.3812890000
Sn	3.5750140000	-0.4409530000	0.2051780000
C	-7.4930340000	2.4037640000	1.9072440000
H	-7.9832350000	2.9726090000	2.7260380000
H	-8.0963450000	1.4862400000	1.7314280000
C	-6.0352570000	2.0609330000	2.2415870000
H	-7.5617620000	3.0214260000	0.9854590000
H	-5.4667410000	2.9955620000	2.4491220000
C	-5.3097750000	1.2750860000	1.1319180000
H	-5.9955330000	1.4726370000	3.1871640000
H	-5.3544900000	1.8689900000	0.1901720000
H	-5.8857980000	0.3432440000	0.9217300000
C	-3.8488570000	0.9463570000	1.4748930000
H	-3.2603160000	1.8729310000	1.6431680000
H	-3.7877780000	0.3534990000	2.4146500000
C	-6.6816750000	-4.4251120000	0.0658610000
H	-6.8994010000	-5.5105430000	0.1592700000
H	-7.0867000000	-4.0871450000	-0.9129050000
C	-5.1805660000	-4.1285520000	0.1820130000
H	-7.2602340000	-3.9001300000	0.8569260000
H	-4.7972900000	-4.5112320000	1.1558760000
C	-4.8264330000	-2.6335060000	0.0593890000
H	-4.6244280000	-4.6963400000	-0.5991000000

H	-5.3916490000	-2.0719310000	0.8395280000
H	-5.2188790000	-2.2558080000	-0.9146600000
C	-3.3248280000	-2.3325000000	0.1796240000
H	-2.9377380000	-2.6736890000	1.1657850000
H	-2.7523530000	-2.9032550000	-0.5861100000
C	-4.0544980000	3.5084600000	-4.2853130000
H	-4.1999740000	3.6756800000	-5.3741990000
H	-3.2313200000	4.1742240000	-3.9489600000
C	-3.7433310000	2.0398210000	-3.9664110000
H	-4.9791720000	3.8467950000	-3.7687110000
H	-4.5694210000	1.3910120000	-4.3422640000
C	-3.5217630000	1.7692440000	-2.4669330000
H	-2.8347940000	1.7212340000	-4.5273070000
H	-4.4217080000	2.1102460000	-1.9044350000
H	-2.6881590000	2.4058690000	-2.0923020000
C	-3.2287860000	0.2977610000	-2.1450030000
H	-4.0914460000	-0.3515920000	-2.4206870000
H	-2.3617820000	-0.0625460000	-2.7420340000
C	1.3555980000	-5.6024710000	1.5183150000
H	1.0528230000	-6.3241370000	2.3069990000
H	2.0974170000	-6.1133390000	0.8658830000
C	1.9300510000	-4.3103230000	2.1141220000
H	0.4595460000	-5.3944910000	0.8949840000
H	1.1751570000	-3.8372830000	2.7820850000
C	2.3638080000	-3.2789390000	1.0553860000
H	2.7997880000	-4.5534170000	2.7684240000
H	1.4819570000	-3.0205380000	0.4256710000
H	3.1033760000	-3.7571830000	0.3703170000
C	2.9402850000	-1.9907820000	1.6567120000
H	2.1919470000	-1.5029750000	2.3188650000
H	3.8358780000	-2.2067490000	2.2828060000
C	1.3864860000	-2.3962180000	-4.7938410000
H	1.5807910000	-2.7406380000	-5.8322490000
H	0.7211910000	-1.5083930000	-4.8528060000
C	2.6850810000	-2.0666520000	-4.0455590000
H	0.8149970000	-3.1972300000	-4.2768390000

H	3.3470200000	-2.9642610000	-4.0299650000
C	2.4592800000	-1.5764520000	-2.6027570000
H	3.2524090000	-1.2888200000	-4.6076230000
H	1.8847470000	-2.3498700000	-2.0442080000
H	1.7950050000	-0.6821410000	-2.6222530000
C	3.7583640000	-1.2456170000	-1.8544060000
H	4.4128950000	-2.1452180000	-1.7838180000
H	4.3443050000	-0.4837620000	-2.4169870000
C	8.3902590000	2.6119900000	-0.5758640000
H	9.4117790000	2.8793880000	-0.2301700000
H	7.7884850000	3.5461040000	-0.5961750000
C	7.7388610000	1.5507490000	0.3211910000
H	8.4756890000	2.2566440000	-1.6259900000
H	8.3799960000	0.6388750000	0.3493410000
C	6.3163220000	1.1546680000	-0.1176320000
H	7.7018410000	1.9206600000	1.3716800000
H	6.3564750000	0.8001120000	-1.1745140000
H	5.6763340000	2.0668730000	-0.1391810000
C	5.6588450000	0.0879670000	0.7695270000
H	6.2568440000	-0.8526800000	0.7657580000
H	5.6226350000	0.4322200000	1.8273510000

$^{n}Bu_3SnF$

Charge = 0 Multiplicity = 1

Sn	-3.1253460000	3.2317340000	-0.3232650000
F	-2.1336030000	1.5769990000	0.1278980000
C	-1.3591230000	8.4325730000	-1.9761830000
H	-0.5077120000	9.1019830000	-2.2183260000
H	-1.9381040000	8.9134560000	-1.1584340000
C	-0.8809210000	7.0315000000	-1.5760450000
H	-2.0188700000	8.3971180000	-2.8698570000
H	-0.2730860000	6.5916470000	-2.3993470000
C	-2.0253260000	6.0610770000	-1.2290120000
H	-0.1927620000	7.1035150000	-0.7031130000
H	-2.7144050000	5.9946400000	-2.1032270000
H	-2.6337010000	6.5059920000	-0.4071620000

C	-1.5395880000	4.6572750000	-0.8289390000
H	-0.9450780000	4.1955990000	-1.6476340000
H	-0.8638270000	4.7083400000	0.0528730000
C	-3.1518520000	3.8968410000	5.3268320000
H	-3.7280620000	4.0728090000	6.2589510000
H	-2.3655190000	4.6798860000	5.2680210000
C	-4.0566840000	3.9181610000	4.0883820000
H	-2.6351390000	2.9189590000	5.4326960000
H	-4.8563920000	3.1498520000	4.1942710000
C	-3.3004470000	3.6714460000	2.7703110000
H	-4.5877380000	4.8958230000	4.0269390000
H	-2.7670270000	2.6960680000	2.8317880000
H	-2.4999140000	4.4402070000	2.6647430000
C	-4.2069290000	3.6852210000	1.5273100000
H	-5.0151570000	2.9262980000	1.6180360000
H	-4.7139290000	4.6691250000	1.4111710000
C	-3.6649930000	0.6732810000	-5.3758340000
H	-4.3253250000	0.3205190000	-6.1951930000
H	-3.1322670000	-0.2134610000	-4.9704430000
C	-4.4581610000	1.3963990000	-4.2799720000
H	-2.8988470000	1.3390910000	-5.8282240000
H	-5.0090850000	2.2587950000	-4.7208570000
C	-3.5828020000	1.8984840000	-3.1173370000
H	-5.2421460000	0.7172420000	-3.8735780000
H	-2.7979690000	2.5777330000	-3.5243290000
H	-3.0296900000	1.0378580000	-2.6779230000
C	-4.3769410000	2.6179530000	-2.0134100000
H	-4.8987530000	3.5154890000	-2.4143400000
H	-5.1687840000	1.9554740000	-1.5992400000

$(Me_3Si)_3As_7$

Charge = 0 Multiplicity = 1

As	0.8856410000	0.1249830000	-0.9161920000
As	2.8222650000	1.0787410000	0.2566120000
As	2.1511300000	0.8977120000	2.6275220000
Si	2.5878190000	3.4746740000	-0.1208780000

C	2.0207870000	3.7317510000	-1.9149830000
H	2.6779590000	3.1980130000	-2.6323730000
H	2.0496090000	4.8148660000	-2.1653560000
H	0.9814760000	3.3736720000	-2.0666050000
C	4.3560470000	4.1399230000	0.0954690000
H	4.7290650000	3.9715930000	1.1274910000
H	4.3815200000	5.2345190000	-0.0991920000
H	5.0632940000	3.6500060000	-0.6056270000
C	1.4280250000	4.3700150000	1.0811840000
H	0.3866240000	4.0011660000	0.9840330000
H	1.4360330000	5.4601440000	0.8607720000
H	1.7466610000	4.2305690000	2.1350370000
As	-0.8820660000	1.2976250000	0.3259890000
As	-0.3355940000	0.7478690000	2.6725740000
Si	-2.8479990000	-0.0935390000	-0.0377640000
C	-2.8291690000	-0.6665050000	-1.8479740000
H	-2.7111860000	0.1869740000	-2.5472740000
H	-3.7871500000	-1.1766730000	-2.0901720000
H	-2.0030390000	-1.3832200000	-2.0351470000
C	-4.3010120000	1.1008980000	0.2437380000
H	-4.3186250000	1.4798440000	1.2871170000
H	-5.2662970000	0.5813550000	0.0563780000
H	-4.2449200000	1.9768540000	-0.4353200000
C	-3.0187040000	-1.5755940000	1.1307810000
H	-2.1816110000	-2.2909400000	0.9970340000
H	-3.9720370000	-2.1069830000	0.9162040000
H	-3.0357020000	-1.2578680000	2.1939480000
As	0.7797780000	-2.0198990000	0.2775350000
As	1.0374640000	-1.3307640000	2.6354470000
Si	2.9579980000	-3.0190840000	-0.1596070000
C	3.3896560000	-2.6946180000	-1.9803080000
H	2.5723860000	-3.0168520000	-2.6583210000
H	4.3064070000	-3.2599480000	-2.2569140000
H	3.5842350000	-1.6174090000	-2.1627120000
C	2.6658990000	-4.8783360000	0.1119080000
H	2.3748860000	-5.0954320000	1.1610240000

H	3.5967590000	-5.4467540000	-0.1054940000
H	1.8645190000	-5.2659040000	-0.5508990000
C	4.3603760000	-2.4338310000	0.9731920000
H	4.5574240000	-1.3500610000	0.8427740000
H	5.2906910000	-2.9914080000	0.7264440000
H	4.1248870000	-2.6164970000	2.0421610000

$[(Me_3Si)_2As_7]^-$

Charge = -1 Multiplicity = 1

As	1.0909120000	0.2883870000	-0.8209150000
As	2.8226940000	1.3428700000	0.4456950000
As	2.1343080000	0.8025890000	2.6786340000
As	-0.8195480000	1.3372180000	0.3887280000
As	-0.3805600000	0.6811590000	2.7229840000
Si	-2.7449290000	-0.0475480000	-0.0734230000
C	-2.6897290000	-0.6146970000	-1.8950070000
H	-2.5420990000	0.2460670000	-2.5806110000
H	-3.6362590000	-1.1270650000	-2.1782160000
H	-1.8488100000	-1.3213870000	-2.0538320000
C	-4.2601970000	1.1067580000	0.1300020000
H	-4.3395860000	1.4752050000	1.1749690000
H	-5.2054320000	0.5737960000	-0.1187150000
H	-4.1791590000	1.9946890000	-0.5321580000
C	-3.0429870000	-1.5660370000	1.0359330000
H	-2.2012020000	-2.2844860000	0.9527790000
H	-3.9827620000	-2.0818500000	0.7356720000
H	-3.1304000000	-1.2684530000	2.1017210000
As	0.7258790000	-1.9609240000	0.2295030000
As	0.9581110000	-1.4383030000	2.6086950000
Si	2.8793320000	-2.9851270000	-0.1252860000
C	3.3482490000	-2.7602930000	-1.9616950000
H	2.5374940000	-3.1126380000	-2.6336800000
H	4.2725250000	-3.3306580000	-2.2041730000
H	3.5320600000	-1.6881360000	-2.1832400000
C	2.6488760000	-4.8578860000	0.1977450000
H	2.3522780000	-5.0422520000	1.2521410000

H	3.5943260000	-5.4133400000	0.0057910000
H	1.8573870000	-5.2853660000	-0.4537450000
C	4.3015470000	-2.3534160000	0.9607350000
H	4.3926990000	-1.2513220000	0.8423410000
H	5.2607200000	-2.8380680000	0.6705200000
H	4.1112620000	-2.5624860000	2.0341080000

$(Et_3Ge)_3As_7$

Charge = 0 Multiplicity = 1

Ge	1.2480300000	3.6434100000	-0.3743620000
Ge	2.5533360000	-2.8898980000	-0.8131710000
As	-1.4667020000	-1.5792230000	-0.1166860000
As	2.0961610000	-0.5113100000	-0.1504000000
As	-0.6032600000	2.0123800000	0.0758800000
As	-0.0189890000	0.0414940000	-1.2698010000
As	-1.0449640000	-1.0756050000	2.2636730000
As	1.4148810000	-0.7031550000	2.2160690000
As	-0.1363510000	1.2416800000	2.3771370000
C	2.3707380000	4.0766360000	1.2196530000
H	2.8549400000	5.0476170000	0.9677850000
H	1.6750130000	4.2923440000	2.0593980000
C	0.2488880000	5.3111600000	-0.8409080000
H	-0.3428720000	5.5957080000	0.0565360000
H	1.0127340000	6.1105660000	-0.9705170000
C	1.3079080000	-3.6214900000	-2.1897850000
H	1.6009740000	-4.6911560000	-2.2953620000
H	0.2853730000	-3.6181760000	-1.7551990000
C	2.3740460000	3.0779470000	-1.9223520000
H	2.8804300000	2.1323410000	-1.6338260000
H	1.6891160000	2.8187950000	-2.7581420000
C	4.3865110000	-2.7746400000	-1.6028700000
H	4.6021100000	-3.7801350000	-2.0308420000
H	4.3392280000	-2.0745110000	-2.4649020000
H	3.2594990000	-4.9897960000	0.3845930000
H	3.2256200000	-3.6454660000	1.5471000000
C	-3.8097500000	0.1072300000	-2.2964280000

H	-3.4420500000	-0.7069610000	-2.9576860000
H	-4.8759970000	-2.9826560000	-2.2484600000
C	3.4216090000	3.0383550000	1.6293180000
H	4.0210250000	3.3896530000	2.4972290000
H	2.9553610000	2.0743770000	1.9224680000
H	4.1333490000	2.8182380000	0.8060330000
C	1.3279000000	-2.9150230000	-3.5513250000
H	0.6393030000	-3.4054300000	-4.2732990000
H	1.0067950000	-1.8544280000	-3.4670800000
H	2.3388420000	-2.9182640000	-4.0109480000
C	-0.6525450000	5.2092340000	-2.0780590000
H	-1.1927420000	6.1606640000	-2.2753870000
H	-0.0736330000	4.9672340000	-2.9946450000
H	-1.4212530000	4.4156510000	-1.9576600000
C	5.4874830000	-2.3508540000	-0.6210630000
H	6.4812040000	-2.2916550000	-1.1160380000
H	5.2807520000	-1.3505120000	-0.1833070000
H	5.5869790000	-3.0640630000	0.2245840000
C	3.3923460000	4.1448210000	-2.3532460000
H	4.0142670000	3.7922430000	-3.2049140000
H	2.9008760000	5.0859700000	-2.6796080000
H	4.0907260000	4.4083950000	-1.5306700000
C	-5.1908510000	0.5998060000	-2.7563210000
H	-5.1677520000	0.9409590000	-3.8144400000
H	-5.9630600000	-0.1958180000	-2.6897610000
H	-5.5494170000	1.4572890000	-2.1491120000
C	1.2905040000	-4.6399920000	1.2795530000
H	1.4291020000	-5.3610340000	2.1142380000
H	0.6653410000	-3.8080920000	1.6671060000
H	0.6981670000	-5.1550870000	0.4947090000
H	-3.7210980000	1.7619120000	0.5808440000
C	-5.7153690000	1.0336040000	1.1574780000
H	-5.8923680000	1.8315410000	1.9114320000
H	-6.2527620000	1.3378980000	0.2345740000
H	-6.2114500000	0.1158200000	1.5377440000
C	2.6371850000	-4.1383640000	0.7438220000

Ge	-3.7443470000	-0.5810290000	-0.4219010000
C	-4.2113730000	0.8241970000	0.9198990000
H	-3.7037290000	0.5454290000	1.8684070000
C	-4.9887230000	-2.1324340000	-0.2166100000
H	-4.9096740000	-2.4766580000	0.8378370000
H	-6.0192730000	-1.7278190000	-0.3300820000
C	-4.7518050000	-3.2952360000	-1.1898670000
H	-5.4633010000	-4.1308070000	-1.0122710000
H	-3.7259740000	-3.7099630000	-1.0911850000
H	-3.0571350000	0.9220780000	-2.3644510000

$[(Et_3Ge)_2As_7]^-$

Charge = -1 Multiplicity = 1

Ge	3.2945590000	0.8259530000	-0.0587020000
Ge	-3.0748070000	1.5857440000	0.0146900000
As	-1.3923710000	-2.1270250000	1.7028180000
As	-0.6579970000	1.1221840000	-0.3377640000
As	1.9841920000	-1.1133870000	0.7801630000
As	-0.0815680000	-0.1323360000	1.7582740000
As	-1.1139530000	-2.7895260000	-0.5870750000
As	-0.8503850000	-0.6824020000	-1.9717810000
As	1.1620870000	-2.0433540000	-1.3537060000
C	2.9955660000	1.2984280000	-1.9820680000
H	3.1367470000	0.3565430000	-2.5555820000
H	1.9184170000	1.5536520000	-2.0777150000
C	5.2254310000	0.2862950000	0.1309400000
H	5.3933220000	-0.5485800000	-0.5849040000
H	5.8557370000	1.1322480000	-0.2264410000
C	-3.4267000000	2.0563460000	1.9301720000
H	-4.4922760000	2.3780380000	1.9858730000
H	-3.3494970000	1.1114730000	2.5090920000
C	2.9727300000	2.4117730000	1.1327130000
H	1.9960600000	2.8379800000	0.8172100000
H	2.8085620000	2.0132030000	2.1570270000
C	-3.4465500000	3.2411520000	-1.0667460000
H	-4.4995300000	3.5378920000	-0.8526930000

H	-2.8032420000	4.0549570000	-0.6659940000
H	-5.1910970000	0.7654250000	-1.1394780000
H	-3.8867970000	-0.4366880000	-1.3343870000
C	3.8769750000	2.4205390000	-2.5498430000
H	3.6828110000	2.5860320000	-3.6340100000
H	3.6926330000	3.3910440000	-2.0413670000
H	4.9619280000	2.2003460000	-2.4469360000
C	-2.5010550000	3.1273040000	2.5215290000
H	-2.7614350000	3.3639530000	3.5779550000
H	-1.4431490000	2.7886140000	2.5152270000
H	-2.5456790000	4.0813690000	1.9529240000
C	5.6315550000	-0.1330200000	1.5503380000
H	6.6948500000	-0.4593890000	1.6081830000
H	5.5058820000	0.6983490000	2.2776800000
H	5.0037390000	-0.9746800000	1.9141050000
C	-3.2222180000	3.0783000000	-2.5761750000
H	-3.4278410000	4.0166120000	-3.1399930000
H	-2.1738640000	2.7818080000	-2.7963860000
H	-3.8745240000	2.2883790000	-3.0073940000
C	4.0692710000	3.4875000000	1.1430580000
H	3.8244010000	4.3198170000	1.8417180000
H	5.0520860000	3.0781490000	1.4622620000
H	4.2212900000	3.9428810000	0.1413610000
C	-5.0149710000	-0.6595760000	0.5219780000
H	-5.7370970000	-1.3994400000	0.1083750000
H	-4.2264900000	-1.2293550000	1.0620960000
H	-5.5651210000	-0.0493380000	1.2708600000
C	-4.4022140000	0.2045100000	-0.5877180000

$(^{n}Bu_3Sn)_3As_7$

Charge = 0 Multiplicity = 1

Sn	-3.5810840000	-1.1999540000	0.1954450000
Sn	3.0871480000	-2.3124930000	0.0283210000
As	1.7104710000	1.5129700000	-0.3933880000
As	0.4319050000	-1.9687380000	-0.3195160000
As	-1.9441110000	0.8826920000	-0.3140250000

As	0.0897200000	0.1590720000	0.8597160000
As	1.0013260000	1.1651780000	-2.7308110000
As	0.4306640000	-1.2628960000	-2.6847500000
As	-1.3854160000	0.4437710000	-2.6738440000
Sn	0.7528490000	3.9927050000	0.0819900000
C	6.0172000000	-7.0862040000	1.3630100000
H	6.0317380000	-8.1941270000	1.4280010000
H	6.2154200000	-6.6898610000	2.3821350000
C	4.6831500000	-6.5675940000	0.8112960000
H	6.8694180000	-6.7791840000	0.7191660000
H	4.4942820000	-7.0080500000	-0.1942780000
C	4.6131500000	-5.0320510000	0.7055780000
H	3.8461760000	-6.9233970000	1.4546720000
H	5.4544460000	-4.6808910000	0.0640280000
H	4.8090560000	-4.5959410000	1.7125820000
C	3.2728200000	-4.5137410000	0.1566830000
H	3.0820900000	-4.9181370000	-0.8620940000
H	2.4295090000	-4.8673200000	0.7900160000
C	2.6579680000	-1.7640720000	5.7337690000
H	3.0472340000	-1.3063620000	6.6670530000
H	2.7163680000	-2.8673080000	5.8546510000
C	3.4413820000	-1.2930630000	4.5019820000
H	1.5819980000	-1.4978280000	5.6555040000
H	3.3941080000	-0.1826740000	4.4286050000
C	2.9380500000	-1.9015110000	3.1796910000
H	4.5209390000	-1.5389240000	4.6267570000
H	1.8577510000	-1.6543480000	3.0593760000
H	2.9818570000	-3.0128300000	3.2558190000
C	3.7195410000	-1.4230170000	1.9466710000
H	3.6438690000	-0.3199580000	1.8302510000
H	4.8034760000	-1.6552270000	2.0526740000
C	8.1360530000	-1.1190740000	-2.4318980000
H	8.6826900000	-0.6999130000	-3.3021900000
H	8.4732370000	-2.1700370000	-2.3018430000
C	6.6166380000	-1.0378570000	-2.6255130000
H	8.4613020000	-0.5550310000	-1.5312780000

H	6.3138850000	0.0210620000	-2.7912850000
C	5.8108770000	-1.6068840000	-1.4418840000
H	6.3260770000	-1.5801990000	-3.5540460000
H	6.1049480000	-1.0628490000	-0.5146750000
H	6.1200960000	-2.6648710000	-1.2759150000
C	4.2888340000	-1.5203170000	-1.6442380000
H	3.9710820000	-0.4653330000	-1.7901270000
H	3.9772660000	-2.0718390000	-2.5584110000
C	-5.5690230000	-5.9782300000	-2.3021450000
H	-5.3941740000	-6.8059470000	-3.0206890000
H	-6.4861000000	-5.4422120000	-2.6289380000
C	-4.3642630000	-5.0319000000	-2.2246500000
H	-5.7899370000	-6.4364740000	-1.3140300000
H	-3.4537580000	-5.6046020000	-1.9354680000
C	-4.5564630000	-3.8656320000	-1.2364620000
H	-4.1465840000	-4.6159900000	-3.2347320000
H	-4.7738680000	-4.2846330000	-0.2268470000
H	-5.4718050000	-3.3001330000	-1.5271960000
C	-3.3458610000	-2.9192060000	-1.1709870000
H	-2.4295220000	-3.4578880000	-0.8464270000
H	-3.1197060000	-2.5021460000	-2.1768420000
C	-4.1029090000	-4.8509670000	4.6141680000
H	-3.9070280000	-5.0620340000	5.6861050000
H	-3.6339370000	-5.6667170000	4.0229540000
C	-3.5616140000	-3.4768930000	4.1996050000
H	-5.2008760000	-4.9195620000	4.4568050000
H	-4.0218590000	-2.6846470000	4.8332630000
C	-3.8062340000	-3.1364280000	2.7170800000
H	-2.4680060000	-3.4255090000	4.4050700000
H	-4.9010130000	-3.1849390000	2.5145140000
H	-3.3510860000	-3.9351980000	2.0874410000
C	-3.2489310000	-1.7626350000	2.3078310000
H	-3.6969230000	-0.9542460000	2.9272170000
H	-2.1523600000	-1.7186970000	2.4849750000
C	-9.1864460000	-0.9893620000	1.4949650000
H	-10.1683350000	-0.4931340000	1.3479730000

H	-8.9474560000	-0.9398840000	2.5791900000
C	-8.0876750000	-0.3338570000	0.6488370000
H	-9.3134550000	-2.0622720000	1.2345810000
H	-8.3724220000	-0.3657930000	-0.4276170000
C	-6.7027810000	-0.9873640000	0.8193620000
H	-8.0099520000	0.7474810000	0.9050060000
H	-6.7847330000	-2.0694320000	0.5655950000
H	-6.4247120000	-0.9568810000	1.8983100000
C	-5.6023060000	-0.3240740000	-0.0264130000
H	-5.8601470000	-0.3630560000	-1.1081400000
H	-5.5122970000	0.7542020000	0.2309440000
C	-3.9612690000	5.4236380000	-2.9169870000
H	-4.3912920000	5.9586710000	-3.7892540000
H	-4.4339230000	5.8428760000	-2.0026110000
C	-2.4336550000	5.5546020000	-2.8683580000
H	-4.2734480000	4.3598690000	-2.9906360000
H	-1.9931010000	5.1591920000	-3.8118080000
C	-1.7912890000	4.8263000000	-1.6729710000
H	-2.1496670000	6.6315960000	-2.8342660000
H	-2.0806510000	3.7509250000	-1.7051560000
H	-2.2371430000	5.2205170000	-0.7304830000
C	-0.2617900000	4.9553040000	-1.6292880000
H	0.1953900000	4.5450440000	-2.5560360000
H	0.0428040000	6.0254240000	-1.5807790000
C	5.6316680000	4.8056750000	3.0066610000
H	6.5442660000	5.4162550000	3.1690810000
H	5.9606120000	3.7711590000	2.7689720000
C	4.7532320000	5.3836450000	1.8898290000
H	5.0832820000	4.7625990000	3.9723540000
H	4.4706740000	6.4322620000	2.1386540000
C	3.4733510000	4.5686640000	1.6254590000
H	5.3409250000	5.4494060000	0.9456360000
H	2.8911050000	4.4982200000	2.5738130000
H	3.7587850000	3.5197190000	1.3771560000
C	2.5907460000	5.1459690000	0.5082590000
H	2.2662110000	6.1818850000	0.7573940000

H	3.1612730000	5.2207980000	-0.4439500000
C	-1.8865350000	6.7876350000	4.3213960000
H	-2.5301320000	6.7467230000	5.2247450000
H	-2.3850470000	7.4567700000	3.5873470000
C	-1.6458710000	5.3915870000	3.7331970000
H	-0.9314340000	7.2744710000	4.6145390000
H	-1.1810150000	4.7337430000	4.5025330000
C	-0.7542620000	5.3965040000	2.4764250000
H	-2.6208140000	4.9153060000	3.4821490000
H	0.2175100000	5.8804780000	2.7293860000
H	-1.2225730000	6.0570090000	1.7098980000
C	-0.5115870000	3.9948210000	1.8921430000
H	-0.0203020000	3.3344060000	2.6397610000
H	-1.4700270000	3.5014160000	1.6213760000

$[(^{n}Bu_3Sn)_2As_7]^-$

Charge = -1 Multiplicity = 1

Sn	-3.3419360000	0.0208260000	-0.2613180000
Sn	3.0388590000	0.9881060000	0.3582600000
As	1.8957520000	-2.3175720000	-1.7145140000
As	0.4011440000	0.5331240000	0.4226180000
As	-1.7517220000	-1.8559620000	-1.3103010000
As	0.2990670000	-0.5395390000	-1.8309380000
As	1.3405870000	-3.2847020000	0.4084640000
As	0.5275890000	-1.4103830000	1.9059560000
As	-1.1209160000	-2.9505600000	0.8056010000
C	6.3506070000	5.1218330000	2.6400650000
H	6.4497740000	5.9820620000	3.3361820000
H	6.6339790000	5.4795740000	1.6262010000
C	4.9323930000	4.5358250000	2.6490390000
H	7.1045680000	4.3618500000	2.9401460000
H	4.6626290000	4.2214750000	3.6835300000
C	4.7450470000	3.3369920000	1.6982820000
H	4.1974690000	5.3288720000	2.3790630000
H	5.4844580000	2.5481980000	1.9739590000
H	5.0285950000	3.6554920000	0.6676120000
C	3.3255830000	2.7505010000	1.6946780000

H	3.0344110000	2.4295340000	2.7202640000
H	2.5833590000	3.5233620000	1.3940800000
C	2.5083730000	4.2806020000	-4.3302680000
H	2.9032800000	4.5828050000	-5.3238650000
H	2.4553270000	5.1951770000	-3.6999680000
C	3.3753680000	3.1981620000	-3.6733200000
H	1.4660250000	3.9252610000	-4.4788590000
H	3.4365050000	2.3102990000	-4.3430860000
C	2.8617640000	2.7438980000	-2.2937850000
H	4.4224030000	3.5674950000	-3.5699360000
H	1.8186060000	2.3683940000	-2.4063830000
H	2.7887850000	3.6356580000	-1.6271670000
C	3.7263580000	1.6575960000	-1.6390500000
H	3.7632710000	0.7473960000	-2.2753140000
H	4.7767710000	2.0106670000	-1.5167260000
C	7.3527320000	-2.7504120000	-0.3140950000
H	8.0006780000	-3.5387960000	0.1256050000
H	8.0183040000	-1.9441240000	-0.6934720000
C	6.3393970000	-2.2067910000	0.7021670000
H	6.8388580000	-3.1916800000	-1.1949170000
H	5.7118840000	-3.0419650000	1.0878270000
C	5.4136000000	-1.1182160000	0.1264980000
H	6.8791360000	-1.8014150000	1.5899990000
H	4.8560460000	-1.5416040000	-0.7411030000
H	6.0431280000	-0.2937930000	-0.2846320000
C	4.4050490000	-0.5687670000	1.1442950000
H	3.7570540000	-1.3861110000	1.5283490000
H	4.9242300000	-0.1234150000	2.0237310000
C	-5.6240980000	1.2311310000	4.9056890000
H	-5.4648330000	1.3551190000	5.9981060000
H	-6.3848330000	0.4318050000	4.7688040000
C	-4.3197410000	0.8932980000	4.1714970000
H	-6.0706960000	2.1756180000	4.5249140000
H	-3.5661220000	1.6921390000	4.3578970000
C	-4.4906540000	0.7120960000	2.6503340000
H	-3.8778290000	-0.0361050000	4.5972570000

H	-4.9375040000	1.6442590000	2.2315190000
H	-5.2498060000	-0.0850310000	2.4720580000
C	-3.1815350000	0.3733380000	1.9224870000
H	-2.4265260000	1.1775220000	2.0583010000
H	-2.7203070000	-0.5464050000	2.3447000000
C	-3.6093850000	5.7695280000	-0.4982010000
H	-3.4558900000	6.7008370000	-1.0840690000
H	-2.9804540000	5.8431310000	0.4152980000
C	-3.2624420000	4.5163410000	-1.3130280000
H	-4.6702320000	5.7560530000	-0.1650120000
H	-3.8788710000	4.4899500000	-2.2412760000
C	-3.4599140000	3.1979280000	-0.5400960000
H	-2.2053600000	4.5746750000	-1.6586580000
H	-4.5184510000	3.1442240000	-0.1921310000
H	-2.8434910000	3.2352820000	0.3874630000
C	-3.1009880000	1.9433060000	-1.3502530000
H	-3.7213780000	1.8776770000	-2.2723530000
H	-2.0423590000	1.9852580000	-1.6850820000
C	-8.9447550000	1.0855840000	-1.2163430000
H	-9.9560610000	0.6887810000	-1.4487570000
H	-8.6741630000	1.8015970000	-2.0225770000
C	-7.9028270000	-0.0342780000	-1.0928930000
H	-9.0245470000	1.6702000000	-0.2740280000
H	-8.2192940000	-0.7563780000	-0.3054460000
C	-6.4819510000	0.4686240000	-0.7697870000
H	-7.8705400000	-0.6221750000	-2.0389840000
H	-6.5195550000	1.0510150000	0.1801430000
H	-6.1807050000	1.2037800000	-1.5520610000
C	-5.4314940000	-0.6479770000	-0.6659150000
H	-5.7094550000	-1.3728690000	0.1320130000
H	-5.3948820000	-1.2335340000	-1.6114560000

6.4. Optimised Structures BP86/SV(p) Level of Theory for HIA calculations

$B(C_6F_5)_3$

Charge = 0 Multiplicity = 1

B	-0.1531740000	0.4666880000	-0.1571150000
C	-0.5934870000	1.3637820000	-1.3742430000
C	-0.1079390000	-1.0994570000	-0.3181920000
C	0.2408290000	1.1287850000	1.2159520000
C	-0.0324160000	-3.9375360000	-0.6161290000
C	0.4129910000	-3.1094450000	-1.6626570000
C	0.3574730000	-1.7171430000	-1.5010100000
C	-0.5343990000	-1.9731600000	0.7083660000
C	-0.5146630000	-3.3696020000	0.5772810000
F	0.0030740000	-5.2606340000	-0.7550970000
F	0.8792690000	-3.6538160000	-2.7891410000
F	0.8046300000	-0.9684080000	-2.5225490000
F	-1.0156790000	-1.4785000000	1.8607370000
F	-0.9456400000	-4.1599010000	1.5634640000
C	0.9497970000	2.3233350000	3.7105370000
C	1.6610960000	1.2047720000	3.2409850000
C	1.2913990000	0.6259710000	2.0185200000
C	-0.4359970000	2.2606300000	1.7269600000
C	-0.1096870000	2.8544980000	2.9539960000
F	1.2797400000	2.8801740000	4.8725090000
F	2.6729720000	0.7111010000	3.9581240000
F	2.0114880000	-0.4299320000	1.6073640000
F	-1.4644400000	2.7964460000	1.0514890000
F	-0.7878770000	3.9098860000	3.4095480000
C	-1.3748140000	2.9632760000	-3.5726670000
C	-2.0217000000	1.7569770000	-3.3284360000
C	-1.6181230000	0.9796550000	-2.2517330000
C	0.0186790000	2.5937840000	-1.6592780000
C	-0.3452560000	3.3860540000	-2.7391020000
F	-1.7381680000	3.7070780000	-4.5945040000
F	-3.0063680000	1.3667580000	-4.1186080000
F	-2.2788050000	-0.1603680000	-2.0528190000
F	1.0207800000	3.0365140000	-0.9000130000
F	0.2713940000	4.5287500000	-2.9835370000

$[HB(C_6F_5)_3]^-$

Charge = -1 Multiplicity = 1

B	-0.8351440000	0.4097510000	0.1454970000
C	-0.9128380000	1.2985030000	-1.2384890000
C	-0.3821490000	-1.1441140000	-0.1514660000
C	0.0158010000	1.1509140000	1.3427450000
C	0.2564940000	-3.8744060000	-0.6694120000
C	0.8865760000	-2.8594650000	-1.3782350000
C	0.5605020000	-1.5319060000	-1.1030320000
C	-0.9783850000	-2.2019970000	0.5364870000
C	-0.6826410000	-3.5452400000	0.2992220000
F	0.5559290000	-5.1569520000	-0.9138370000
F	1.8029000000	-3.1718720000	-2.3057280000
F	1.2329190000	-0.6071590000	-1.8082340000
F	-1.8902590000	-1.9656980000	1.4924740000
F	-1.2907490000	-4.5217170000	0.9890550000
C	1.3043530000	2.5140540000	3.5251700000
C	1.8979470000	1.3863420000	2.9412050000
C	1.2528190000	0.7411730000	1.8689720000
C	-0.5339020000	2.2895500000	1.9631380000
C	0.0725980000	2.9714370000	3.0319030000
F	1.9071620000	3.1500350000	4.5487290000
F	3.0841410000	0.9431720000	3.4049690000
F	1.9098250000	-0.3225140000	1.3530720000
F	-1.7163800000	2.7871310000	1.5380550000
F	-0.5071170000	4.0553660000	3.5873090000
C	-1.2174130000	2.8299100000	-3.6512060000
C	-2.1860690000	1.8830380000	-3.2867370000
C	-2.0130780000	1.1448070000	-2.1025630000
C	0.0324660000	2.2508250000	-1.6554170000
C	-0.0982080000	3.0182200000	-2.8273750000
F	-1.3602880000	3.5495260000	-4.7811440000
F	-3.2647020000	1.6958530000	-4.0746250000
F	-2.9830680000	0.2495170000	-1.8173070000
F	1.1505860000	2.4744200000	-0.9301120000
F	0.8408660000	3.9206490000	-3.1769340000
H	-1.9904910000	0.3508480000	0.5658520000

SbF_5

Charge = 0 Multiplicity = 1

F	-1.9354430000	0.7880830000	0.0118850000
F	0.1865520000	1.0762600000	-1.6358360000
F	-1.0232240000	-1.7224270000	-0.3860040000
F	0.2213570000	0.5881340000	1.6245680000
F	1.5235260000	-0.8318660000	-0.2673920000
Sb	-0.2057670000	-0.0211940000	-0.1292210000

$[HSbF_5]^-$

Charge = -1 Multiplicity = 1

F	-1.9858220000	0.8997830000	0.3130360000
F	0.3346960000	1.6056330000	-1.0594700000
F	-1.0310680000	-1.7040220000	0.5537970000
F	0.4494240000	0.4496570000	1.4417800000
F	1.3118730000	-0.9606060000	-0.7175670000
Sb	-0.3612480000	-0.0442780000	-0.2546640000
H	-1.0848550000	-0.4851660000	-1.7689130000

H^-

Charge = -1 Multiplicity = 1

H	5.2740000000	0.7150000000	-1.0680000000

Me_3Si^+

Charge = +1 Multiplicity = 1

Si	4.5593300000	-1.1629140000	0.4317530000
C	4.1895900000	-1.5136870000	2.2040410000
C	5.4289170000	0.3947850000	-0.0352990000
C	4.1975700000	-2.4349380000	-0.8534960000
H	4.0356760000	-0.5869410000	2.7940150000
H	4.0413610000	-1.9874920000	-1.8565400000
H	6.5277720000	0.1993070000	0.0282680000
H	5.0926610000	-3.1002390000	-0.9299300000
H	3.3378420000	-3.0799270000	-0.5787650000
H	3.3260030000	-2.1991290000	2.3269270000

H	5.0802930000	-2.0317310000	2.6375710000
H	5.2079900000	1.2267050000	0.6645500000
H	5.2149960000	0.7002010000	-1.0800960000

Me_3SiH

Charge = 0 Multiplicity = 1

Si	4.0525710000	-0.9204570000	0.3574060000
C	4.1847450000	-1.4995980000	2.1604720000
C	5.3954250000	0.3656530000	-0.0264160000
C	4.1916850000	-2.3984650000	-0.8254150000
H	4.0814320000	-0.6470970000	2.8645360000
H	4.0925040000	-2.0769450000	-1.8836420000
H	6.4114740000	-0.0636060000	0.1062170000
H	2.7007650000	-0.2742770000	0.1601330000
H	5.1729510000	-2.9077000000	-0.7165120000
H	3.3972710000	-3.1483440000	-0.6259510000
H	3.3897840000	-2.2354850000	2.4046640000
H	5.1656490000	-1.9832810000	2.3558240000
H	5.3102770000	1.2472950000	0.6433060000
H	5.3154660000	0.7293060000	-1.0726210000

$(Me_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	1.0893750000	3.4626110000	0.1735510000
Ge	2.5645720000	-2.6021410000	-0.2240980000
P	-1.1788730000	-1.5067070000	-0.0311690000
P	1.9612790000	-0.3485790000	0.3249150000
P	-0.6308050000	1.8001370000	0.2923960000
P	0.1391490000	0.0729760000	-0.8842700000
P	-1.0639170000	-1.0982330000	2.1713650000
P	1.1284910000	-0.5634810000	2.3974060000
P	-0.4443830000	1.0700670000	2.4052340000
C	2.5301900000	3.2486280000	1.5061170000
H	3.2484850000	4.0883430000	1.3971310000
H	2.1179610000	3.2640360000	2.5346470000
C	0.1293590000	5.1633570000	0.4965380000

H	-0.3185400000	5.1748510000	1.5105380000
H	0.8399040000	6.0125350000	0.4170190000
C	1.6169760000	-3.9811810000	0.8231290000
H	1.9963920000	-4.9818430000	0.5269930000
H	1.7952450000	-3.8393630000	1.9076390000
C	1.8112360000	3.4369940000	-1.6667130000
H	2.3566460000	2.4915320000	-1.8568030000
H	0.9967480000	3.5356030000	-2.4116510000
C	2.2588380000	-2.8399570000	-2.1630770000
H	2.6557340000	-3.8281380000	-2.4766510000
H	1.1754130000	-2.8011040000	-2.3919220000
H	4.8934610000	-3.6896990000	-0.1013760000
H	5.0543880000	-1.9219820000	-0.4175750000
C	-3.3867070000	-0.1076320000	-2.4065110000
H	-2.9256240000	-0.8345860000	-3.1043230000
H	-3.6080220000	1.4181070000	0.6912350000
C	4.5032490000	-2.6856200000	0.1668200000
Ge	-3.4120990000	-0.8231030000	-0.5637490000
C	-4.1952330000	0.4788100000	0.6965010000
H	-4.2078360000	0.0678010000	1.7255210000
C	-4.4504220000	-2.5079200000	-0.5114730000
H	-4.4344810000	-2.9469250000	0.5062930000
H	-5.5056620000	-2.3032740000	-0.7892770000
H	-2.8146420000	0.8405120000	-2.4484440000
H	0.5279380000	-3.9307950000	0.6276530000
H	2.7757810000	-2.0503830000	-2.7437850000
H	4.6943900000	-2.5112440000	1.2446940000
H	-4.0331090000	-3.2483880000	-1.2226080000
H	-4.4284250000	0.0887110000	-2.7355540000
H	-5.2389330000	0.6969600000	0.3869550000
H	-0.6790160000	5.3051050000	-0.2481180000
H	2.5141440000	4.2865350000	-1.7948990000
H	3.0613850000	2.2900650000	1.3457580000

$[(Me_3Ge)_2P_7]^-$

Charge = -1 Multiplicity = 1

Ge	1.0792570000	3.3467980000	0.2572700000
Ge	2.5273620000	-2.5204650000	-0.2616390000
P	-1.4134760000	-1.4664330000	0.0248210000
P	1.9329610000	-0.2937530000	0.2829310000
P	-0.6691180000	1.7469030000	0.3902330000
P	-0.0256980000	-0.0314170000	-0.8368140000
P	-0.9944830000	-1.1853820000	2.1473270000
P	1.2265340000	-0.6056240000	2.3692780000
P	-0.3937210000	0.9995120000	2.4867340000
C	2.5689610000	3.2116540000	1.5612350000
H	3.3030940000	4.0254050000	1.3763380000
H	2.1814400000	3.3010250000	2.5960150000
C	0.2109160000	5.1201500000	0.5463510000
H	-0.2318420000	5.1720230000	1.5622400000
H	0.9540600000	5.9399850000	0.4421850000
C	1.5550370000	-3.9505810000	0.6995350000
H	1.8692950000	-4.9464580000	0.3191520000
H	1.7617940000	-3.8935750000	1.7870650000
C	1.8254150000	3.3522930000	-1.5851460000
H	2.3447020000	2.3928610000	-1.7793380000
H	1.0135770000	3.4680280000	-2.3315400000
C	2.3030950000	-2.7724170000	-2.2198100000
H	2.7054630000	-3.7614800000	-2.5270050000
H	1.2268040000	-2.7223330000	-2.4787290000
H	4.8366930000	-3.7105750000	-0.1385870000
H	5.0574590000	-1.9402450000	-0.4111360000
C	4.4715710000	-2.7001360000	0.1455940000
H	0.4673110000	-3.8043430000	0.5380840000
H	2.8370110000	-1.9786990000	-2.7806740000
H	4.6528870000	-2.5517410000	1.2298570000
H	-0.6006100000	5.2789910000	-0.1930060000
H	2.5468760000	4.1887450000	-1.7060010000
H	3.0703740000	2.2292790000	1.4551800000

Me_3GeH

Charge = 0 Multiplicity = 1

Ge	1.1327170000	3.4765370000	0.2269070000
C	2.5846630000	3.2241110000	1.5451730000
H	3.3243040000	4.0472480000	1.4684310000
H	2.1787240000	3.2147820000	2.5771480000
C	0.1852740000	5.1770110000	0.5739070000
H	-0.2526280000	5.1802370000	1.5928300000
H	0.8831130000	6.0356490000	0.4914510000
C	1.8699510000	3.4716830000	-1.6078330000
H	2.3924460000	2.5162300000	-1.8174800000
H	1.0596400000	3.5960220000	-2.3547650000
H	-0.6355590000	5.3229080000	-0.1573500000
H	2.5947350000	4.3015310000	-1.7374300000
H	3.1111630000	2.2639320000	1.3698210000
H	0.1174580000	2.2981170000	0.3631900000

$(Et_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	1.0610860000	3.4195100000	-0.0358480000
Ge	2.6547150000	-2.6345920000	-0.4241120000
P	-1.3053010000	-1.5330400000	0.1705010000
P	1.8953280000	-0.4384280000	0.1802550000
P	-0.6353510000	1.7538110000	0.2973680000
P	-0.0199770000	-0.0377550000	-0.8753610000
P	-0.9610280000	-1.0501120000	2.3291670000
P	1.2552400000	-0.5753600000	2.3224990000
P	-0.2669720000	1.1076490000	2.4095720000
C	2.6059400000	3.3631520000	1.2343210000
H	2.7161580000	4.4081730000	1.6003220000
H	2.2843170000	2.7629910000	2.1123790000
C	0.0593800000	5.1142130000	0.3003050000
H	-0.2550980000	5.0965910000	1.3668400000
H	0.8048770000	5.9368600000	0.2155990000
C	1.2771310000	-3.9756750000	-0.9381590000
H	1.7975380000	-4.9585970000	-0.8751020000
H	0.4926160000	-3.9758940000	-0.1527820000
C	1.5989480000	3.3126540000	-1.9539540000

H	2.2116970000	2.3941540000	-2.0730010000
H	0.6721000000	3.1436330000	-2.5427920000
C	3.8570090000	-2.2739170000	-1.9760540000
H	4.1584620000	-3.2715360000	-2.3688660000
H	3.2439420000	-1.8018030000	-2.7739780000
H	4.4303910000	-4.0761080000	0.6331810000
H	4.4002680000	-2.4981470000	1.4510920000
C	-3.6343040000	-0.1966140000	-2.0892670000
H	-3.1843900000	-1.0125280000	-2.6948780000
H	-4.5212570000	-3.3036760000	-1.9001580000
C	3.9338380000	2.8371710000	0.6747840000
H	4.7265330000	2.8424670000	1.4541430000
H	3.8326160000	1.7930090000	0.3120800000
H	4.3050150000	3.4532020000	-0.1711330000
C	0.6545150000	-3.7754670000	-2.3255470000
H	-0.0807540000	-4.5759290000	-2.5579460000
H	0.1134150000	-2.8078540000	-2.3904370000
H	1.4164760000	-3.7855260000	-3.1331730000
C	-1.1418410000	5.3616290000	-0.6208900000
H	-1.6703070000	6.3054470000	-0.3643150000
H	-0.8382810000	5.4377760000	-1.6867160000
H	-1.8837400000	4.5380600000	-0.5510280000
C	5.0887270000	-1.4164130000	-1.6554720000
H	5.7063180000	-1.2312550000	-2.5609390000
H	4.7985400000	-0.4259040000	-1.2455430000
H	5.7479410000	-1.9012520000	-0.9047590000
C	2.3492840000	4.5532940000	-2.4635820000
H	2.6268420000	4.4469990000	-3.5349390000
H	1.7355280000	5.4748520000	-2.3774620000
H	3.2904090000	4.7345930000	-1.9023900000
C	-5.0456740000	0.1429620000	-2.5943310000
H	-5.0339670000	0.4228350000	-3.6703250000
H	-5.7452920000	-0.7136220000	-2.4900920000
H	-5.4897520000	0.9988980000	-2.0438130000
C	2.9649260000	-3.9466110000	2.2574970000
H	3.6470160000	-4.3368890000	3.0436180000

H	2.2984610000	-3.2033580000	2.7458110000
H	2.3284890000	-4.7939140000	1.9257560000
H	-3.7271620000	1.6255750000	0.6724540000
C	-5.6516680000	0.7619430000	1.3045400000
H	-5.9036890000	1.5981510000	1.9924810000
H	-6.2122660000	0.9386550000	0.3623410000
H	-6.0601020000	-0.1645410000	1.7601290000
C	3.7494360000	-3.3248730000	1.0945840000
Ge	-3.5533300000	-0.7650500000	-0.1783360000
C	-4.1342610000	0.6746730000	1.0763370000
H	-3.6042000000	0.5029560000	2.0376780000
C	-4.6538840000	-2.4047340000	0.1087380000
H	-4.5172750000	-2.7065180000	1.1701420000
H	-5.7178150000	-2.0937260000	0.0135930000
C	-4.3392430000	-3.5712250000	-0.8375770000
H	-4.9664690000	-4.4613230000	-0.6139330000
H	-3.2773840000	-3.8860780000	-0.7574410000
H	-2.9544490000	0.6758880000	-2.1938790000

$[(Et_3Ge)_2P_7]^-$

Charge = -1 Multiplicity = 1

Ge	2.9837360000	0.7807880000	0.1454530000
P	-1.8362630000	-1.4875220000	-0.7233740000
P	1.2083830000	-2.6713150000	-1.3406670000
P	0.6421800000	0.4217930000	0.3051790000
P	0.1438130000	-0.7888720000	-1.5482870000
P	-1.2565960000	-2.2872910000	1.2897970000
P	0.8091030000	-3.1214690000	0.7543590000
P	0.6149510000	-1.1243280000	1.8979330000
C	4.2284480000	-0.7036720000	0.6602500000
H	5.0218600000	-0.2281440000	1.2809640000
H	3.6515190000	-1.3701670000	1.3366610000
C	3.3544370000	2.2765680000	1.4364960000
H	3.1832670000	1.8613610000	2.4542820000
H	4.4440080000	2.5018970000	1.3742720000
C	3.3567890000	1.4443190000	-1.7067550000

H	3.2657100000	0.5651800000	-2.3795500000
H	2.5224680000	2.1244500000	-1.9825790000
C	-2.7522640000	1.8414040000	-1.5196070000
H	-2.9496460000	1.3508150000	-2.4973130000
H	-5.3473880000	0.1005150000	-2.3279330000
C	4.8341790000	-1.5145500000	-0.4919920000
H	5.5171000000	-2.3084140000	-0.1133820000
H	4.0314440000	-2.0150820000	-1.0761930000
H	5.4249190000	-0.8812510000	-1.1894880000
C	2.5161900000	3.5434370000	1.2240990000
H	2.7261210000	4.3242730000	1.9901000000
H	2.7061030000	4.0031050000	0.2297450000
H	1.4304580000	3.3127280000	1.2683740000
C	4.7125460000	2.1432740000	-1.8843380000
H	4.8734680000	2.4804720000	-2.9336130000
H	4.8050940000	3.0428870000	-1.2380900000
H	5.5623090000	1.4745870000	-1.6275660000
C	-3.5866300000	3.1215160000	-1.3711500000
H	-3.4016720000	3.8387580000	-2.2031390000
H	-4.6784230000	2.9108740000	-1.3633710000
H	-3.3535600000	3.6603560000	-0.4274860000
H	-1.8307260000	1.9325020000	1.5884970000
C	-3.8737490000	1.9108480000	2.4050000000
H	-3.5888200000	2.3236960000	3.3993800000
H	-4.2817970000	2.7568160000	1.8103850000
H	-4.7136510000	1.2046350000	2.5795820000
Ge	-3.0484360000	0.4597080000	-0.0984730000
C	-2.6818290000	1.2306430000	1.7155990000
H	-2.2900150000	0.3979600000	2.3380570000
C	-4.9818810000	-0.0877270000	-0.1627030000
H	-5.1287210000	-0.8406090000	0.6429270000
H	-5.5968100000	0.7955080000	0.1227390000
C	-5.4342180000	-0.6534630000	-1.5156040000
H	-6.4950750000	-0.9920900000	-1.4980360000
H	-4.8097780000	-1.5224600000	-1.8144260000
H	-1.6650470000	2.0684740000	-1.5070390000

Et_3GeH

Charge = 0 Multiplicity = 1

Ge	1.1987880000	3.5797640000	-0.1387690000
C	2.8000140000	3.6353940000	1.0418520000
H	3.3384380000	4.5876740000	0.8406020000
H	2.4287010000	3.7108030000	2.0876120000
C	-0.0005420000	5.1134500000	0.2739470000
H	-0.1877050000	5.0926920000	1.3701620000
H	0.5663750000	6.0505190000	0.0796200000
C	1.7265000000	3.5825880000	-2.0596810000
H	2.3198620000	2.6598500000	-2.2414140000
H	0.7969260000	3.4648670000	-2.6585050000
C	3.7456990000	2.4342380000	0.8901900000
H	4.6136260000	2.5003630000	1.5819570000
H	3.2285100000	1.4748230000	1.1050250000
H	4.1570580000	2.3583260000	-0.1389690000
C	-1.3274490000	5.1110290000	-0.5002890000
H	-1.9703610000	5.9747970000	-0.2231920000
H	-1.1665050000	5.1663040000	-1.5980960000
H	-1.9156010000	4.1892430000	-0.3040650000
C	2.5072770000	4.8277970000	-2.5071960000
H	2.7779390000	4.7817030000	-3.5845410000
H	1.9205810000	5.7596530000	-2.3605310000
H	3.4549880000	4.9485260000	-1.9403260000
H	0.4208820000	2.2515970000	0.1426090000

$(^nBu_3Sn)_3P_7$

Charge = 0 Multiplicity = 1

Sn	-3.3518850000	-1.2301790000	-0.0465410000
Sn	3.0394800000	-2.0690670000	-0.2335600000
P	1.5094680000	1.4970080000	-0.6511450000
P	0.4755140000	-1.7136890000	-0.5515430000
P	-1.7828290000	0.7878520000	-0.5583130000
P	0.0959480000	0.2161560000	0.4945170000
P	0.8873610000	1.1214930000	-2.7699490000

P	0.4278700000	-1.1021320000	-2.7060440000
P	-1.2677360000	0.4061280000	-2.7031890000
Sn	0.5792670000	3.8973160000	-0.2262440000
C	5.9329390000	-6.8818100000	1.0045780000
H	5.9398720000	-7.9907490000	1.0503030000
H	6.1466580000	-6.5046470000	2.0278050000
C	4.5960740000	-6.3441750000	0.4785150000
H	6.7793630000	-6.5700310000	0.3554080000
H	4.3908050000	-6.7670720000	-0.5313490000
C	4.5369240000	-4.8068080000	0.3977600000
H	3.7646100000	-6.7034960000	1.1270310000
H	5.3714920000	-4.4521680000	-0.2507860000
H	4.7508090000	-4.3875920000	1.4083530000
C	3.1926480000	-4.2697060000	-0.1227720000
H	2.9785880000	-4.6632930000	-1.1410370000
H	2.3562110000	-4.6157410000	0.5234020000
C	2.5557860000	-1.5283210000	5.4619610000
H	2.9415520000	-1.0785920000	6.4005660000
H	2.5984760000	-2.6325880000	5.5799830000
C	3.3578450000	-1.0640050000	4.2397150000
H	1.4843510000	-1.2476120000	5.3733760000
H	3.3260080000	0.0470810000	4.1694390000
C	2.8594690000	-1.6615580000	2.9106560000
H	4.4327450000	-1.3246240000	4.3746840000
H	1.7845480000	-1.3990770000	2.7783610000
H	2.8892560000	-2.7736170000	2.9830670000
C	3.6603740000	-1.1880650000	1.6880020000
H	3.5956650000	-0.0849630000	1.5697500000
H	4.7406250000	-1.4320500000	1.8047080000
C	8.0386780000	-0.7476550000	-2.7189010000
H	8.5694440000	-0.3245310000	-3.5970470000
H	8.4126380000	-1.7838100000	-2.5715870000
C	6.5172550000	-0.7230430000	-2.9119040000
H	8.3448550000	-0.1572710000	-1.8285230000
H	6.1772540000	0.3214480000	-3.0955900000
C	5.7327460000	-1.2992900000	-1.7176440000

H	6.2452180000	-1.2913150000	-3.8304450000
H	6.0057070000	-0.7276400000	-0.8006740000
H	6.0810180000	-2.3420570000	-1.5325420000
C	4.2087370000	-1.2721030000	-1.9229590000
H	3.8516840000	-0.2335240000	-2.0903860000
H	3.9183390000	-1.8559490000	-2.8236400000
C	-5.2061840000	-5.9958190000	-2.6723590000
H	-5.0058770000	-6.7958740000	-3.4151470000
H	-6.1374860000	-5.4765700000	-2.9857730000
C	-4.0292430000	-5.0181900000	-2.5621380000
H	-5.4162530000	-6.4901280000	-1.6993600000
H	-3.1035560000	-5.5728050000	-2.2864640000
C	-4.2575640000	-3.8880730000	-1.5404180000
H	-3.8204300000	-4.5659250000	-3.5582540000
H	-4.4683470000	-4.3431060000	-0.5449340000
H	-5.1861100000	-3.3382230000	-1.8193390000
C	-3.0706440000	-2.9150780000	-1.4409860000
H	-2.1428210000	-3.4366170000	-1.1226310000
H	-2.8465970000	-2.4640890000	-2.4326500000
C	-3.6477990000	-4.9140830000	4.3493500000
H	-3.4352220000	-5.1230450000	5.4184860000
H	-3.1381290000	-5.6980490000	3.7488860000
C	-3.1842930000	-3.5091750000	3.9440140000
H	-4.7412020000	-5.0407760000	4.1963940000
H	-3.6839380000	-2.7483570000	4.5862490000
C	-3.4553600000	-3.1720790000	2.4653360000
H	-2.0941110000	-3.3998740000	4.1445210000
H	-4.5464720000	-3.2848260000	2.2674680000
H	-2.9561820000	-3.9371230000	1.8273160000
C	-2.9834210000	-1.7645780000	2.0636220000
H	-3.4834680000	-0.9870130000	2.6823520000
H	-1.8919710000	-1.6507310000	2.2391390000
C	-8.9531790000	-1.0999270000	1.2422440000
H	-9.9389650000	-0.6080380000	1.1074440000
H	-8.7146720000	-1.0755660000	2.3274360000
C	-7.8597650000	-0.4146090000	0.4130200000

H	-9.0715740000	-2.1669590000	0.9550880000
H	-8.1444740000	-0.4209740000	-0.6638650000
C	-6.4700120000	-1.0617360000	0.5665740000
H	-7.7899690000	0.6602990000	0.6969080000
H	-6.5438300000	-2.1374680000	0.2844280000
H	-6.1922810000	-1.0575870000	1.6461030000
C	-5.3747680000	-0.3678170000	-0.2615280000
H	-5.6282830000	-0.3862000000	-1.3445860000
H	-5.2940110000	0.7049480000	0.0202470000
C	-4.1492190000	5.0875940000	-3.2972190000
H	-4.5876350000	5.5782480000	-4.1911400000
H	-4.6397510000	5.5266730000	-2.4017360000
C	-2.6262560000	5.2624650000	-3.2443080000
H	-4.4311580000	4.0135460000	-3.3338500000
H	-2.1686450000	4.8444660000	-4.1696570000
C	-1.9732060000	4.5957280000	-2.0193840000
H	-2.3719500000	6.3474340000	-3.2482060000
H	-2.2278100000	3.5115650000	-2.0157760000
H	-2.4382120000	5.0087700000	-1.0943500000
C	-0.4485720000	4.7739670000	-1.9702540000
H	0.0288500000	4.3468290000	-2.8790210000
H	-0.1761380000	5.8537450000	-1.9547060000
C	5.4997840000	4.7098050000	2.6120300000
H	6.4192690000	5.3150850000	2.7540860000
H	5.8172450000	3.6707790000	2.3785980000
C	4.6078600000	5.2840930000	1.5040820000
H	4.9667350000	4.6796420000	3.5867450000
H	4.3370420000	6.3370340000	1.7476290000
C	3.3183450000	4.4757200000	1.2676980000
H	5.1808710000	5.3366550000	0.5500990000
H	2.7494430000	4.4197940000	2.2250160000
H	3.5914100000	3.4226040000	1.0250160000
C	2.4236250000	5.0481280000	0.1577330000
H	2.1080170000	6.0880880000	0.4013380000
H	2.9795920000	5.1095950000	-0.8039180000
C	-2.0506840000	6.6987230000	4.0103470000

H	-2.6876250000	6.6577010000	4.9183760000
H	-2.5600790000	7.3590490000	3.2758070000
C	-1.8019690000	5.3012160000	3.4291160000
H	-1.0978420000	7.1955240000	4.2939730000
H	-1.3260900000	4.6521640000	4.1991480000
C	-0.9189590000	5.3060190000	2.1663320000
H	-2.7742920000	4.8148530000	3.1875280000
H	0.0498070000	5.8008300000	2.4098120000
H	-1.3988730000	5.9568930000	1.3986350000
C	-0.6683690000	3.9017910000	1.5913770000
H	-0.1662350000	3.2506070000	2.3394800000
H	-1.6222910000	3.3970500000	1.3275140000

$[(^{n}Bu_3Sn)_2P_7]^-$

Charge = -1 Multiplicity = 1

Sn	-2.7327960000	0.1179380000	0.1601200000
P	2.2196830000	-2.0996490000	0.2403190000
P	-0.9398310000	-3.1009810000	0.8210800000
P	-0.1944250000	0.1183120000	-0.3387700000
P	0.3412440000	-1.3926580000	1.2578420000
P	1.4793700000	-2.5552800000	-1.8223010000
P	-0.6325740000	-3.2828790000	-1.3308480000
P	-0.2972440000	-1.1552600000	-2.1646670000
Sn	3.4652460000	0.0896560000	-0.2996030000
C	-7.6236940000	-1.5664770000	-2.4130620000
H	-8.1714160000	-2.3665990000	-2.9554370000
H	-7.6150320000	-0.6671160000	-3.0669050000
C	-6.2002210000	-1.9997130000	-2.0380380000
H	-8.2197930000	-1.3080130000	-1.5106040000
H	-6.2401780000	-2.9214350000	-1.4139390000
C	-5.3983300000	-0.9205320000	-1.2839040000
H	-5.6398860000	-2.2878830000	-2.9564060000
H	-5.9689980000	-0.6296940000	-0.3705740000
H	-5.3624980000	-0.0017080000	-1.9148310000
C	-3.9777470000	-1.3669620000	-0.9085830000
H	-3.9870650000	-2.2686760000	-0.2599890000

H	-3.3978690000	-1.6540450000	-1.8126160000
C	-6.1059990000	-1.0057360000	4.6745120000
H	-6.2341370000	-1.0327290000	5.7777950000
H	-6.2765330000	-2.0361420000	4.2939150000
C	-4.7198170000	-0.4859980000	4.2706890000
H	-6.9157790000	-0.3660370000	4.2602290000
H	-4.5622470000	0.5322590000	4.6956190000
C	-4.4937320000	-0.4351810000	2.7470560000
H	-3.9311550000	-1.1255420000	4.7281680000
H	-5.2883410000	0.2007170000	2.2897530000
H	-4.6525220000	-1.4565360000	2.3311260000
C	-3.1024640000	0.0769680000	2.3459140000
H	-2.9326710000	1.1072870000	2.7319600000
H	-2.3072990000	-0.5652450000	2.7801390000
C	-6.3895360000	4.6036260000	0.2833910000
H	-6.6527400000	5.6185530000	-0.0840340000
H	-6.2930560000	4.6643150000	1.3893730000
C	-5.1010980000	4.0751100000	-0.3612140000
H	-7.2526290000	3.9367700000	0.0678080000
H	-5.2149990000	4.0607740000	-1.4696470000
C	-4.6951390000	2.6673100000	0.1180740000
H	-4.2630590000	4.7810410000	-0.1582190000
H	-5.5392760000	1.9678090000	-0.0847190000
H	-4.5936510000	2.6888650000	1.2284520000
C	-3.4005480000	2.1369720000	-0.5175020000
H	-3.4958240000	2.1014320000	-1.6262100000
H	-2.5564910000	2.8309760000	-0.3068580000
C	1.4925730000	4.4638400000	-3.5064300000
H	1.2558560000	4.8563100000	-4.5185760000
H	2.1900480000	5.1837120000	-3.0243220000
C	2.0943940000	3.0535810000	-3.5647690000
H	0.5513330000	4.4745000000	-2.9158050000
H	1.3859810000	2.3651910000	-4.0787280000
C	2.4308340000	2.4667280000	-2.1807370000
H	3.0145110000	3.0641760000	-4.1948140000
H	1.5002770000	2.4405120000	-1.5685470000

H	3.1248520000	3.1641720000	-1.6545160000
C	3.0326680000	1.0565610000	-2.2442900000
H	2.3417240000	0.3657550000	-2.7754820000
H	3.9901760000	1.0553150000	-2.8132380000
C	8.0654640000	-2.6242650000	1.8582820000
H	9.1228160000	-2.9429390000	1.7358660000
H	7.4520390000	-3.5416720000	1.9888410000
C	7.5737100000	-1.7926290000	0.6658690000
H	7.9977950000	-2.0493320000	2.8075350000
H	8.2284080000	-0.8994840000	0.5361010000
C	6.1090080000	-1.3319190000	0.7918400000
H	7.6861890000	-2.3826040000	-0.2728850000
H	6.0001170000	-0.7468500000	1.7353970000
H	5.4574700000	-2.2258150000	0.9270430000
C	5.6050660000	-0.5066560000	-0.4006880000
H	6.2110020000	0.4202090000	-0.5259610000
H	5.7207520000	-1.0832870000	-1.3460910000
C	5.3345470000	4.5832100000	2.7875730000
H	5.1752660000	5.2699630000	3.6461120000
H	5.4000000000	5.2071280000	1.8696270000
C	4.2161700000	3.5387110000	2.6738070000
H	6.3269190000	4.1012220000	2.9261100000
H	4.1511980000	2.9531550000	3.6194560000
C	4.3919490000	2.5632330000	1.4935570000
H	3.2323620000	4.0515240000	2.5740890000
H	5.3811890000	2.0581250000	1.5937490000
H	4.4602290000	3.1573010000	0.5518600000
C	3.2711430000	1.5183350000	1.3835880000
H	3.2057910000	0.9110350000	2.3127150000
H	2.2797800000	2.0068530000	1.2658210000

$^{n}Bu_3SnH$

Charge = 0 Multiplicity = 1

Sn	0.4730700000	4.1649100000	-0.1855330000
C	-4.0336180000	4.5916720000	-3.7010130000
H	-4.5398900000	5.1339110000	-4.5266550000

H	-4.7370730000	4.5625230000	-2.8411100000
C	-2.7057330000	5.2559510000	-3.3156870000
H	-3.8800060000	3.5432140000	-4.0358340000
H	-2.0373630000	5.3032150000	-4.2057980000
C	-1.9643350000	4.5386560000	-2.1722010000
H	-2.8867170000	6.3154260000	-3.0221490000
H	-1.7890080000	3.4781750000	-2.4678910000
H	-2.6381060000	4.4888890000	-1.2852870000
C	-0.6321520000	5.2018880000	-1.7841420000
H	0.0454050000	5.2594540000	-2.6650150000
H	-0.7984730000	6.2518210000	-1.4553100000
C	5.5115720000	4.4408730000	2.5342550000
H	6.4865220000	4.9546510000	2.6666900000
H	5.7258380000	3.3820220000	2.2736320000
C	4.6536300000	5.1195580000	1.4589720000
H	4.9993750000	4.4393340000	3.5205510000
H	4.4872650000	6.1874200000	1.7298230000
C	3.2886720000	4.4415820000	1.2367440000
H	5.2082930000	5.1398590000	0.4930000000
H	2.7401550000	4.4165380000	2.2071390000
H	3.4579610000	3.3731010000	0.9674660000
C	2.4259350000	5.1232130000	0.1612190000
H	2.2368430000	6.1869180000	0.4278830000
H	2.9617800000	5.1420330000	-0.8137820000
C	-1.9770390000	6.8472090000	4.2600270000
H	-2.5605850000	6.7723840000	5.2012100000
H	-2.5363860000	7.5197050000	3.5743450000
C	-1.7421580000	5.4701350000	3.6265770000
H	-1.0165640000	7.3508240000	4.5029580000
H	-1.2142670000	4.8085540000	4.3510300000
C	-0.9341430000	5.5202550000	2.3163600000
H	-2.7203890000	4.9749240000	3.4291490000
H	0.0404170000	6.0231510000	2.5173390000
H	-1.4647830000	6.1852150000	1.5956720000
C	-0.6937920000	4.1395430000	1.6833970000
H	-0.1566290000	3.4729170000	2.3942500000

H	-1.6614360000	3.6352120000	1.4658310000
H	0.7489130000	2.5051640000	-0.6891130000

$(Et_3Ge)_3As_7$

Charge = 0 Multiplicity = 1

Ge	-1.0932100000	3.6830880000	0.3669020000
Ge	-2.7448720000	-2.7532550000	0.7979380000
As	1.4281310000	-1.6412830000	0.1241360000
As	-2.0966990000	-0.4245970000	0.1365940000
As	0.6966190000	1.9799740000	-0.0651100000
As	0.0327010000	0.0294020000	1.2751060000
As	1.0352530000	-1.1227370000	-2.2561300000
As	-1.4072310000	-0.6517080000	-2.2239240000
As	0.2212790000	1.2304770000	-2.3714920000
C	-2.2085580000	4.1447150000	-1.2243450000
H	-2.6573910000	5.1330360000	-0.9740840000
H	-1.5101450000	4.3323470000	-2.0685790000
C	-0.0297370000	5.3170680000	0.8118530000
H	0.5733280000	5.5657580000	-0.0887180000
H	-0.7616240000	6.1476750000	0.9298590000
C	-1.3430170000	-3.8907030000	1.6415080000
H	-1.7771220000	-4.9165680000	1.6598280000
H	-0.4713800000	-3.9257620000	0.9541960000
C	-2.2294950000	3.1772550000	1.9275540000
H	-2.7706280000	2.2464860000	1.6544410000
H	-1.5488540000	2.9053470000	2.7627770000
C	-4.2057370000	-2.4481820000	2.1282960000
H	-4.4502250000	-3.4508290000	2.5474770000
H	-3.7789640000	-1.8589210000	2.9686420000
H	-4.2109930000	-4.4598870000	-0.3521150000
H	-4.1644690000	-2.9760170000	-1.3297610000
C	3.8525750000	-0.1040950000	2.3284440000
H	3.4337700000	-0.9129880000	2.9653550000
H	4.8150730000	-3.2041080000	2.1960660000
C	-3.2973490000	3.1423590000	-1.6237650000
H	-3.8914960000	3.5130170000	-2.4872410000

H	-2.8665880000	2.1628290000	-1.9190960000
H	-4.0091460000	2.9471740000	-0.7943050000
C	-0.9094180000	-3.4591030000	3.0483530000
H	-0.1425050000	-4.1466620000	3.4662930000
H	-0.4652150000	-2.4401920000	3.0459620000
H	-1.7600630000	-3.4439860000	3.7620410000
C	0.8664880000	5.1975850000	2.0513620000
H	1.4468350000	6.1283620000	2.2326310000
H	0.2778980000	4.9968240000	2.9717190000
H	1.6007010000	4.3699740000	1.9457150000
C	-5.4627760000	-1.7668050000	1.5705200000
H	-6.2339220000	-1.6178630000	2.3574240000
H	-5.2307480000	-0.7668240000	1.1455200000
H	-5.9341120000	-2.3643310000	0.7617330000
C	-3.2078780000	4.2839320000	2.3509630000
H	-3.8315880000	3.9660640000	3.2149010000
H	-2.6823560000	5.2137390000	2.6559180000
H	-3.9063400000	4.5567840000	1.5315090000
C	5.2652850000	0.2786560000	2.7972850000
H	5.2704800000	0.5757810000	3.8688300000
H	5.9829250000	-0.5624720000	2.6905730000
H	5.6761020000	1.1354230000	2.2231780000
C	-2.5087110000	-4.3568400000	-1.7280340000
H	-3.0159520000	-4.8734630000	-2.5715470000
H	-1.8153000000	-3.6116390000	-2.1740780000
H	-1.8847840000	-5.1138250000	-1.2077960000
H	3.7668300000	1.6277650000	-0.5270530000
C	5.7589270000	0.8808630000	-1.0885130000
H	5.9576080000	1.6873210000	-1.8278480000
H	6.2869780000	1.1642360000	-0.1537170000
H	6.2479950000	-0.0378800000	-1.4754700000
C	-3.5214830000	-3.6982580000	-0.7824650000
Ge	3.7406010000	-0.7315810000	0.4339980000
C	4.2489170000	0.6892470000	-0.8754440000
H	3.7507630000	0.4335160000	-1.8354960000
C	4.9218650000	-2.3242710000	0.1770090000

H	4.8102480000	-2.6463260000	-0.8814730000
H	5.9691450000	-1.9613610000	0.2776800000
C	4.6582860000	-3.4938380000	1.1352740000
H	5.3327980000	-4.3533990000	0.9299950000
H	3.6151030000	-3.8662500000	1.0507570000
H	3.1558730000	0.7561010000	2.4264740000

$[(Et_3Ge)_2As_7]^-$

Charge = -1 Multiplicity = 1

Ge	-3.3045950000	1.3758650000	0.0073500000
As	0.7498270000	0.9775210000	0.5284430000
As	-2.1745110000	-0.6522040000	-0.9047730000
As	1.0143150000	-2.1100460000	-1.8642890000
As	0.0622470000	0.0763740000	-1.7135770000
As	0.6029330000	-1.0133070000	1.9388500000
As	-1.6029910000	-1.9066490000	1.1438990000
As	0.5289880000	-2.9618570000	0.3256430000
C	-2.4328840000	3.1211740000	-0.4473970000
H	-3.0447650000	3.9063820000	0.0543160000
H	-1.4364060000	3.1254140000	0.0443570000
C	-5.0947640000	1.3861760000	-0.9145010000
H	-5.6008320000	2.3387260000	-0.6333680000
H	-4.9025030000	1.4446350000	-2.0083580000
H	-4.5316820000	2.1497200000	2.0891300000
H	-4.1902420000	0.4039430000	2.2087620000
C	3.5535110000	1.8527620000	-1.6012140000
H	2.7328730000	2.5760780000	-1.7967720000
H	3.4362590000	4.2365690000	0.6759970000
C	-2.2925650000	3.4099000000	-1.9476710000
H	-1.8224700000	4.4013700000	-2.1366050000
H	-1.6550740000	2.6467730000	-2.4441380000
H	-3.2750620000	3.4101640000	-2.4680170000
C	-5.9860210000	0.1784750000	-0.5949550000
H	-6.9512450000	0.2045570000	-1.1502160000
H	-5.4786490000	-0.7745650000	-0.8592820000
H	-6.2344870000	0.1233900000	0.4869280000

C	4.9199670000	2.5261630000	-1.7983320000
H	5.0318400000	2.9409590000	-2.8260980000
H	5.0737120000	3.3705350000	-1.0921600000
H	5.7622390000	1.8195900000	-1.6420260000
C	-2.5566030000	1.6730040000	2.9163280000
H	-2.8829920000	1.6923920000	3.9808600000
H	-1.7646830000	0.8998830000	2.8274180000
H	-2.0773680000	2.6516930000	2.7006730000
H	3.5822340000	-1.4027300000	-0.2686020000
C	5.6381260000	-0.7110570000	0.0944840000
H	6.0861650000	-1.7172890000	0.2589330000
H	5.8422180000	-0.4415740000	-0.9638150000
H	6.2078590000	0.0030010000	0.7292980000
C	-3.7277090000	1.3858830000	1.9689020000
Ge	3.2080310000	1.0527980000	0.2098830000
C	4.1337180000	-0.7062730000	0.4012500000
H	3.9381060000	-1.0550370000	1.4386660000
C	3.9324930000	2.3025280000	1.6108090000
H	3.7934140000	1.7912770000	2.5889130000
H	5.0326390000	2.3853600000	1.4582350000
C	3.2779490000	3.6902450000	1.6313700000
H	3.6773650000	4.3358620000	2.4462900000
H	2.1789910000	3.6112180000	1.7755940000
H	3.4045870000	1.0261830000	-2.3292580000

$(^{n}Bu_3Sn)_3As_7$

Charge = 0 Multiplicity = 1

Sn	-3.5810840000	-1.1999540000	0.1954450000
Sn	3.0871480000	-2.3124930000	0.0283210000
As	1.7104710000	1.5129700000	-0.3933880000
As	0.4319050000	-1.9687380000	-0.3195160000
As	-1.9441110000	0.8826920000	-0.3140250000
As	0.0897200000	0.1590720000	0.8597160000
As	1.0013260000	1.1651780000	-2.7308110000
As	0.4306640000	-1.2628960000	-2.6847500000

As	-1.3854160000	0.4437710000	-2.6738440000
Sn	0.7528490000	3.9927050000	0.0819900000
C	6.0172000000	-7.0862040000	1.3630100000
H	6.0317380000	-8.1941270000	1.4280010000
H	6.2154200000	-6.6898610000	2.3821350000
C	4.6831500000	-6.5675940000	0.8112960000
H	6.8694180000	-6.7791840000	0.7191660000
H	4.4942820000	-7.0080500000	-0.1942780000
C	4.6131500000	-5.0320510000	0.7055780000
H	3.8461760000	-6.9233970000	1.4546720000
H	5.4544460000	-4.6808910000	0.0640280000
H	4.8090560000	-4.5959410000	1.7125820000
C	3.2728200000	-4.5137410000	0.1566830000
H	3.0820900000	-4.9181370000	-0.8620940000
H	2.4295090000	-4.8673200000	0.7900160000
C	2.6579680000	-1.7640720000	5.7337690000
H	3.0472340000	-1.3063620000	6.6670530000
H	2.7163680000	-2.8673080000	5.8546510000
C	3.4413820000	-1.2930630000	4.5019820000
H	1.5819980000	-1.4978280000	5.6555040000
H	3.3941080000	-0.1826740000	4.4286050000
C	2.9380500000	-1.9015110000	3.1796910000
H	4.5209390000	-1.5389240000	4.6267570000
H	1.8577510000	-1.6543480000	3.0593760000
H	2.9818570000	-3.0128300000	3.2558190000
C	3.7195410000	-1.4230170000	1.9466710000
H	3.6438690000	-0.3199580000	1.8302510000
H	4.8034760000	-1.6552270000	2.0526740000
C	8.1360530000	-1.1190740000	-2.4318980000
H	8.6826900000	-0.6999130000	-3.3021900000
H	8.4732370000	-2.1700370000	-2.3018430000
C	6.6166380000	-1.0378570000	-2.6255130000
H	8.4613020000	-0.5550310000	-1.5312780000
H	6.3138850000	0.0210620000	-2.7912850000
C	5.8108770000	-1.6068840000	-1.4418840000
H	6.3260770000	-1.5801990000	-3.5540460000

H	6.1049480000	-1.0628490000	-0.5146750000
H	6.1200960000	-2.6648710000	-1.2759150000
C	4.2888340000	-1.5203170000	-1.6442380000
H	3.9710820000	-0.4653330000	-1.7901270000
H	3.9772660000	-2.0718390000	-2.5584110000
C	-5.5690230000	-5.9782300000	-2.3021450000
H	-5.3941740000	-6.8059470000	-3.0206890000
H	-6.4861000000	-5.4422120000	-2.6289380000
C	-4.3642630000	-5.0319000000	-2.2246500000
H	-5.7899370000	-6.4364740000	-1.3140300000
H	-3.4537580000	-5.6046020000	-1.9354680000
C	-4.5564630000	-3.8656320000	-1.2364620000
H	-4.1465840000	-4.6159900000	-3.2347320000
H	-4.7738680000	-4.2846330000	-0.2268470000
H	-5.4718050000	-3.3001330000	-1.5271960000
C	-3.3458610000	-2.9192060000	-1.1709870000
H	-2.4295220000	-3.4578880000	-0.8464270000
H	-3.1197060000	-2.5021460000	-2.1768420000
C	-4.1029090000	-4.8509670000	4.6141680000
H	-3.9070280000	-5.0620340000	5.6861050000
H	-3.6339370000	-5.6667170000	4.0229540000
C	-3.5616140000	-3.4768930000	4.1996050000
H	-5.2008760000	-4.9195620000	4.4568050000
H	-4.0218590000	-2.6846470000	4.8332630000
C	-3.8062340000	-3.1364280000	2.7170800000
H	-2.4680060000	-3.4255090000	4.4050700000
H	-4.9010130000	-3.1849390000	2.5145140000
H	-3.3510860000	-3.9351980000	2.0874410000
C	-3.2489310000	-1.7626350000	2.3078310000
H	-3.6969230000	-0.9542460000	2.9272170000
H	-2.1523600000	-1.7186970000	2.4849750000
C	-9.1864460000	-0.9893620000	1.4949650000
H	-10.1683350000	-0.4931340000	1.3479730000
H	-8.9474560000	-0.9398840000	2.5791900000
C	-8.0876750000	-0.3338570000	0.6488370000
H	-9.3134550000	-2.0622720000	1.2345810000

H	-8.3724220000	-0.3657930000	-0.4276170000
C	-6.7027810000	-0.9873640000	0.8193620000
H	-8.0099520000	0.7474810000	0.9050060000
H	-6.7847330000	-2.0694320000	0.5655950000
H	-6.4247120000	-0.9568810000	1.8983100000
C	-5.6023060000	-0.3240740000	-0.0264130000
H	-5.8601470000	-0.3630560000	-1.1081400000
H	-5.5122970000	0.7542020000	0.2309440000
C	-3.9612690000	5.4236380000	-2.9169870000
H	-4.3912920000	5.9586710000	-3.7892540000
H	-4.4339230000	5.8428760000	-2.0026110000
C	-2.4336550000	5.5546020000	-2.8683580000
H	-4.2734480000	4.3598690000	-2.9906360000
H	-1.9931010000	5.1591920000	-3.8118080000
C	-1.7912890000	4.8263000000	-1.6729710000
H	-2.1496670000	6.6315960000	-2.8342660000
H	-2.0806510000	3.7509250000	-1.7051560000
H	-2.2371430000	5.2205170000	-0.7304830000
C	-0.2617900000	4.9553040000	-1.6292880000
H	0.1953900000	4.5450440000	-2.5560360000
H	0.0428040000	6.0254240000	-1.5807790000
C	5.6316680000	4.8056750000	3.0066610000
H	6.5442660000	5.4162550000	3.1690810000
H	5.9606120000	3.7711590000	2.7689720000
C	4.7532320000	5.3836450000	1.8898290000
H	5.0832820000	4.7625990000	3.9723540000
H	4.4706740000	6.4322620000	2.1386540000
C	3.4733510000	4.5686640000	1.6254590000
H	5.3409250000	5.4494060000	0.9456360000
H	2.8911050000	4.4982200000	2.5738130000
H	3.7587850000	3.5197190000	1.3771560000
C	2.5907460000	5.1459690000	0.5082590000
H	2.2662110000	6.1818850000	0.7573940000
H	3.1612730000	5.2207980000	-0.4439500000
C	-1.8865350000	6.7876350000	4.3213960000
H	-2.5301320000	6.7467230000	5.2247450000

H	-2.3850470000	7.4567700000	3.5873470000
C	-1.6458710000	5.3915870000	3.7331970000
H	-0.9314340000	7.2744710000	4.6145390000
H	-1.1810150000	4.7337430000	4.5025330000
C	-0.7542620000	5.3965040000	2.4764250000
H	-2.6208140000	4.9153060000	3.4821490000
H	0.2175100000	5.8804780000	2.7293860000
H	-1.2225730000	6.0570090000	1.7098980000
C	-0.5115870000	3.9948210000	1.8921430000
H	-0.0203020000	3.3344060000	2.6397610000
H	-1.4700270000	3.5014160000	1.6213760000

$[(^{n}Bu_3Sn)_2As_7]^-$

Charge = -1 Multiplicity = 1

Sn	-3.3419360000	0.0208260000	-0.2613180000
Sn	3.0388590000	0.9881060000	0.3582600000
As	1.8957520000	-2.3175710000	-1.7145140000
As	0.4011440000	0.5331240000	0.4226180000
As	-1.7517220000	-1.8559620000	-1.3103010000
As	0.2990670000	-0.5395390000	-1.8309380000
As	1.3405870000	-3.2847020000	0.4084640000
As	0.5275890000	-1.4103830000	1.9059560000
As	-1.1209160000	-2.9505600000	0.8056010000
C	6.3506070000	5.1218330000	2.6400650000
H	6.4497740000	5.9820620000	3.3361820000
H	6.6339790000	5.4795740000	1.6262010000
C	4.9323930000	4.5358250000	2.6490390000
H	7.1045680000	4.3618500000	2.9401460000
H	4.6626290000	4.2214750000	3.6835300000
C	4.7450470000	3.3369920000	1.6982820000
H	4.1974690000	5.3288720000	2.3790640000
H	5.4844580000	2.5481980000	1.9739590000
H	5.0285950000	3.6554920000	0.6676120000
C	3.3255830000	2.7505010000	1.6946780000
H	3.0344110000	2.4295340000	2.7202640000
H	2.5833590000	3.5233620000	1.3940800000
C	2.5083730000	4.2806020000	-4.3302680000

H	2.9032800000	4.5828050000	-5.3238650000
H	2.4553270000	5.1951770000	-3.6999680000
C	3.3753680000	3.1981620000	-3.6733200000
H	1.4660240000	3.9252610000	-4.4788590000
H	3.4365050000	2.3102990000	-4.3430860000
C	2.8617640000	2.7438980000	-2.2937850000
H	4.4224030000	3.5674950000	-3.5699360000
H	1.8186060000	2.3683940000	-2.4063830000
H	2.7887850000	3.6356580000	-1.6271670000
C	3.7263580000	1.6575960000	-1.6390500000
H	3.7632710000	0.7473970000	-2.2753140000
H	4.7767710000	2.0106670000	-1.5167260000
C	7.3527320000	-2.7504120000	-0.3140950000
H	8.0006780000	-3.5387960000	0.1256050000
H	8.0183040000	-1.9441240000	-0.6934720000
C	6.3393970000	-2.2067910000	0.7021670000
H	6.8388580000	-3.1916800000	-1.1949170000
H	5.7118840000	-3.0419650000	1.0878270000
C	5.4136000000	-1.1182160000	0.1264980000
H	6.8791360000	-1.8014160000	1.5899990000
H	4.8560460000	-1.5416040000	-0.7411030000
H	6.0431280000	-0.2937930000	-0.2846320000
C	4.4050490000	-0.5687670000	1.1442950000
H	3.7570540000	-1.3861110000	1.5283490000
H	4.9242300000	-0.1234150000	2.0237310000
C	-5.6240980000	1.2311310000	4.9056890000
H	-5.4648330000	1.3551190000	5.9981060000
H	-6.3848330000	0.4318050000	4.7688040000
C	-4.3197420000	0.8932980000	4.1714970000
H	-6.0706970000	2.1756180000	4.5249140000
H	-3.5661230000	1.6921390000	4.3578970000
C	-4.4906540000	0.7120960000	2.6503340000
H	-3.8778290000	-0.0361050000	4.5972570000
H	-4.9375050000	1.6442590000	2.2315190000
H	-5.2498060000	-0.0850320000	2.4720580000
C	-3.1815350000	0.3733380000	1.9224870000

H	-2.4265270000	1.1775220000	2.0583010000
H	-2.7203070000	-0.5464050000	2.3447000000
C	-3.6093850000	5.7695280000	-0.4982010000
H	-3.4558910000	6.7008370000	-1.0840690000
H	-2.9804550000	5.8431310000	0.4152980000
C	-3.2624430000	4.5163410000	-1.3130280000
H	-4.6702320000	5.7560530000	-0.1650120000
H	-3.8788710000	4.4899500000	-2.2412760000
C	-3.4599150000	3.1979280000	-0.5400960000
H	-2.2053600000	4.5746750000	-1.6586580000
H	-4.5184510000	3.1442230000	-0.1921310000
H	-2.8434910000	3.2352820000	0.3874630000
C	-3.1009880000	1.9433060000	-1.3502530000
H	-3.7213780000	1.8776770000	-2.2723530000
H	-2.0423590000	1.9852580000	-1.6850820000
C	-8.9447550000	1.0855840000	-1.2163430000
H	-9.9560610000	0.6887810000	-1.4487570000
H	-8.6741630000	1.8015970000	-2.0225770000
C	-7.9028270000	-0.0342780000	-1.0928930000
H	-9.0245470000	1.6701990000	-0.2740280000
H	-8.2192940000	-0.7563790000	-0.3054460000
C	-6.4819510000	0.4686240000	-0.7697870000
H	-7.8705400000	-0.6221760000	-2.0389840000
H	-6.5195550000	1.0510140000	0.1801430000
H	-6.1807050000	1.2037800000	-1.5520610000
C	-5.4314940000	-0.6479770000	-0.6659150000
H	-5.7094550000	-1.3728690000	0.1320130000
H	-5.3948820000	-1.2335340000	-1.6114560000

6.5. Optimised structures at the PBE1PBE/6-311G(d,p) level of theory for Compounds 6–11 N,N,N and O,O,O tetrel coordination modes

$(Me_3Ge\text{-}PhNCO)_3P_7$ – NNN

Charge = 0 Multiplicity = 1

Ge	-4.7943260000	1.9577400000	-0.1736020000
Ge	4.1920080000	3.0899180000	-0.1656220000

Ge	0.6889320000	-5.0785980000	-0.1448510000
P	-0.5096720000	1.8838980000	1.4627480000
P	1.8236360000	-0.4852860000	1.4748730000
P	1.2471050000	-0.1294810000	3.6046320000
P	-0.5124010000	1.2200480000	3.5972360000
P	-0.0234610000	0.0221650000	0.3715100000
P	-1.3850760000	-1.3220200000	1.4807450000
P	-0.8020130000	-0.9787100000	3.6105790000
O	2.9134720000	1.9153700000	2.1496780000
O	0.0791990000	-3.4980560000	2.1958260000
O	-3.1292450000	1.6589610000	2.1640790000
N	-2.8748950000	2.1010650000	-0.0258480000
N	3.2873440000	1.3923370000	-0.0047200000
N	-0.3722770000	-3.4709270000	-0.0082030000
C	-0.7376130000	4.2404730000	-2.1805250000
H	-0.3207940000	5.2422380000	-2.1737130000
C	-1.5066920000	3.8095190000	-1.1073490000
H	-1.6945240000	4.4644580000	-0.2634000000
C	2.3992400000	0.7093650000	-2.1726560000
H	1.7614830000	1.5870540000	-2.1705480000
C	-0.5189470000	3.3989780000	-3.2661630000
H	0.0677230000	3.7423280000	-4.1120080000
C	-0.2266490000	-6.4700180000	0.8638060000
H	-0.5188130000	-6.0772510000	1.8380950000
H	0.4462390000	-7.3183980000	1.0153110000
H	-1.1119130000	-6.8190990000	0.3276120000
C	2.4769690000	-4.6643740000	0.4933730000
H	2.8369690000	-3.7516950000	0.0128420000
H	3.1546890000	-5.4869580000	0.2479320000
H	2.4643110000	-4.5093090000	1.5717300000
C	-2.5640960000	-3.1648080000	-1.0423170000
H	-3.0180480000	-3.6327170000	-0.1753680000
C	2.3859520000	-0.1702460000	-3.2475560000
H	1.7487500000	0.0380540000	-4.1009800000
C	-2.3941050000	1.8658550000	1.2200750000
C	-3.3469970000	-2.7406870000	-2.1084220000

H	-4.4227940000	-2.8768140000	-2.0714060000
C	-1.8173280000	1.6776580000	-2.1858540000
H	-2.2161870000	0.6691780000	-2.1685280000
C	4.0189590000	-0.6854120000	-1.0605350000
H	4.6594270000	-0.8710860000	-0.2050470000
C	-1.3729080000	-1.9964650000	-3.2622470000
H	-0.9015740000	-1.5444520000	-4.1291070000
C	3.9904520000	-1.5707540000	-2.1303910000
H	4.6148370000	-2.4579090000	-2.1097530000
C	-5.5791700000	3.3640740000	0.9188600000
H	-5.2663950000	3.2363350000	1.9552030000
H	-6.6699860000	3.3122210000	0.8623280000
H	-5.2605540000	4.3464400000	0.5628810000
C	-5.1574730000	2.2738570000	-2.0651020000
H	-4.7655400000	3.2411570000	-2.3866660000
H	-6.2407790000	2.2731370000	-2.2163530000
H	-4.7212940000	1.4960740000	-2.6945760000
C	-2.0507790000	2.5242260000	-1.1028830000
C	2.8765380000	4.4834950000	0.1620460000
H	2.0913840000	4.4478280000	-0.5965260000
H	3.3576740000	5.4648040000	0.1276240000
H	2.4263650000	4.3368500000	1.1441320000
C	2.7672870000	1.1449170000	1.2224400000
C	-5.2875730000	0.1547490000	0.3592040000
H	-4.6315910000	-0.5677540000	-0.1316500000
H	-6.3222550000	-0.0496100000	0.0702930000
H	-5.1790810000	0.0440360000	1.4379550000
C	-1.1787640000	-2.9968320000	-1.0765860000
C	-2.7533300000	-2.1622910000	-3.2253320000
H	-3.3640540000	-1.8470680000	-4.0650370000
C	3.2220100000	0.4602500000	-1.0751230000
C	5.6867140000	3.0885840000	1.0797110000
H	5.3142050000	2.9661790000	2.0964540000
H	6.2311680000	4.0338780000	1.0038580000
H	6.3753900000	2.2731750000	0.8469910000
C	-0.5879120000	-2.4026080000	-2.1909470000

H	0.4855670000	-2.2481270000	-2.2027700000
C	0.6992790000	-5.5004780000	-2.0518440000
H	-0.2950290000	-5.3934890000	-2.4898640000
H	1.0201710000	-6.5386450000	-2.1767040000
H	1.3922670000	-4.8572340000	-2.5981270000
C	-0.4375730000	-2.9508210000	1.2435400000
C	3.1797270000	-1.3118960000	-3.2306380000
H	3.1717970000	-1.9951130000	-4.0736850000
C	4.8350350000	3.1147360000	-2.0085060000
H	5.4000870000	2.2089720000	-2.2391370000
H	5.4972270000	3.9757070000	-2.1369360000
H	4.0137860000	3.2017800000	-2.7224110000
C	-1.0616460000	2.1185790000	-3.2644730000
H	-0.8939830000	1.4544690000	-4.1062840000

$(Me_3Ge\text{-}PhNCO)_3P_7$ – OOO

Charge = 0 Multiplicity = 1

P	-1.3052580000	1.3782370000	-0.7234930000
P	-0.5507840000	-1.8435240000	-0.6730220000
P	-0.5330760000	-1.2019360000	-2.8125590000
P	-0.7139640000	1.0109170000	-2.8448810000
P	-0.0020940000	0.0017980000	0.4198180000
P	1.8667520000	0.4202770000	-0.6921490000
P	1.2926060000	0.0612450000	-2.8208560000
O	-3.1341600000	-1.5289350000	-1.3742260000
O	2.8622260000	-2.0065230000	-1.3195020000
O	0.3143840000	3.4283670000	-1.3908410000
N	-0.3557590000	3.5392120000	0.7460140000
N	-2.9102640000	-2.0121750000	0.8238070000
N	3.2264650000	-1.4741220000	0.8507050000
C	-3.2593700000	2.7974970000	2.9181670000
H	-4.3402010000	2.8945780000	2.8984470000
C	-2.5173020000	3.1954920000	1.8138080000
H	-3.0068380000	3.6111830000	0.9393420000
C	-2.0478020000	-1.4849150000	3.0210160000
H	-2.5206890000	-0.5110690000	2.9525240000

C	-2.6251770000	2.2854720000	4.0447450000
H	-3.2062770000	1.9825300000	4.9093490000
C	3.9866140000	0.5580700000	1.9567800000
H	4.6350880000	0.7643300000	1.1116660000
C	-1.3382320000	-1.8484930000	4.1563760000
H	-1.2681490000	-1.1493850000	4.9835530000
C	-0.3565910000	2.9627660000	-0.3652400000
C	3.9713880000	1.4017940000	3.0596070000
H	4.6076660000	2.2810460000	3.0682420000
C	-0.4884370000	2.5724510000	2.9578850000
H	0.5924320000	2.4802300000	2.9620710000
C	-1.5292400000	-3.6195520000	2.0278220000
H	-1.6233730000	-4.3118390000	1.1977650000
C	2.3495660000	-0.0135080000	4.1239930000
H	1.7060350000	-0.2444190000	4.9669470000
C	-0.8234630000	-3.9763190000	3.1695280000
H	-0.3541470000	-4.9534700000	3.2235660000
C	-1.1235040000	3.0798120000	1.8212520000
C	-2.3976100000	-1.7975900000	-0.3176590000
C	3.1738280000	-0.5794720000	1.9274940000
C	3.1536710000	1.1215460000	4.1486710000
H	3.1494710000	1.7780710000	5.0123950000
C	-2.1421150000	-2.3656070000	1.9400660000
C	2.3595550000	-0.8631350000	3.0269890000
H	1.7251280000	-1.7427460000	3.0039110000
C	2.7548490000	-1.1896820000	-0.2935970000
C	-0.7231300000	-3.0938450000	4.2393670000
H	-0.1773780000	-3.3775770000	5.1330600000
C	-1.2382050000	2.1750090000	4.0557450000
H	-0.7303790000	1.7776780000	4.9288460000
Ge	1.4601600000	4.8970020000	-1.1745860000
Ge	-4.9832760000	-1.2856600000	-1.1711950000
Ge	3.6028990000	-3.7129560000	-1.0860550000
C	-5.7603310000	-2.9929210000	-0.6660890000
C	-5.4036760000	-0.7761930000	-2.9986010000
C	-5.2472930000	0.1697140000	0.0881260000

H	-5.4506680000	-3.7695960000	-1.3686280000
H	-6.8516120000	-2.9230220000	-0.6855140000
H	-5.4334200000	-3.2646030000	0.3375930000
H	-6.4654750000	-0.5327390000	-3.0908500000
H	-5.1715020000	-1.5912680000	-3.6869160000
H	-4.8183080000	0.0998920000	-3.2857140000
H	-5.2974900000	-0.2091780000	1.1088040000
H	-6.1699920000	0.7049020000	-0.1522330000
H	-4.4056490000	0.8626950000	0.0127620000
C	2.7554630000	4.4316360000	0.1938930000
C	0.3671220000	6.4589110000	-0.8019860000
C	2.2259800000	4.9201560000	-2.9601210000
H	3.0367020000	3.3822990000	0.0776710000
H	2.3275630000	4.5720820000	1.1861730000
H	3.6480390000	5.0541620000	0.0856150000
H	-0.1279330000	6.3417850000	0.1622300000
H	-0.3867120000	6.5865530000	-1.5817310000
H	0.9969210000	7.3527060000	-0.7782930000
H	2.7702280000	3.9923110000	-3.1481890000
H	2.9171740000	5.7600650000	-3.0689680000
H	1.4366810000	5.0185050000	-3.7081620000
C	3.3505520000	-4.3811440000	-2.8929660000
C	2.5152150000	-4.6490070000	0.2209970000
C	5.4759890000	-3.4980290000	-0.6181160000
H	2.7043730000	-5.7242820000	0.1583700000
H	1.4596080000	-4.4602600000	0.0130340000
H	2.7441810000	-4.2944770000	1.2256810000
H	5.5635090000	-3.0840920000	0.3865360000
H	5.9646780000	-2.8261460000	-1.3269880000
H	5.9798060000	-4.4679520000	-0.6565740000
H	3.8573200000	-3.7323820000	-3.6102070000
H	2.2871320000	-4.4086520000	-3.1393760000
H	3.7580800000	-5.3911870000	-2.9868020000

$(Et_3Ge\text{-}PhNCO)_3P_7$ – NNN

Charge = 0 Multiplicity = 1

Ge	0.0697020000	5.2317290000	0.0412610000
Ge	-4.5796240000	-2.6659510000	0.1652120000
Ge	4.8035070000	-2.4798410000	0.0158580000
P	-1.4863690000	1.1933370000	-1.4965350000
P	-0.3327940000	-1.9198110000	-1.4374800000
P	-0.4048810000	-1.3029730000	-3.5819040000
P	-0.8861340000	0.8619250000	-3.6236840000
P	-0.0006820000	-0.0088460000	-0.3807770000
P	1.7913520000	0.6279050000	-1.5086280000
P	1.2278850000	0.1971880000	-3.6263400000
O	-2.9676050000	-1.9079230000	-2.1287880000
O	3.1896450000	-1.5956160000	-2.2173420000
O	-0.1278130000	3.4418890000	-2.2348140000
N	-0.7765340000	3.4968690000	-0.0744570000
N	-2.6543860000	-2.4605040000	0.0345560000
N	3.4651900000	-1.0821550000	-0.0393580000
C	-3.6523110000	2.5123680000	2.0613800000
H	-4.7341260000	2.5947590000	2.0579250000
C	-2.9195020000	3.0323640000	1.0027480000
H	-3.4172660000	3.5210250000	0.1721170000
C	-1.4877610000	-1.9637060000	2.1248330000
H	-1.8885290000	-0.9566490000	2.0909800000
C	-3.0016240000	1.8987910000	3.1267120000
H	-3.5741150000	1.5031740000	3.9592090000
C	6.2832970000	-1.8378020000	-1.0994220000
H	5.8519080000	-1.5415340000	-2.0590050000
C	7.3822020000	-2.8800930000	-1.2969250000
H	6.6885910000	-0.9340220000	-0.6313620000
C	4.0372660000	-4.1643700000	-0.6237070000
C	2.5915230000	-4.4290960000	-0.2165110000
H	4.6960310000	-4.9612950000	-0.2560430000
H	4.1274770000	-4.1471910000	-1.7127140000
C	3.9589300000	1.0633550000	1.0209350000
H	4.5783410000	1.3190930000	0.1679390000
C	-0.6836950000	-2.3717050000	3.1822210000
H	-0.4751850000	-1.6813790000	3.9934670000

C	-0.6782250000	2.9027450000	-1.2901280000
C	3.8270260000	1.9416430000	2.0887340000
H	4.3513760000	2.8913490000	2.0710250000
C	-0.8789270000	2.3052390000	2.0565450000
H	0.2006550000	2.2027910000	2.0329890000
C	-1.2313320000	-4.1309640000	1.1055240000
H	-1.4519630000	-4.8088980000	0.2877230000
C	2.3708760000	0.3788390000	3.1936210000
H	1.7524150000	0.1054250000	4.0426160000
C	-0.4218690000	-4.5323200000	2.1596560000
H	-0.0051410000	-5.5338860000	2.1659640000
C	-0.7403210000	6.3939050000	-1.3121600000
H	-0.3246350000	6.1061090000	-2.2803290000
H	-0.3941880000	7.4117640000	-1.0948300000
C	-2.2645010000	6.3444430000	-1.3467480000
C	-0.3732290000	5.8893180000	1.8443380000
H	-1.3787430000	5.5378940000	2.0978950000
H	-0.4474820000	6.9795740000	1.7554170000
C	0.6165680000	5.5191380000	2.9459260000
C	-1.5278080000	2.9305760000	0.9929050000
C	-5.3906260000	-0.9267020000	-0.2235510000
H	-4.9176260000	-0.1910670000	0.4357160000
C	-6.9092250000	-0.9121700000	-0.0539740000
H	-5.1048720000	-0.6601620000	-1.2432660000
C	-2.2102840000	-2.0918270000	-1.1903920000
C	1.9897870000	4.9474050000	-0.2041310000
H	2.3461130000	4.3404940000	0.6344510000
C	2.7795290000	6.2501110000	-0.3145530000
H	2.1049850000	4.3394460000	-1.1048010000
C	3.2915180000	-0.1624070000	1.0314880000
C	3.0372260000	1.5993340000	3.1812080000
H	2.9455290000	2.2799840000	4.0213140000
C	-1.7732630000	-2.8450500000	1.0837330000
C	-5.1096840000	-4.1307630000	-1.0369100000
C	-5.6277150000	-3.7194410000	-2.4120990000
H	-5.8642060000	-4.7151970000	-0.4968640000

H	-4.2354730000	-4.7831350000	-1.1370860000
C	2.4909450000	-0.4975560000	2.1221470000
H	1.9549760000	-1.4404150000	2.1149630000
C	5.3787310000	-2.5631450000	1.8956970000
H	5.3973400000	-1.5414300000	2.2891690000
H	6.4247990000	-2.8916200000	1.8627780000
C	4.5760950000	-3.4810930000	2.8133240000
C	2.9207730000	-0.8818210000	-1.2656130000
C	-0.1510640000	-3.6556610000	3.2049970000
H	0.4715020000	-3.9738870000	4.0348210000
C	-4.8890400000	-3.2133050000	2.0310340000
H	-4.1118680000	-3.9336100000	2.3075900000
H	-5.8307030000	-3.7749400000	2.0196740000
C	-4.9656040000	-2.0862540000	3.0574640000
C	-1.6149670000	1.7980710000	3.1207730000
H	-1.0998440000	1.3202920000	3.9481240000
H	3.5378480000	-3.1518100000	2.9091780000
H	5.0034250000	-3.5055610000	3.8211960000
H	4.5593810000	-4.5100990000	2.4415170000
H	6.9996780000	-3.7778280000	-1.7920260000
H	7.8276330000	-3.1936240000	-0.3469080000
H	8.1934550000	-2.4891560000	-1.9190750000
H	1.9144600000	-3.6733620000	-0.6223860000
H	2.4632050000	-4.4392040000	0.8696470000
H	2.2547740000	-5.4008080000	-0.5937550000
H	-5.1768870000	-2.4766070000	4.0584350000
H	-5.7551790000	-1.3698070000	2.8131790000
H	-4.0277370000	-1.5289060000	3.1181080000
H	-4.8768030000	-3.1451580000	-2.9563220000
H	-6.5270190000	-3.1012830000	-2.3354090000
H	-5.8889910000	-4.5987210000	-3.0099010000
H	-7.4015270000	-1.6167720000	-0.7309990000
H	-7.3192440000	0.0793060000	-0.2715230000
H	-7.2164250000	-1.1728300000	0.9639680000
H	-2.6672180000	7.0418570000	-2.0879810000
H	-2.7073800000	6.6046450000	-0.3796840000

H	-2.6179220000	5.3455210000	-1.6178930000
H	3.8493180000	6.0563970000	-0.4427720000
H	2.6689950000	6.8777990000	0.5761970000
H	2.4555260000	6.8442670000	-1.1743880000
H	0.6869240000	4.4361960000	3.0786130000
H	0.3160690000	5.9455050000	3.9085740000
H	1.6231800000	5.8876990000	2.7260660000

$(Et_3Ge\text{-}PhNCO)_3P_7$ – OOO

Charge = 0 Multiplicity = 1

P	-1.1354820000	1.4779360000	-0.3729970000
P	-0.6661740000	-1.7821500000	-0.4288910000
P	-0.6047770000	-1.0863230000	-2.5471570000
P	-0.5964720000	1.1336250000	-2.5097400000
P	0.0414950000	-0.0352320000	0.7281370000
P	1.9261330000	0.2613660000	-0.3939660000
P	1.3223630000	0.0162640000	-2.5281930000
O	-3.2278750000	-1.3306660000	-1.1298610000
O	2.8014210000	-2.1760050000	-1.1394760000
O	0.5128190000	3.4888380000	-1.0609470000
N	-0.0010230000	3.5436380000	1.1445700000
N	-3.0365400000	-1.8891090000	1.0578820000
N	3.1867100000	-1.7753650000	1.0566310000
C	-2.7902340000	2.8251260000	3.4723860000
H	-3.8685970000	2.9412490000	3.5154500000
C	-2.1053510000	3.2223260000	2.3313230000
H	-2.6384060000	3.6543310000	1.4909440000
C	-2.1263220000	-1.4651040000	3.2608580000
H	-2.5315110000	-0.4598080000	3.2174950000
C	-2.1020540000	2.2911790000	4.5560590000
H	-2.6382640000	1.9892010000	5.4496010000
C	4.0408050000	0.1672130000	2.2531120000
H	4.6837030000	0.3954410000	1.4094200000
C	-1.4369860000	-1.9008780000	4.3832830000
H	-1.3134720000	-1.2254410000	5.2237110000
C	-0.0920750000	2.9978070000	-0.0000850000

C	4.0760250000	0.9499260000	3.3996670000
H	4.7481390000	1.8010800000	3.4446360000
C	-0.0260940000	2.5557600000	3.3525450000
H	1.0515280000	2.4456960000	3.2963280000
C	-1.7592890000	-3.6075660000	2.2183360000
H	-1.9024870000	-4.2727790000	1.3733120000
C	2.4151100000	-0.4560790000	4.4145780000
H	1.7748010000	-0.7066920000	5.2541860000
C	-1.0746320000	-4.0368140000	3.3478620000
H	-0.6734220000	-5.0449380000	3.3780690000
C	-0.7153120000	3.0847500000	2.2580040000
C	-2.5101100000	-1.6511240000	-0.0743000000
C	3.1838730000	-0.9354960000	2.1773290000
C	3.2645610000	0.6434510000	4.4863300000
H	3.3000700000	1.2517150000	5.3840650000
C	-2.2860710000	-2.3131400000	2.1617930000
C	2.3767110000	-1.2461470000	3.2747670000
H	1.7094980000	-2.0993280000	3.2155950000
C	2.7235250000	-1.4125210000	-0.0703270000
C	-0.9092220000	-3.1870480000	4.4359620000
H	-0.3802030000	-3.5272630000	5.3200050000
C	-0.7188070000	2.1578100000	4.4867460000
H	-0.1685680000	1.7414150000	5.3244210000
Ge	1.4572300000	5.1086230000	-0.9459420000
Ge	-5.1047140000	-1.2965080000	-1.0355160000
Ge	3.6855590000	-3.8321670000	-1.0593290000
C	-5.6809920000	-3.1188470000	-0.6139800000
C	-5.4475460000	-0.7435130000	-2.8819260000
C	-5.6618280000	0.0543090000	0.2624350000
H	-5.1330580000	-3.7944060000	-1.2791810000
C	-7.1876780000	-3.3316750000	-0.7512460000
H	-5.3439130000	-3.3315790000	0.4035050000
C	-6.8689580000	-0.2470750000	-3.1419180000
H	-5.2018860000	-1.5848680000	-3.5377390000
H	-4.7181220000	0.0414530000	-3.1066790000
H	-5.3435310000	-0.3018040000	1.2451600000

H	-6.7591160000	0.0565520000	0.2606390000
C	-5.1163560000	1.4513920000	-0.0196950000
C	2.9754260000	4.8860790000	0.2642940000
C	0.1850760000	6.4899970000	-0.3997860000
C	1.9883820000	5.2453480000	-2.8222290000
C	3.9480660000	3.7832850000	-0.1441200000
H	2.5602000000	4.6983730000	1.2574540000
H	3.4823290000	5.8581540000	0.3079720000
H	-0.0019800000	6.3497120000	0.6676500000
C	-1.1204090000	6.4781250000	-1.1893970000
H	0.6961330000	7.4540290000	-0.5118940000
H	2.5317450000	4.3295720000	-3.0756160000
C	2.8340510000	6.4813800000	-3.1214520000
H	1.0772860000	5.2379120000	-3.4285680000
C	3.4791820000	-4.3397130000	-2.9361550000
C	2.7223700000	-5.0123250000	0.1643610000
C	5.5425920000	-3.4886850000	-0.5516870000
H	3.3016720000	-5.9424650000	0.2189240000
C	1.2773770000	-5.2924720000	-0.2380790000
H	2.7742340000	-4.5473550000	1.1519380000
H	5.5475060000	-3.2664580000	0.5182760000
C	6.2067000000	-2.3679540000	-1.3460240000
H	6.0860950000	-4.4319380000	-0.6861910000
H	3.9661030000	-3.5720400000	-3.5455950000
H	2.4117860000	-4.2866770000	-3.1726430000
C	4.0402170000	-5.7244280000	-3.2529090000
H	2.2954710000	7.4075210000	-2.8958700000
H	3.1201440000	6.5241360000	-4.1768110000
H	3.7589310000	6.4918080000	-2.5356800000
H	4.7811140000	3.7133180000	0.5630890000
H	4.3777170000	3.9654330000	-1.1344910000
H	3.4565170000	2.8066380000	-0.1706680000
H	-1.7947540000	7.2709570000	-0.8509480000
H	-1.6480780000	5.5272020000	-1.0731990000
H	-0.9513320000	6.6281070000	-2.2601330000
H	-7.7545250000	-2.6639250000	-0.0949210000

H	-7.4666750000	-4.3560660000	-0.4856060000
H	-7.5331660000	-3.1583530000	-1.7748270000
H	-5.4660220000	2.1682330000	0.7305750000
H	-5.4360200000	1.8233910000	-0.9986260000
H	-4.0229050000	1.4644720000	-0.0053500000
H	-6.9877350000	0.0899600000	-4.1763380000
H	-7.1282520000	0.5969660000	-2.4951090000
H	-7.6155510000	-1.0282160000	-2.9698160000
H	3.9017430000	-5.9798790000	-4.3079490000
H	3.5489760000	-6.5060970000	-2.6644490000
H	5.1133360000	-5.7865430000	-3.0450010000
H	1.2129660000	-5.7587620000	-1.2264930000
H	0.6866670000	-4.3723840000	-0.2655460000
H	0.7966010000	-5.9716810000	0.4735980000
H	6.2192530000	-2.5808500000	-2.4193290000
H	7.2440570000	-2.2199470000	-1.0300970000
H	5.6832670000	-1.4175130000	-1.2089650000

$(Me_3Ge\text{-}TsNCO)_3P_7$ – NNN

Charge = 0 Multiplicity = 1

S	-2.9800130000	4.3341160000	0.8247670000
S	4.0505680000	0.4648140000	-1.3367610000
P	-0.0140430000	0.0429270000	-0.3689690000
P	-1.3456130000	-1.3549170000	0.7297630000
P	-0.7391530000	1.9024110000	0.5769650000
P	1.7190830000	-0.1973720000	1.0010840000
S	-1.2511070000	-3.7395450000	-1.6400670000
P	-1.0070310000	-0.8321820000	2.8726810000
P	-0.9964100000	1.3914890000	2.7435100000
P	0.8995320000	0.2720940000	3.0251800000
O	2.4089810000	2.3799630000	1.5054190000
O	-2.8662020000	0.9713180000	-0.8239200000
O	0.4520000000	-3.1427950000	1.7036350000
O	-1.3771850000	-2.3091350000	-1.8463230000
O	2.8669010000	-0.3609530000	-1.4911450000
O	4.5592360000	1.2443460000	-2.4472860000

O	-1.9865450000	4.3247830000	1.8814100000
O	-0.5580060000	-4.5752300000	-2.5988510000
O	-4.2453190000	5.0267570000	1.0025630000
N	-0.4649210000	-3.9559470000	-0.1660010000
N	3.7357350000	1.5524950000	-0.0930370000
N	-3.4397560000	2.7618050000	0.4353590000
C	-2.5239130000	1.8234860000	-0.0374040000
C	2.6568270000	1.4439260000	0.7717840000
C	-0.2950210000	-2.9455420000	0.7649150000
C	-2.9825110000	5.2318760000	-1.7646730000
H	-4.0533220000	5.0671000000	-1.7390700000
C	-2.2020680000	4.9513330000	-0.6478580000
C	-2.3731180000	5.7378620000	-2.8998440000
H	-2.9767120000	5.9594580000	-3.7746030000
C	5.3682780000	-0.5628850000	-0.7348760000
C	-2.8819640000	-4.4044510000	-1.4088000000
C	-0.9956780000	5.9752230000	-2.9355150000
C	-0.2427460000	5.6998390000	-1.7951670000
H	0.8263460000	5.8879730000	-1.8004270000
C	-3.8048210000	-3.6850240000	-0.6546840000
H	-3.5170850000	-2.7402250000	-0.2035110000
C	5.1104100000	-1.4585670000	0.2995310000
C	-0.8340430000	5.1867690000	-0.6483460000
H	-0.2522580000	4.9686220000	0.2388690000
C	-3.2287020000	-5.5961290000	-2.0277030000
H	-2.5000900000	-6.1177100000	-2.6372120000
C	-0.3439800000	6.4936790000	-4.1827770000
H	-0.1446590000	5.6730340000	-4.8805170000
H	0.6093460000	6.9786250000	-3.9631120000
H	-0.9852980000	7.2127830000	-4.6982420000
C	-5.0833810000	-4.1927670000	-0.5030960000
H	-5.8073880000	-3.6369290000	0.0851620000
C	7.4033310000	-2.2349640000	0.1581050000
C	-5.4615020000	-5.3981170000	-1.1038650000
C	-4.5196740000	-6.0850190000	-1.8678290000
H	-4.8001540000	-7.0149940000	-2.3526330000

C	-6.8585450000	-5.9201600000	-0.9423620000
H	-7.1410660000	-5.9696080000	0.1131690000
H	-6.9644430000	-6.9188800000	-1.3699310000
H	-7.5788270000	-5.2632700000	-1.4405890000
C	8.4947010000	-3.1391730000	0.6492660000
H	8.7134170000	-2.9509120000	1.7049050000
H	9.4168090000	-2.9975660000	0.0827490000
H	8.2012410000	-4.1896410000	0.5616340000
H	4.1189730000	-1.5083670000	0.7406100000
C	6.6128010000	-0.5023860000	-1.3428540000
H	6.7765290000	0.1833540000	-2.1659220000
C	7.6233720000	-1.3415210000	-0.8882860000
H	8.5992660000	-1.3030410000	-1.3621770000
C	6.1322010000	-2.2801270000	0.7416050000
H	5.9380250000	-2.9788260000	1.5497860000
Ge	-5.3335860000	2.2763070000	0.5241150000
Ge	0.5207470000	-5.5939070000	0.3028980000
Ge	4.7483480000	3.2213570000	0.1517570000
C	-5.4076510000	0.3324850000	0.4425600000
C	-6.2229080000	3.1331010000	-0.9769330000
C	-5.9682840000	2.8541470000	2.2686580000
C	-0.0309430000	-7.0141360000	-0.9093040000
C	-0.0435050000	-6.0776510000	2.1009230000
C	2.3968880000	-5.1462400000	0.0845950000
C	6.3980370000	3.0919080000	-0.8738660000
C	5.1995030000	3.3250030000	2.0405650000
C	3.5873170000	4.6237470000	-0.5233690000
H	-1.1042770000	-7.1997570000	-0.8358300000
H	0.4914990000	-7.9226250000	-0.5930730000
H	0.2280020000	-6.7862790000	-1.9418470000
H	3.0087440000	-6.0383090000	0.2439730000
H	2.6817130000	-4.3763770000	0.8016320000
H	2.5697180000	-4.7775280000	-0.9284640000
H	0.3904380000	-5.4103010000	2.8431550000
H	0.2652000000	-7.1075600000	2.3021350000
H	-1.1327290000	-6.0280540000	2.1715620000

H	-5.1797060000	-0.0346360000	-0.5567460000
H	-6.4186770000	0.0292740000	0.7327200000
H	-4.6977130000	-0.1089120000	1.1454190000
H	-5.2844070000	2.5055690000	3.0461000000
H	-6.9506480000	2.4076610000	2.4488270000
H	-6.0399600000	3.9390630000	2.3210060000
H	-7.2633090000	2.8000000000	-1.0231720000
H	-5.7302780000	2.8615280000	-1.9127770000
H	-6.2078530000	4.2167320000	-0.8494490000
H	3.3453610000	4.4226980000	-1.5691460000
H	4.0957950000	5.5892840000	-0.4564530000
H	2.6709530000	4.6550570000	0.0663760000
H	6.9549480000	4.0177180000	-0.6980250000
H	6.2024980000	2.9841440000	-1.9394160000
H	7.0130930000	2.2579160000	-0.5302120000
H	5.9827370000	4.0766650000	2.1745790000
H	5.5880050000	2.3626910000	2.3823380000
H	4.3286940000	3.5881680000	2.6381310000

$(Me_3Ge\text{-}TsNCO)_3P_7$ – OOO

Charge = 0 Multiplicity = 1

Ge	-2.7645200000	-3.1275280000	-2.0302290000
Ge	-1.7819170000	4.4749840000	1.3193370000
Ge	5.2284860000	-0.5124440000	0.9672990000
S	-4.5705010000	-0.6982830000	1.4677200000
S	1.3544990000	3.4694580000	-1.9335440000
P	0.3964660000	-0.0607940000	-0.4794330000
P	0.9342800000	-1.8756750000	0.6690580000
P	-1.5139130000	0.3368090000	0.5513470000
P	1.5115820000	1.4411240000	0.7518820000
S	2.8496600000	-3.5097470000	-1.5378350000
P	0.8269870000	-1.2058160000	2.7901120000
P	-1.0985760000	-0.0918330000	2.7190690000
P	0.8343510000	0.9999880000	2.8441940000
O	-0.3715580000	3.2153640000	1.4349230000
O	-1.9356150000	-1.7274850000	-1.0527880000

O	3.4123350000	-0.9962200000	1.2500560000
O	1.4551310000	-3.1530550000	-1.7893550000
O	2.2284060000	2.3130950000	-1.7387250000
O	0.5165720000	3.5584150000	-3.1116600000
O	-3.9802050000	0.6139350000	1.7466830000
O	3.7948960000	-3.5643630000	-2.6327840000
O	-4.8467720000	-1.6117620000	2.5582630000
N	3.5165610000	-2.4837220000	-0.4119300000
N	0.3709710000	3.6950960000	-0.6196450000
N	-3.6870920000	-1.5076440000	0.3291000000
C	-2.5132630000	-1.1265640000	-0.0557280000
C	0.3997430000	2.9358270000	0.4238900000
C	2.8118430000	-1.8096000000	0.4326600000
C	-1.4614320000	-3.3394930000	-3.4425080000
H	-1.4717820000	-2.4669960000	-4.0990270000
H	-1.7013020000	-4.2258760000	-4.0365780000
H	-0.4609660000	-3.4485140000	-3.0192140000
C	-0.9498870000	6.2268570000	1.2267180000
H	-0.2766240000	6.3688280000	2.0746440000
H	-1.7207620000	7.0017590000	1.2622460000
H	-0.3852260000	6.3221680000	0.2988580000
C	-7.0812360000	-1.3873230000	0.6328510000
H	-6.9439490000	-2.2668580000	1.2516000000
C	-6.0779870000	-0.4292990000	0.5688120000
C	-4.4732530000	-2.4545520000	-2.6642060000
H	-5.1884630000	-2.3661640000	-1.8468710000
H	-4.8652990000	-3.1378210000	-3.4233690000
H	-4.3367360000	-1.4741560000	-3.1262470000
C	-2.8648650000	-4.6169880000	-0.7909570000
H	-1.8600440000	-4.8937080000	-0.4656190000
H	-3.3208270000	-5.4789370000	-1.2857190000
H	-3.4657580000	-4.3404280000	0.0761350000
C	-8.2506420000	-1.1843650000	-0.0851250000
H	-9.0406830000	-1.9278600000	-0.0386680000
C	2.3648390000	4.9279840000	-1.8503320000
C	2.8649160000	-5.0796210000	-0.7055180000

C	-8.4312760000	-0.0385240000	-0.8622520000
C	-2.8665500000	3.9536840000	-0.1996910000
H	-2.3449800000	4.1411120000	-1.1380660000
H	-3.8063320000	4.5130570000	-0.1792750000
H	-3.0836900000	2.8868320000	-0.1091490000
C	-7.4058460000	0.9083680000	-0.9024220000
H	-7.5321950000	1.8067640000	-1.4990020000
C	1.8032490000	-5.4199310000	0.1254860000
H	0.9798340000	-4.7257110000	0.2580650000
C	3.5079020000	4.9222190000	-1.0590430000
C	-6.2292350000	0.7222510000	-0.1923400000
H	-5.4391580000	1.4643590000	-0.2130960000
C	6.3044710000	-2.0729300000	1.3829510000
H	6.0312950000	-2.4684250000	2.3634870000
H	7.3617480000	-1.7938770000	1.4034860000
H	6.1476740000	-2.8424920000	0.6272650000
C	5.3417830000	0.8763110000	2.3199520000
H	4.6232960000	1.6666560000	2.0933360000
H	6.3469470000	1.3058470000	2.3393300000
H	5.1166440000	0.4696080000	3.3079200000
C	3.9345410000	-5.9425040000	-0.8979230000
H	4.7391030000	-5.6564180000	-1.5658180000
C	5.3434900000	0.1620110000	-0.8445720000
H	5.3160120000	-0.6596130000	-1.5603790000
H	6.2797590000	0.7155130000	-0.9620850000
H	4.5091660000	0.8390210000	-1.0456580000
C	-9.7128110000	0.1872540000	-1.6090330000
H	-10.1654600000	-0.7573540000	-1.9191000000
H	-9.5530660000	0.7999460000	-2.4991150000
H	-10.4406740000	0.7082490000	-0.9772800000
C	-2.6339690000	4.0903640000	3.0170930000
H	-3.0572030000	3.0834010000	2.9966680000
H	-3.4398860000	4.8051230000	3.2043710000
H	-1.9109270000	4.1585430000	3.8323420000
C	1.8266090000	-6.6429440000	0.7768320000
H	1.0026950000	-6.9137640000	1.4302610000

C	3.9402060000	7.2161580000	-1.7123760000
C	2.8891860000	-7.5337920000	0.6035240000
C	3.9371770000	-7.1652470000	-0.2408170000
H	4.7688170000	-7.8474370000	-0.3886270000
C	2.8845020000	-8.8689730000	1.2877650000
H	2.4431850000	-8.8031550000	2.2852500000
H	3.8949690000	-9.2714230000	1.3855710000
H	2.2941690000	-9.5935760000	0.7162200000
C	4.7876330000	8.4511000000	-1.6214090000
H	4.6821330000	8.9236500000	-0.6391070000
H	4.5044540000	9.1864190000	-2.3769280000
H	5.8467860000	8.2148760000	-1.7559460000
H	3.7837130000	4.0241170000	-0.5170470000
C	1.9988160000	6.0504220000	-2.5778150000
H	1.1155370000	6.0164490000	-3.2054730000
C	2.7925350000	7.1876620000	-2.5038940000
H	2.5179900000	8.0672870000	-3.0779820000
C	4.2857650000	6.0664290000	-0.9957080000
H	5.1839830000	6.0676880000	-0.3852690000

$(Et_3Ge\text{-}TsNCO)_3P_7$ – NNN

Charge = 0 Multiplicity = 1

S	-4.4411900000	-2.1593930000	0.8799000000
S	-0.1695050000	3.8541930000	-1.3821690000
P	0.3018890000	-0.0001320000	-0.3338880000
P	1.5461380000	-1.5212090000	0.6930600000
P	-1.6095980000	-0.4144160000	0.6600030000
P	0.7604050000	1.6888600000	1.0544710000
S	3.8223170000	-1.5439850000	-1.7735450000
P	1.1049880000	-1.1780690000	2.8548930000
P	-1.0951420000	-0.8178480000	2.8018820000
P	0.3213660000	0.8683890000	3.0955230000
O	-1.4925680000	2.8246290000	1.9764090000
O	-1.1029270000	-2.6525720000	-0.7600910000
O	3.5203410000	0.0605760000	1.6655240000
O	2.3896300000	-1.7337020000	-1.9028020000

O	0.9163860000	2.8901740000	-1.4058590000
O	-0.9537390000	4.1224820000	-2.5687260000
O	-4.1399250000	-0.9611460000	1.6426070000
O	4.5917630000	-0.9122560000	-2.8236720000
O	-5.2747190000	-3.2088480000	1.4373770000
N	4.0889930000	-0.6390090000	-0.3776340000
N	-1.2397640000	3.3921970000	-0.1758340000
N	-2.9985680000	-2.9102130000	0.4555130000
C	-1.8955590000	-2.1753620000	0.0180230000
C	-0.8229040000	2.7209770000	0.9653630000
C	3.2051840000	-0.5848250000	0.6821280000
C	-6.3138650000	-2.3164700000	-1.1086610000
H	-6.7396660000	-3.1160940000	-0.5143250000
C	-5.1751520000	-1.6610120000	-0.6637040000
C	-6.8923430000	-1.9225040000	-2.3087760000
H	-7.7853190000	-2.4304050000	-2.6597110000
C	0.4929120000	5.3971870000	-0.7993770000
C	4.5541370000	-3.1266400000	-1.4345950000
C	-6.3466950000	-0.8895030000	-3.0687130000
C	-5.2035700000	-0.2418200000	-2.5894210000
H	-4.7652120000	0.5687090000	-3.1635020000
C	3.8553780000	-4.0486070000	-0.6611710000
H	2.8710590000	-3.7995760000	-0.2769210000
C	1.4384650000	5.3844000000	0.2225840000
C	-4.6207840000	-0.6108040000	-1.3893050000
H	-3.7447210000	-0.0896440000	-1.0172000000
C	5.7953930000	-3.4318780000	-1.9732060000
H	6.2976530000	-2.7108400000	-2.6077640000
C	-6.9744350000	-0.4617400000	-4.3620440000
H	-7.7564690000	-1.1555770000	-4.6759920000
H	-6.2295530000	-0.4021770000	-5.1604070000
H	-7.4256640000	0.5311150000	-4.2648520000
C	4.4336300000	-5.2810890000	-0.4070780000
H	3.8938160000	-6.0059000000	0.1950760000
C	1.5177860000	7.8069450000	0.1408600000
C	5.6902900000	-5.6136920000	-0.9224360000

C	6.3544640000	-4.6762730000	-1.7122800000
H	7.3212810000	-4.9256530000	-2.1385060000
C	6.3035710000	-6.9503760000	-0.6266330000
H	6.6228560000	-7.0073960000	0.4192910000
H	7.1778480000	-7.1363220000	-1.2532620000
H	5.5868550000	-7.7594680000	-0.7918190000
C	2.0790890000	9.1002470000	0.6531140000
H	1.9339890000	9.1904350000	1.7336700000
H	1.6055080000	9.9592570000	0.1744190000
H	3.1555670000	9.1600910000	0.4643260000
H	1.7780850000	4.4415620000	0.6408890000
C	0.0649000000	6.5867500000	-1.3687250000
H	-0.6497260000	6.5665710000	-2.1836340000
C	0.5826590000	7.7853160000	-0.8923160000
H	0.2556450000	8.7201360000	-1.3368380000
C	1.9374690000	6.5890230000	0.6869980000
H	2.6722010000	6.5861410000	1.4866450000
Ge	-2.9740510000	-4.8853870000	0.3577620000
Ge	5.6503580000	0.5404210000	-0.0649970000
Ge	-3.0461090000	4.1768670000	0.0931680000
C	-1.2088030000	-5.5322480000	-0.1901120000
C	-4.3443050000	-5.3617050000	-0.9633730000
C	-3.3349200000	-5.4759400000	2.1909960000
C	6.8828770000	0.4119340000	-1.5870520000
C	6.5405430000	-0.1413170000	1.5424940000
C	4.8921370000	2.3467740000	0.0441520000
C	-3.7167220000	4.8290210000	-1.6322820000
C	-2.7628660000	5.6754100000	1.3274500000
C	-4.1672160000	2.7034990000	0.7407990000
H	7.1786300000	-0.6294220000	-1.7390810000
C	8.1135290000	1.2857550000	-1.3428050000
H	6.3516240000	0.7177930000	-2.4894250000
H	5.4072460000	2.9455180000	-0.7153730000
C	4.9863700000	3.0086700000	1.4148250000
H	3.8483830000	2.2742690000	-0.2768430000
H	5.9629700000	0.1792620000	2.4107240000

H	7.5123170000	0.3645900000	1.5926090000
C	6.7296990000	-1.6551770000	1.5436510000
H	-0.9671540000	-5.1171850000	-1.1695720000
H	-1.3671130000	-6.6107940000	-0.3234990000
C	-0.0755510000	-5.2884270000	0.7997880000
H	-2.6337750000	-4.9475750000	2.8458460000
C	-3.1981370000	-6.9879040000	2.3637670000
H	-4.3344550000	-5.1335270000	2.4612390000
C	-4.1671760000	-6.7564930000	-1.5619520000
H	-4.3118360000	-4.6030910000	-1.7517080000
H	-5.3177360000	-5.2691660000	-0.4737830000
H	-3.5819300000	1.7824510000	0.6671640000
H	-5.0012680000	2.6055130000	0.0373100000
C	-4.6838010000	2.8704980000	2.1663520000
H	-4.6098760000	5.4052040000	-1.3546510000
C	-4.0796380000	3.7566710000	-2.6539840000
H	-3.0069990000	5.5407880000	-2.0591380000
C	-3.9203180000	6.6709640000	1.3661200000
H	-1.8372510000	6.1756090000	1.0234640000
H	-2.5779670000	5.2457670000	2.3147360000
H	4.5687870000	4.0210170000	1.3866570000
H	6.0218900000	3.0960600000	1.7590800000
H	4.4308450000	2.4381880000	2.1619830000
H	7.8447020000	2.3327250000	-1.1666730000
H	8.7820980000	1.2701410000	-2.2091740000
H	8.6960100000	0.9481720000	-0.4799030000
H	7.2665370000	-1.9847090000	2.4388590000
H	7.3005460000	-1.9996650000	0.6754380000
H	5.7690430000	-2.1777490000	1.5295160000
H	-5.2634090000	1.9917360000	2.4635430000
H	-5.3321310000	3.7464600000	2.2710250000
H	-3.8567080000	2.9723410000	2.8715350000
H	-4.8597570000	6.1957480000	1.6655260000
H	-4.0867180000	7.1423040000	0.3928280000
H	-3.7243860000	7.4728880000	2.0850990000
H	-4.5407280000	4.2022200000	-3.5415700000

H	-4.7934640000	3.0347900000	-2.2448890000
H	-3.1893830000	3.2166830000	-2.9818790000
H	-3.2155420000	-6.8514450000	-2.0923950000
H	-4.9625230000	-6.9775270000	-2.2806900000
H	-4.1968100000	-7.5395820000	-0.7980540000
H	-2.1983390000	-7.3479730000	2.1009280000
H	-3.9170270000	-7.5344910000	1.7452530000
H	-3.3834100000	-7.2800250000	3.4021600000
H	0.8307580000	-5.8180880000	0.4866280000
H	-0.3237000000	-5.6360110000	1.8073790000
H	0.1770720000	-4.2276070000	0.8589590000

$(Et_3Ge\text{-}TsNCO)_3P_7$ – OOO

Charge = 0 Multiplicity = 1

Ge	0.5983640000	4.6091210000	-1.2665360000
Ge	4.0079010000	-2.9360600000	0.9291770000
Ge	-4.8700310000	-2.2012040000	0.7810890000
S	3.6852450000	2.9693140000	1.7284810000
S	0.7979460000	-3.4620760000	-2.3262160000
P	-0.2330150000	0.0497010000	-0.5355280000
P	-1.7334760000	1.0711520000	0.7384030000
P	1.5553580000	0.6224750000	0.6316680000
P	-0.3809650000	-1.9588310000	0.4297030000
S	-4.1195500000	1.5815180000	-1.5558230000
P	-1.3047970000	0.3046460000	2.7840910000
P	0.9187520000	0.4456360000	2.7829270000
P	-0.0907310000	-1.5279260000	2.6090920000
O	2.1618010000	-2.5000490000	1.0755030000
O	0.7339950000	2.8137870000	-0.6301460000
O	-3.4063710000	-1.0201260000	1.1095580000
O	-2.7473100000	2.0666940000	-1.6835400000
O	-0.4383690000	-2.6917600000	-2.2171340000
O	1.6393370000	-3.3339740000	-3.4985390000
O	3.6126020000	1.5673170000	2.1470530000
O	-4.8681570000	1.1921950000	-2.7320330000
O	3.8049590000	4.0172850000	2.7205570000

N	-4.1806090000	0.2856990000	-0.5211110000
N	1.7758950000	-3.1913940000	-1.0133020000
N	2.4103580000	3.3533210000	0.7501770000
C	1.5927320000	2.4676840000	0.2774630000
C	1.3557530000	-2.6128660000	0.0628000000
C	-3.2644660000	0.0270640000	0.3519060000
C	-0.5233760000	4.2608810000	-2.8216120000
H	-0.0020030000	3.4890780000	-3.3984930000
C	-0.7870300000	5.4887410000	-3.6918820000
H	-1.4538120000	3.8010120000	-2.4800400000
C	4.0995790000	-4.8835780000	0.7995300000
C	3.3698940000	-5.6082650000	1.9270030000
H	5.1634670000	-5.1502560000	0.7917340000
H	3.6955320000	-5.1632290000	-0.1767790000
C	5.8704720000	4.2209880000	0.6438060000
H	5.6797860000	4.9941210000	1.3794850000
C	5.0468640000	3.1073470000	0.5946410000
C	2.3804560000	5.2590040000	-1.7701030000
C	2.9711580000	6.3065200000	-0.8329150000
H	2.2941250000	5.6505450000	-2.7901140000
H	3.0331220000	4.3825140000	-1.8269920000
C	-0.2355600000	5.5201410000	0.2505580000
H	-0.9441180000	4.8051210000	0.6813830000
C	-0.9372350000	6.8322010000	-0.0948570000
H	0.5468520000	5.6760850000	0.9984970000
C	6.9310930000	4.3114630000	-0.2492270000
H	7.5827580000	5.1792690000	-0.2152500000
C	0.3886860000	-5.1783530000	-2.1136710000
C	-5.0524730000	2.8188410000	-0.6850830000
C	7.1731440000	3.3084310000	-1.1871020000
C	4.7353770000	-1.9348860000	-0.5864670000
C	5.0777000000	-2.7559270000	-1.8250770000
H	5.6168830000	-1.4068230000	-0.2035390000
H	3.9903730000	-1.1674130000	-0.8204620000
C	6.3243910000	2.1969530000	-1.2105830000
H	6.4982210000	1.4052850000	-1.9333970000

C	-4.4125690000	3.6171570000	0.2567760000
H	-3.3534930000	3.4793420000	0.4486750000
C	-0.6333810000	-5.5284540000	-1.2383700000
C	5.2670420000	2.0860580000	-0.3232380000
H	4.6170590000	1.2171590000	-0.3335310000
C	-6.5221340000	-1.2108790000	1.1165050000
C	-6.4703230000	-0.2933850000	2.3347750000
H	-7.3101500000	-1.9646790000	1.2372300000
H	-6.7503380000	-0.6440910000	0.2110470000
C	-4.5108740000	-3.5084530000	2.1914930000
C	-3.2671900000	-4.3641400000	1.9731140000
H	-5.4054320000	-4.1379560000	2.2720340000
H	-4.4398290000	-2.9565920000	3.1345200000
C	-6.4054630000	2.9679300000	-0.9548370000
H	-6.8724630000	2.3435400000	-1.7081130000
C	-4.6272510000	-2.8962190000	-1.0260130000
H	-4.8755810000	-2.0902100000	-1.7200700000
C	-5.4721500000	-4.1402460000	-1.2997060000
H	-3.5612700000	-3.1058730000	-1.1613410000
C	8.3338580000	3.3992400000	-2.1334770000
H	8.6977750000	4.4248230000	-2.2222460000
H	8.0621380000	3.0444510000	-3.1309110000
H	9.1674020000	2.7807670000	-1.7832520000
C	4.5643230000	-2.2285830000	2.6596410000
H	4.3769620000	-1.1499330000	2.6473310000
C	6.0274590000	-2.5236700000	2.9851780000
H	3.9025530000	-2.6528860000	3.4212750000
C	-5.1500710000	4.5709300000	0.9404750000
H	-4.6574340000	5.1956240000	1.6796210000
C	-0.2396080000	-7.8642510000	-1.7538550000
C	-6.5141630000	4.7450310000	0.6913600000
C	-7.1262970000	3.9320370000	-0.2630710000
H	-8.1845310000	4.0573870000	-0.4712290000
C	-7.2920640000	5.8052800000	1.4137110000
H	-6.9667090000	5.8992340000	2.4526710000
H	-8.3625140000	5.5894850000	1.4077630000

H	-7.1488900000	6.7811760000	0.9369980000
C	-0.6015520000	-9.3099030000	-1.5800340000
H	-0.8894010000	-9.5272280000	-0.5484920000
H	0.2298050000	-9.9649200000	-1.8489440000
H	-1.4508840000	-9.5746980000	-2.2193050000
H	-1.1770090000	-4.7550930000	-0.7051230000
C	1.0990440000	-6.1424120000	-2.8133420000
H	1.8807850000	-5.8372240000	-3.4996980000
C	0.7769700000	-7.4804840000	-2.6284640000
H	1.3259500000	-8.2409550000	-3.1755070000
C	-0.9358940000	-6.8689580000	-1.0620650000
H	-1.7300770000	-7.1505820000	-0.3768460000
H	6.7054670000	-2.0946960000	2.2401010000
H	6.2283270000	-3.5991860000	3.0308050000
H	6.3082960000	-2.0993480000	3.9534960000
H	3.4517780000	-6.6939360000	1.8164460000
H	2.3050900000	-5.3596960000	1.9384320000
H	3.7767330000	-5.3474120000	2.9087690000
H	5.5103650000	-2.1218560000	-2.6055520000
H	4.1848840000	-3.2248780000	-2.2431660000
H	5.8075750000	-3.5413660000	-1.6045550000
H	-1.3512580000	6.2585760000	-3.1573370000
H	-1.3717450000	5.2174550000	-4.5758900000
H	0.1392600000	5.9512180000	-4.0483110000
H	3.9738600000	6.6016630000	-1.1578520000
H	3.0521150000	5.9199320000	0.1855400000
H	2.3596710000	7.2136620000	-0.7998800000
H	-1.7753430000	6.6757360000	-0.7799100000
H	-0.2589050000	7.5523700000	-0.5628850000
H	-1.3378680000	7.3088960000	0.8053630000
H	-5.3052230000	-4.5050060000	-2.3174510000
H	-6.5431890000	-3.9351360000	-1.2033980000
H	-5.2330740000	-4.9624010000	-0.6172590000
H	-6.2323690000	-0.8413760000	3.2514290000
H	-7.4321550000	0.2044390000	2.4914320000
H	-5.7159600000	0.4882220000	2.2121630000

H	-2.3659760000	-3.7487770000	1.9137470000
H	-3.3328160000	-4.9367510000	1.0423550000
H	-3.1263610000	-5.0784420000	2.7903220000

($^{n}Bu_3Sn$-TsNCO)$_3P_7$ – NNN

Charge = 0 Multiplicity = 1

S	3.7915920000	-2.7736010000	-1.6565320000
S	0.8007350000	3.6762160000	1.7074070000
P	-0.3742860000	0.1502310000	0.1781120000
P	-1.8511450000	-1.0399570000	-0.9639940000
P	1.4221070000	-0.4493910000	-0.9488990000
P	-0.5983900000	2.0532480000	-0.9686290000
S	-4.1484370000	-1.2707780000	1.4711930000
P	-1.4495550000	-0.4835600000	-3.0841280000
P	0.7774490000	-0.4788310000	-3.1027010000
P	-0.3606220000	1.4324730000	-3.1097550000
O	1.8244810000	2.8642120000	-1.8411860000
O	0.5141550000	-2.7037630000	0.2397900000
O	-3.6477440000	0.9142900000	-1.5909080000
O	-2.7252940000	-1.4345360000	1.7053130000
O	-0.4074160000	2.8675210000	1.7004260000
O	1.7481360000	3.5919940000	2.8004360000
O	3.5796000000	-1.4913580000	-2.3114280000
O	-5.0323230000	-0.7820000000	2.5113410000
O	4.1627640000	-3.9442730000	-2.4243400000
N	-4.3475480000	-0.2105080000	0.1901060000
N	1.6451960000	3.3695510000	0.3048990000
N	2.4045110000	-3.1572080000	-0.8176370000
C	1.4100650000	-2.2769410000	-0.4783680000
C	1.1304180000	2.8022540000	-0.8303650000
C	-3.4063540000	0.0370670000	-0.7732490000
C	6.0756380000	-3.4237240000	-0.2894500000
H	6.1656510000	-4.2339810000	-1.0040910000
C	5.0042140000	-2.5490280000	-0.3771630000
C	7.0180480000	-3.2320780000	0.7147140000
H	7.8620100000	-3.9108860000	0.7883580000

C	0.3203130000	5.3769460000	1.5232060000
C	-4.7931860000	-2.8250690000	0.8996510000
C	6.8992840000	-2.1842020000	1.6253120000
C	5.8120210000	-1.3111980000	1.5021670000
H	5.7071420000	-0.4831390000	2.1966560000
C	-3.9591230000	-3.6986070000	0.2101790000
H	-2.9281990000	-3.4217620000	0.0178810000
C	-0.6813770000	5.6979250000	0.6110450000
C	4.8679500000	-1.4810330000	0.5051210000
H	4.0324120000	-0.7949870000	0.4045140000
C	-6.1166170000	-3.1517980000	1.1664410000
H	-6.7370860000	-2.4672330000	1.7335780000
C	7.9104910000	-1.9845510000	2.7151960000
H	8.7016260000	-2.7349730000	2.6681200000
H	7.4397530000	-2.0494180000	3.7010460000
H	8.3755200000	-0.9967510000	2.6425590000
C	-4.4750880000	-4.9079580000	-0.2296960000
H	-3.8305190000	-5.5918820000	-0.7740660000
C	-0.4352920000	8.0354920000	1.2068430000
C	-5.8033510000	-5.2627360000	0.0163810000
C	-6.6116460000	-4.3688300000	0.7202780000
H	-7.6443490000	-4.6319350000	0.9281930000
C	-6.3368420000	-6.5900710000	-0.4358280000
H	-5.8822510000	-6.9006510000	-1.3794790000
H	-7.4202860000	-6.5607280000	-0.5700570000
H	-6.1173740000	-7.3666070000	0.3051890000
C	-0.8508880000	9.4658200000	1.0285310000
H	-0.7064300000	9.7897260000	-0.0066570000
H	-0.2768770000	10.1324250000	1.6746460000
H	-1.9114390000	9.5969470000	1.2641730000
H	-1.1708430000	4.9137300000	0.0413160000
C	0.9389840000	6.3544780000	2.2865560000
H	1.7000770000	6.0722820000	3.0051090000
C	0.5537230000	7.6800830000	2.1216830000
H	1.0295620000	8.4506150000	2.7203260000
C	-1.0467480000	7.0238730000	0.4573170000

H	-1.8277230000	7.2811410000	-0.2519560000
Sn	1.9020910000	-5.0682060000	0.1546800000
Sn	-6.0477090000	1.1261800000	-0.1745590000
Sn	3.6384940000	4.1256350000	-0.2608520000
C	1.9505840000	-4.5936930000	2.2702660000
C	3.5783700000	-6.3398310000	-0.4093500000
C	0.0303310000	-5.6407200000	-0.7925300000
C	-7.6117660000	0.5169760000	1.2104390000
C	-6.6654400000	0.6986930000	-2.2099430000
C	-5.3049820000	3.0937060000	0.3330260000
C	4.4200460000	4.9457260000	1.6021200000
C	3.1583470000	5.7427810000	-1.6323090000
C	4.7393120000	2.3630830000	-0.8738870000
H	-8.0464390000	-0.4205220000	0.8448740000
H	-7.1418860000	0.3032060000	2.1731270000
C	-4.5096980000	3.1193470000	1.6375100000
H	-4.6937450000	3.4421370000	-0.5042110000
H	-6.0649450000	1.3317330000	-2.8685780000
C	-8.1579780000	0.8654640000	-2.4807330000
H	2.5064960000	-3.6523870000	2.3319620000
C	2.5743690000	-5.6585440000	3.1690070000
H	4.4768250000	-5.8920420000	0.0299940000
H	3.6946700000	-6.2619450000	-1.4938450000
H	5.5687660000	2.2161280000	-0.1728140000
C	5.2416570000	2.3991080000	-2.3147120000
H	3.9973530000	5.9484580000	1.7323850000
H	4.0326200000	4.3308780000	2.4191480000
H	2.1814040000	6.1018420000	-1.2888790000
H	2.9958380000	5.3096190000	-2.6215550000
H	4.0433980000	1.5273670000	-0.7440540000
C	4.1637070000	6.8911730000	-1.6602090000
C	5.9462980000	5.0078770000	1.6398860000
H	-6.1763790000	3.7566440000	0.4002870000
H	-6.3543000000	-0.3336150000	-2.4090240000
C	-8.6966040000	1.5844490000	1.3529720000
H	0.9246480000	-4.3650010000	2.5738030000

C	3.4576020000	-7.7997100000	0.0268180000
H	-0.7445100000	-5.0552220000	-0.2895250000
C	-0.2950190000	-7.1301640000	-0.7623550000
H	0.0914640000	-5.2700590000	-1.8207730000
H	-8.4649930000	1.9043090000	-2.2975120000
H	-8.7434160000	0.2533200000	-1.7813990000
C	-8.5489600000	0.4885590000	-3.9076810000
H	-7.9668810000	1.0986720000	-4.6092020000
C	-10.0357550000	0.6595180000	-4.1861320000
H	-8.2528270000	-0.5512590000	-4.0941130000
H	-10.3494250000	1.6976580000	-4.0343220000
H	-10.6382320000	0.0332170000	-3.5198090000
H	-10.2863670000	0.3852430000	-5.2146430000
H	-8.2528100000	2.5218000000	1.7145460000
C	-9.8164290000	1.1767570000	2.3078870000
H	-9.1408670000	1.8203680000	0.3759210000
C	-10.8881330000	2.2466230000	2.4629070000
H	-9.3800330000	0.9416480000	3.2863310000
H	-10.2712710000	0.2458170000	1.9463000000
H	-10.4633890000	3.1771150000	2.8534880000
H	-11.6770600000	1.9289050000	3.1503430000
H	-11.3588210000	2.4774670000	1.5015160000
H	-5.0816770000	2.6504610000	2.4490160000
C	-4.1171880000	4.5304330000	2.0651980000
H	-3.5988550000	2.5185630000	1.5284690000
H	-3.5567660000	5.0052450000	1.2502010000
C	-3.2828620000	4.5507240000	3.3382270000
H	-5.0259950000	5.1320350000	2.2005140000
H	-3.8349060000	4.1152830000	4.1777040000
H	-3.0020280000	5.5707880000	3.6169860000
H	-2.3647260000	3.9712930000	3.2071940000
C	6.4890180000	5.5621530000	2.9549410000
H	6.3293850000	5.6261060000	0.8163960000
H	6.3688700000	4.0066510000	1.4804940000
H	6.0753850000	6.5656650000	3.1159480000
C	8.0096460000	5.6194340000	2.9986680000

H	6.1151010000	4.9450410000	3.7812100000
H	8.3702830000	6.0173820000	3.9513470000
H	8.4051180000	6.2577440000	2.2016740000
H	8.4464530000	4.6237040000	2.8688370000
C	5.9973020000	1.1332270000	-2.7097830000
H	5.8969410000	3.2669370000	-2.4706860000
H	4.3888060000	2.5313580000	-2.9913040000
C	6.4898130000	1.1658270000	-4.1499590000
H	5.3418600000	0.2680200000	-2.5641220000
H	6.8491900000	0.9985590000	-2.0300360000
H	7.0267190000	0.2492170000	-4.4099020000
H	7.1672230000	2.0095190000	-4.3226280000
H	5.6521030000	1.2652830000	-4.8475010000
H	4.2880240000	7.2991990000	-0.6494460000
H	3.7539070000	7.7136590000	-2.2636580000
C	5.5370520000	6.5271370000	-2.2211260000
H	6.2143590000	7.3768190000	-2.0759790000
C	5.5222240000	6.1459950000	-3.6956140000
H	5.9679860000	5.7019060000	-1.6345630000
H	6.5307710000	5.9320700000	-4.0601480000
H	5.1153830000	6.9616700000	-4.3026360000
H	4.9128680000	5.2578810000	-3.8824290000
C	2.6179960000	-5.2696120000	4.6488780000
H	3.5968420000	-5.8816250000	2.8352160000
H	2.0153730000	-6.5984770000	3.0774500000
H	2.9542570000	-6.1376420000	5.2288610000
H	1.5988240000	-5.0493340000	4.9901050000
C	3.5248520000	-4.0842410000	4.9526670000
H	3.5582900000	-3.8788360000	6.0261970000
H	3.1810970000	-3.1717560000	4.4577580000
H	4.5501990000	-4.2787250000	4.6186940000
H	3.3348250000	-7.8702790000	1.1158520000
C	4.6661800000	-8.6395360000	-0.3802260000
H	2.5566350000	-8.2534470000	-0.4060180000
C	4.5490770000	-10.0982720000	0.0387720000
H	5.5701250000	-8.1985800000	0.0588310000

H	4.7947010000	-8.5737870000	-1.4675980000
H	4.4503940000	-10.1919160000	1.1253380000
H	5.4265750000	-10.6758190000	-0.2650810000
H	3.6700890000	-10.5696250000	-0.4132210000
C	-0.3906120000	-7.7058710000	0.6452460000
H	0.4513270000	-7.6951600000	-1.3351220000
H	-1.2516710000	-7.3025110000	-1.2760440000
H	0.5717140000	-7.5675180000	1.1608290000
C	-0.7609670000	-9.1813610000	0.6725800000
H	-1.1230990000	-7.1263690000	1.2211040000
H	-0.8165790000	-9.5630720000	1.6955850000
H	-0.0239520000	-9.7840180000	0.1318670000
H	-1.7345420000	-9.3515230000	0.2017060000

($^{n}Bu_3Sn$-TsNCO)$_3P_7$ – OOO

Charge = 0 Multiplicity = 1

Sn	2.7771000000	-4.1175290000	0.7403470000
Sn	2.4227580000	4.3565920000	-0.7511860000
Sn	-5.3553200000	-0.2315910000	-0.2941120000
S	4.5120650000	-1.1533400000	-2.1881360000
S	-0.8959380000	3.3463780000	2.1537800000
P	-0.1890350000	-0.2307290000	0.2661090000
P	-1.0316930000	-1.8173040000	-1.0367840000
P	1.6564370000	0.1222140000	-0.9064720000
P	-1.2926300000	1.4915590000	-0.6346090000
S	-2.9150770000	-3.3790530000	1.2919610000
P	-1.0466620000	-0.8822140000	-3.0586720000
P	0.9708860000	0.0659000000	-3.0496450000
P	-0.8621820000	1.3027780000	-2.8244190000
O	0.7591480000	3.1206000000	-1.2373630000
O	1.8726830000	-2.2467270000	0.2795920000
O	-3.4606410000	-0.6292040000	-1.2446670000
O	-1.4633810000	-3.2590330000	1.3944060000
O	-1.5901320000	2.0612930000	2.0896250000
O	-0.0963390000	3.6836450000	3.3145120000
O	3.9913660000	0.2066460000	-2.3490060000

O	-3.7339160000	-3.3778490000	2.4871350000
O	4.7769370000	-1.9692750000	-3.3554270000
N	-3.5255090000	-2.1814970000	0.3209880000
N	0.0808160000	3.5472200000	0.8326170000
N	3.5518050000	-2.0184710000	-1.1598210000
C	2.4632600000	-1.5468070000	-0.6271390000
C	-0.0348740000	2.8513070000	-0.2579310000
C	-2.8430580000	-1.5462130000	-0.5887010000
C	1.4335310000	-4.6236180000	2.3551930000
C	1.3477340000	-3.5269680000	3.4161630000
H	0.4450180000	-4.7896600000	1.9177480000
C	1.6493290000	6.3778740000	-0.6312330000
C	2.6531090000	7.3865810000	-0.0735740000
H	0.7597250000	6.3271480000	0.0038910000
C	7.0569320000	-1.9056020000	-1.5183500000
H	6.9629570000	-2.6100660000	-2.3371730000
C	6.0072670000	-1.0460250000	-1.2344750000
C	4.7807380000	-3.6780640000	1.4379450000
C	5.3377650000	-4.7069190000	2.4195020000
H	4.7380320000	-2.6871750000	1.9041230000
C	2.5179930000	-5.2540820000	-1.0850160000
C	8.2154190000	-1.8278830000	-0.7547480000
H	9.0451240000	-2.4920290000	-0.9768390000
C	-2.1128260000	4.6224060000	1.9226900000
C	-3.2706430000	-4.8631960000	0.3792710000
C	8.3329570000	-0.9083180000	0.2864900000
C	3.2859030000	3.5367750000	1.0558580000
C	4.7937390000	3.7397720000	1.1946930000
H	3.0403150000	2.4686550000	1.0346420000
C	7.2597840000	-0.0481720000	0.5418080000
H	7.3378450000	0.6840000000	1.3401450000
C	-2.3968880000	-5.2746280000	-0.6213890000
H	-1.5079140000	-4.6895910000	-0.8341390000
C	-3.1367720000	4.4176780000	1.0040120000
C	6.0992560000	-0.1091300000	-0.2110910000
H	5.2724940000	0.5667590000	-0.0194600000

C	-6.6480630000	-1.9248570000	-0.7021780000
H	-6.7237750000	-2.5010210000	0.2252510000
H	-6.0953800000	-2.5518600000	-1.4107160000
C	-5.8016940000	1.4525520000	-1.6012920000
C	-7.1040560000	2.1883900000	-1.2900460000
H	-5.8103470000	1.0757200000	-2.6304040000
C	-4.4157670000	-5.5876950000	0.6769890000
H	-5.0690610000	-5.2512530000	1.4740070000
C	-4.8563040000	0.3508890000	1.7275340000
H	-5.0215310000	-0.5233040000	2.3640350000
H	-3.7749250000	0.5279870000	1.7168530000
C	9.5748120000	-0.8427430000	1.1257960000
H	10.3888700000	-1.4179430000	0.6805650000
H	9.3876900000	-1.2475300000	2.1260880000
H	9.9146560000	0.1889110000	1.2513060000
C	3.5069990000	3.8994960000	-2.5677200000
H	3.7896230000	2.8423950000	-2.5135330000
H	2.7840410000	3.9854610000	-3.3868920000
C	-2.6877470000	-6.4272050000	-1.3342230000
H	-2.0119470000	-6.7513770000	-2.1202230000
C	-4.0277120000	6.6052040000	1.5486650000
C	-3.8326740000	-7.1793680000	-1.0568110000
C	-4.6872680000	-6.7424700000	-0.0443590000
H	-5.5798330000	-7.3164140000	0.1855710000
C	-4.1162140000	-8.4439610000	-1.8127890000
H	-3.8268710000	-8.3535280000	-2.8626300000
H	-5.1755520000	-8.7055400000	-1.7702940000
H	-3.5515500000	-9.2818810000	-1.3894050000
C	-5.0787200000	7.6595520000	1.3615840000
H	-5.3235150000	7.7931830000	0.3046290000
H	-4.7545410000	8.6222260000	1.7618390000
H	-6.0035550000	7.3797600000	1.8775470000
H	-3.1804570000	3.4873820000	0.4459310000
C	-2.0286610000	5.7948650000	2.6573360000
H	-1.2242540000	5.9188950000	3.3736000000
C	-2.9915210000	6.7783640000	2.4655000000

H	-2.9359660000	7.6974810000	3.0408070000
C	-4.0826580000	5.4124260000	0.8203560000
H	-4.8828880000	5.2614550000	0.1014180000
H	1.8635610000	-4.6377280000	-1.7119320000
C	1.9286390000	-6.6498860000	-0.8977250000
H	3.4838060000	-5.2919030000	-1.5976560000
H	5.4213980000	-3.5787230000	0.5575280000
H	1.7633980000	-5.5718240000	2.7968100000
C	-8.0258590000	-1.5744040000	-1.2556320000
H	-4.9465530000	2.1347610000	-1.5317850000
C	-5.5729560000	1.5866720000	2.2645260000
C	4.7286610000	4.7754810000	-2.8408910000
H	1.3186940000	6.6749110000	-1.6321780000
H	2.7296500000	3.9678950000	1.8911560000
C	2.0825150000	8.7986240000	0.0294250000
H	3.5546730000	7.4168480000	-0.7005890000
H	2.9899530000	7.0707520000	0.9228670000
H	1.1841730000	8.7722700000	0.6586320000
H	1.7475380000	9.1207360000	-0.9644640000
C	3.0767970000	9.8058430000	0.5898890000
H	2.6412130000	10.8067840000	0.6545050000
H	3.9695480000	9.8733020000	-0.0404730000
H	3.4039000000	9.5209830000	1.5951870000
H	5.3075330000	3.3364140000	0.3130770000
C	5.3847360000	3.0836250000	2.4452500000
H	5.0332700000	4.8119940000	1.2188250000
H	6.4773270000	3.1797620000	2.4070100000
H	5.1670970000	2.0076510000	2.4176780000
C	4.8751000000	3.6691610000	3.7554890000
H	5.0782720000	4.7442560000	3.8090090000
H	5.3617910000	3.1978000000	4.6138330000
H	3.7974810000	3.5274730000	3.8726460000
C	5.4445630000	4.4002620000	-4.1358580000
H	5.4456240000	4.7009890000	-2.0118740000
H	4.4381350000	5.8340520000	-2.8916370000
H	4.7364050000	4.4820760000	-4.9697180000

H	5.7322000000	3.3433250000	-4.0871050000
C	6.6694150000	5.2603930000	-4.4129140000
H	7.1612860000	4.9691930000	-5.3451200000
H	7.4063520000	5.1703700000	-3.6078570000
H	6.4006600000	6.3188270000	-4.4965220000
C	6.7409610000	-4.3606770000	2.9119150000
H	5.3677360000	-5.7017720000	1.9536150000
H	4.6729780000	-4.8034010000	3.2882560000
C	7.3025980000	-5.3869530000	3.8859130000
H	6.7151420000	-3.3720180000	3.3872720000
H	7.4072840000	-4.2630160000	2.0457620000
H	7.3657640000	-6.3777120000	3.4239720000
H	6.6684210000	-5.4775770000	4.7737220000
H	8.3067400000	-5.1146990000	4.2230140000
H	2.3391730000	-3.3310270000	3.8493570000
C	0.3734160000	-3.8701650000	4.5390330000
H	1.0232710000	-2.5915220000	2.9463770000
H	0.6807280000	-4.8142260000	5.0083990000
H	-0.6143180000	-4.0460290000	4.0987700000
C	0.2768710000	-2.7758280000	5.5926680000
H	1.2475120000	-2.5912290000	6.0660900000
H	-0.4324560000	-3.0412750000	6.3816370000
H	-0.0597690000	-1.8342360000	5.1481680000
C	1.6980680000	-7.3792460000	-2.2186540000
H	0.9748410000	-6.5898580000	-0.3572490000
H	2.5886700000	-7.2625120000	-0.2686190000
C	1.1020750000	-8.7684010000	-2.0376980000
H	2.6491890000	-7.4504130000	-2.7605390000
H	1.0387850000	-6.7699730000	-2.8500730000
H	1.7598460000	-9.4060100000	-1.4380420000
H	0.9449170000	-9.2666680000	-2.9984930000
H	0.1358690000	-8.7206730000	-1.5240310000
C	-5.0780450000	1.9805140000	3.6539500000
H	-6.6591290000	1.4239690000	2.3026200000
H	-5.4173180000	2.4370340000	1.5879870000
H	-7.9558420000	1.5002160000	-1.3691570000

C	-7.3572530000	3.3818560000	-2.2081430000
H	-7.1026340000	2.5403640000	-0.2501860000
H	-8.5808290000	-0.9580570000	-0.5354350000
C	-8.8646390000	-2.8047650000	-1.5918700000
H	-7.9225150000	-0.9585340000	-2.1588660000
H	-5.2632040000	1.1507820000	4.3471890000
C	-5.7287660000	3.2522220000	4.1795370000
H	-3.9903380000	2.1065700000	3.6112760000
H	-5.3653960000	3.5020900000	5.1802720000
H	-6.8179910000	3.1493980000	4.2381920000
H	-5.5084110000	4.1032790000	3.5261880000
H	-8.3176960000	-3.4198880000	-2.3173120000
C	-10.2405680000	-2.4579140000	-2.1431410000
H	-8.9700450000	-3.4210330000	-0.6903600000
H	-10.8185310000	-1.8696800000	-1.4228030000
H	-10.8186660000	-3.3564790000	-2.3759330000
H	-10.1610000000	-1.8677510000	-3.0619310000
H	-7.3699990000	3.0357390000	-3.2491340000
H	-6.5098000000	4.0757090000	-2.1335330000
C	-8.6535070000	4.1147420000	-1.8921120000
H	-9.5178400000	3.4505620000	-1.9944900000
H	-8.8087930000	4.9650610000	-2.5620130000
H	-8.6527080000	4.4959110000	-0.8654650000

$(Me_3Si\text{-}TsNCO)_3As_7$ – NNN

Charge = 0 Multiplicity = 1

As	-0.4906000000	1.9300850000	0.8348110000
As	-0.2121110000	-0.0377300000	-0.5961240000
As	1.8521380000	-0.7315610000	0.4948210000
As	-1.7755770000	-1.4773310000	0.5941760000
As	-0.0384380000	1.0574770000	3.0955070000
As	-1.2183800000	-1.0617840000	2.9533160000
As	1.2301550000	-1.0219630000	2.8547410000
S	4.2242040000	-3.2582320000	0.6832050000
S	0.8065300000	3.9576670000	-1.7066350000
S	-4.2790260000	-1.0684020000	-1.7839440000

O	0.7053080000	-3.0255650000	-0.6981700000
O	-3.4674970000	0.6150070000	1.5148400000
O	3.9034140000	-2.2040380000	1.6308410000
O	4.6353100000	-4.5644300000	1.1543340000
O	-0.2402330000	2.9514890000	-1.7237430000
O	2.1737530000	2.5409450000	1.5435670000
O	-2.8747670000	-1.3974930000	-1.9493310000
O	-4.9631550000	-0.2486980000	-2.7622270000
O	1.7281360000	4.0727100000	-2.8177670000
N	2.8514230000	-3.4861120000	-0.2703570000
N	1.7220140000	3.6873890000	-0.3164190000
N	-4.4249890000	-0.2838030000	-0.2949770000
C	1.7383370000	-2.6409380000	-0.1939380000
C	5.4800460000	-2.6496260000	-0.4167500000
C	6.5935860000	-3.4370500000	-0.6688270000
H	6.6703880000	-4.4177770000	-0.2147000000
C	-0.9026920000	5.6910770000	-0.4424660000
H	-1.1625740000	4.8533910000	0.1973380000
C	1.3647150000	2.7551050000	0.6652470000
C	-6.5646050000	-4.9964380000	-1.4123380000
C	7.5940610000	-2.9420900000	-1.4962350000
H	8.4684130000	-3.5535070000	-1.6961690000
C	-3.3630880000	-0.1877710000	0.6123850000
C	7.4959910000	-1.6753820000	-2.0688260000
C	-5.1859820000	-2.5871190000	-1.6102270000
C	5.3627060000	-1.3721320000	-0.9568140000
H	4.5040870000	-0.7506560000	-0.7219600000
C	-1.2199720000	7.9978710000	-1.1185350000
C	-4.6863200000	-3.5946690000	-0.7903290000
H	-3.7545210000	-3.4530130000	-0.2513870000
C	0.3537460000	6.5879930000	-2.3075360000
H	1.0774740000	6.4369030000	-3.0999440000
C	-6.3454070000	-2.7710190000	-2.3487290000
H	-6.6960050000	-1.9809230000	-3.0021550000
C	0.0441500000	5.5419370000	-1.4519080000
C	-7.0269030000	-3.9773460000	-2.2426750000

H	-7.9321890000	-4.1285250000	-2.8223030000
C	6.3669010000	-0.9002080000	-1.7837130000
H	6.2781650000	0.0947880000	-2.2093270000
C	-5.3833260000	-4.7861430000	-0.6929190000
H	-4.9978300000	-5.5755440000	-0.0547720000
C	-0.2820820000	7.8112440000	-2.1318090000
H	-0.0452720000	8.6334960000	-2.7997310000
C	-1.5201730000	6.9185340000	-0.2800140000
H	-2.2579230000	7.0412200000	0.5071760000
C	-1.9068990000	9.3176590000	-0.9291250000
H	-1.5587820000	10.0571830000	-1.6524220000
H	-1.7254550000	9.7133070000	0.0748060000
H	-2.9900430000	9.2140450000	-1.0457860000
C	-7.3072330000	-6.2936150000	-1.2878620000
H	-7.7236520000	-6.4083150000	-0.2818470000
H	-6.6436480000	-7.1452560000	-1.4628300000
H	-8.1316500000	-6.3529530000	-2.0007870000
C	8.5808400000	-1.1378880000	-2.9540240000
H	9.0927070000	-0.2975470000	-2.4739980000
H	8.1716570000	-0.7708680000	-3.8995510000
H	9.3281010000	-1.9008890000	-3.1796450000
Si	3.3863440000	4.4512710000	-0.0172600000
Si	2.5677840000	-5.0003760000	-1.3064740000
Si	-5.8889020000	0.7596740000	0.1623640000
C	3.6527750000	5.8262900000	-1.2585290000
C	4.6688660000	3.1199040000	-0.2729740000
C	3.3865030000	5.2340840000	1.6801760000
H	2.9201270000	6.6307420000	-1.1536000000
H	3.6448070000	5.4750980000	-2.2906740000
H	4.6386640000	6.2553630000	-1.0440630000
H	5.6723460000	3.5390030000	-0.1440450000
H	4.5951250000	2.7262590000	-1.2913040000
H	4.5407740000	2.2993800000	0.4349770000
H	2.4948540000	5.8548440000	1.8136840000
H	4.2592700000	5.8898840000	1.7701920000
H	3.4149940000	4.4935090000	2.4787010000

C	1.9624070000	-4.4455760000	-2.9850210000
C	1.3880170000	-6.1128470000	-0.3857890000
C	4.2054240000	-5.8681720000	-1.5601160000
H	1.2412980000	-7.0437220000	-0.9436380000
H	0.4178620000	-5.6318080000	-0.2506610000
H	1.7958140000	-6.3687220000	0.5962960000
H	2.6195310000	-3.6737040000	-3.3975580000
H	0.9463520000	-4.0531420000	-2.9533550000
H	1.9910150000	-5.3001770000	-3.6699000000
H	4.9392510000	-5.2346340000	-2.0649330000
H	4.0105730000	-6.7247030000	-2.2160600000
H	4.6366510000	-6.2372660000	-0.6291420000
C	-7.3253490000	0.3088780000	-0.9484830000
C	-5.4209930000	2.5475570000	-0.0843430000
C	-6.3881670000	0.3194060000	1.9099340000
H	-7.1359750000	0.5368440000	-1.9976100000
H	-8.1829830000	0.9034740000	-0.6126830000
H	-7.6057510000	-0.7438680000	-0.8582360000
H	-6.4702180000	-0.7659710000	2.0246410000
H	-7.3762320000	0.7459960000	2.1146510000
H	-5.6817980000	0.6923600000	2.6508710000
H	-6.2809840000	3.1916520000	0.1275830000
H	-5.1158160000	2.7191710000	-1.1205140000
H	-4.5992570000	2.8329270000	0.5745150000

$(Me_3Si\text{-}TsNCO)_3As_7$ – OOO

Charge = 0 Multiplicity = 1

As	0.9175830000	-1.9838040000	0.6658080000
As	0.2995540000	-0.1008110000	-0.7764740000
As	-1.8921730000	0.1779580000	0.2574340000
As	1.4375680000	1.6447800000	0.4839430000
As	0.2011690000	-1.2524430000	2.9085240000
As	1.0068700000	1.0384370000	2.8234750000
As	-1.3970190000	0.5859830000	2.6421750000
S	-4.2824750000	2.5616280000	1.0001490000
S	0.0780110000	-3.8807360000	-2.1032630000

S	3.9321400000	2.0576020000	-1.8697830000
Si	-1.5076320000	3.6793220000	-2.5350730000
Si	5.0659870000	-0.8844730000	1.4533580000
Si	-3.0355970000	-4.0754140000	1.2981060000
O	-1.4351650000	2.2801270000	-1.4859640000
O	3.5907120000	0.0466580000	1.3329620000
O	-4.2239910000	1.1600320000	1.4247210000
O	-4.1947280000	3.6177530000	1.9878080000
O	1.3107740000	-3.1420040000	-1.8323260000
O	-1.5262410000	-3.2006790000	1.2702270000
O	2.5098390000	2.3731210000	-2.0054230000
O	4.6496300000	1.4543890000	-2.9715480000
O	-0.7313810000	-3.5474490000	-3.2572300000
N	-3.1475270000	2.8679780000	-0.1685020000
N	-0.9300810000	-3.8545340000	-0.7820940000
N	4.1939430000	1.0796340000	-0.5505590000
C	-2.2351850000	2.0158070000	-0.4788680000
C	-5.7745150000	2.7802590000	0.0657050000
C	-6.3292560000	4.0496120000	-0.0323680000
H	-5.8635070000	4.8810020000	0.4844810000
C	1.6226900000	-6.0703530000	-1.5315390000
H	2.2695170000	-5.3727140000	-1.0115330000
C	-0.6837480000	-3.1455780000	0.2616430000
C	6.1140950000	5.8561560000	-0.6132300000
C	-7.4853150000	4.2204260000	-0.7791920000
H	-7.9264870000	5.2092830000	-0.8594660000
C	3.2942820000	0.8528730000	0.3393580000
C	-8.0936330000	3.1425370000	-1.4255010000
C	4.7759580000	3.5435820000	-1.3882210000
C	-6.3575090000	1.6875510000	-0.5623540000
H	-5.9151950000	0.7036310000	-0.4555190000
C	1.0997940000	-8.3163920000	-2.2786510000
C	4.7137250000	-1.8949250000	2.9795990000
H	4.5042950000	-1.2536970000	3.8403770000
H	5.5716440000	-2.5269350000	3.2304190000
H	3.8487140000	-2.5460350000	2.8251260000

C	4.0703580000	4.5602680000	-0.7563050000
H	3.0046940000	4.4534950000	-0.5858560000
C	-0.3527940000	-6.4688970000	-2.8728150000
H	-1.2242990000	-6.0762020000	-3.3841570000
C	6.1344960000	3.6644440000	-1.6494560000
H	6.6540360000	2.8684810000	-2.1708230000
C	-1.0316760000	5.1618020000	-1.5114310000
H	-1.7474230000	5.3285220000	-0.7030700000
H	-0.9974930000	6.0599680000	-2.1367310000
H	-0.0393330000	5.0176530000	-1.0743450000
C	0.4823910000	-5.6067630000	-2.1745350000
C	5.2348500000	-1.9451950000	-0.0669160000
H	4.3029790000	-2.4817320000	-0.2710340000
H	6.0271940000	-2.6865720000	0.0827170000
H	5.4784380000	-1.3450270000	-0.9457440000
C	6.7927830000	4.8217560000	-1.2597670000
H	7.8528900000	4.9276490000	-1.4688130000
C	-3.2215180000	3.8033900000	-3.2630840000
H	-3.5084050000	2.8647070000	-3.7465940000
H	-3.2361180000	4.5861580000	-4.0293980000
H	-3.9683810000	4.0435190000	-2.5043280000
C	-7.5137370000	1.8781560000	-1.3037740000
H	-7.9767830000	1.0285240000	-1.7963370000
C	6.4920250000	0.2872610000	1.7194860000
H	6.6494480000	0.9155430000	0.8405830000
H	7.4105670000	-0.2777170000	1.9106060000
H	6.3130240000	0.9351350000	2.5825250000
C	4.7458300000	5.7093380000	-0.3744440000
H	4.1989710000	6.5116570000	0.1116020000
C	-0.0371260000	-7.8187060000	-2.9182060000
H	-0.6831680000	-8.4990560000	-3.4646960000
C	1.9216840000	-7.4232150000	-1.5882030000
H	2.8133770000	-7.7932310000	-1.0912230000
C	1.4523670000	-9.7722240000	-2.3628610000
H	0.5626510000	-10.3914220000	-2.4968690000
H	1.9730430000	-10.1093330000	-1.4635920000

H	2.1148840000	-9.9591350000	-3.2151560000
C	6.8388620000	7.0925070000	-0.1692840000
H	7.1338530000	7.0096140000	0.8825700000
H	6.2074860000	7.9793820000	-0.2619550000
H	7.7466150000	7.2552080000	-0.7540990000
C	-0.2419060000	3.2527090000	-3.8244120000
H	0.7355190000	3.0567300000	-3.3748940000
H	-0.1352960000	4.0773390000	-4.5371760000
H	-0.5403400000	2.3625020000	-4.3857240000
C	-9.3621890000	3.3319410000	-2.2036980000
H	-10.2354690000	3.1824780000	-1.5592060000
H	-9.4361720000	2.6173480000	-3.0266200000
H	-9.4292210000	4.3403850000	-2.6179690000
C	-2.6710440000	-5.9009550000	1.1829300000
H	-2.2410190000	-6.1548190000	0.2117590000
H	-3.5940590000	-6.4755790000	1.3145340000
H	-1.9711280000	-6.2125550000	1.9637900000
C	-4.1222270000	-3.4435160000	-0.0754000000
H	-4.2344720000	-2.3577760000	-0.0005740000
H	-5.1177790000	-3.8939650000	-0.0006490000
H	-3.7028160000	-3.6808900000	-1.0551700000
C	-3.6852420000	-3.5962650000	2.9763000000
H	-2.9907530000	-3.8886870000	3.7688930000
H	-4.6459150000	-4.0826600000	3.1732360000
H	-3.8367530000	-2.5148780000	3.0410190000

6.6. Optimised Structures at the PBE1PBE/6-311G(d,p) Level of Theory for clusters reactivity towards CO_2

CO_2

Charge = 0 Multiplicity = 1

C	0.0000000000	-0.0001410000	0.0003820000
O	0.0010000000	-0.9469220000	-0.6716860000
O	-0.0010000000	0.9470630000	0.6723040000

$(Me_3Si)_3P_7$

Charge = 0 Multiplicity = 1

P	-0.4535530000	0.0161450000	-0.3258980000
P	0.5066060000	0.3221500000	-2.2808610000
P	0.6068580000	-1.8230210000	0.2466790000
P	-2.3124390000	-0.9154700000	-1.0409460000
P	0.2707350000	-3.1458960000	-1.4975790000
P	-1.5800740000	-2.4092020000	-2.5023900000
P	0.4207010000	-1.6964450000	-3.1881760000
Si	2.7413590000	0.6384700000	-1.8773270000
Si	-0.6164230000	-2.8083820000	1.9152900000
Si	-3.3775980000	0.6341460000	-2.3513500000
C	-3.3005660000	2.2589320000	-1.4147490000
C	-5.1451690000	0.0057270000	-2.4411110000
C	-2.6749460000	0.8236580000	-4.0782560000
C	-1.0659620000	-1.4365650000	3.1149270000
C	0.5893950000	-4.0121340000	2.7049280000
C	-2.1507110000	-3.7203190000	1.3432090000
C	2.8505020000	1.8148850000	-0.4188100000
C	3.3718890000	1.4617130000	-3.4431620000
C	3.7119340000	-0.9289830000	-1.5409900000
H	2.2622700000	2.7215880000	-0.5846500000
H	3.8932950000	2.1128830000	-0.2640990000
H	2.4946460000	1.3415710000	0.5003830000
H	3.3491600000	-1.4301610000	-0.6410330000
H	4.7671380000	-0.6709270000	-1.3954320000
H	3.6506730000	-1.6309970000	-2.3774370000
H	2.8393550000	2.3954930000	-3.6428570000
H	3.2499220000	0.8102220000	-4.3133970000
H	4.4382200000	1.6918880000	-3.3438790000
H	0.1116030000	-4.5248290000	3.5468680000
H	1.4773620000	-3.4963460000	3.0802700000
H	0.9168270000	-4.7742220000	1.9916660000
H	-1.9073050000	-4.5156310000	0.6328260000
H	-2.8604300000	-3.0392450000	0.8683660000
H	-2.6360830000	-4.1817160000	2.2108710000
H	-1.5251360000	-1.8684110000	4.0108930000
H	-1.7819360000	-0.7390840000	2.6718020000

H	-0.1862050000	-0.8678550000	3.4283950000
H	-5.7574150000	0.6896760000	-3.0389180000
H	-5.5909710000	-0.0680070000	-1.4454220000
H	-5.1950020000	-0.9823190000	-2.9078900000
H	-3.9226540000	3.0046310000	-1.9218400000
H	-2.2790820000	2.6463070000	-1.3700470000
H	-3.6697360000	2.1531180000	-0.3909500000
H	-1.6391490000	1.1685730000	-4.0461210000
H	-3.2712490000	1.5599720000	-4.6289910000
H	-2.7086570000	-0.1185810000	-4.6328060000

$(Me_3Si–CO_2)_3P_7$

Charge = 0 Multiplicity = 1

P	0.3599230000	0.0053860000	-0.7033530000
P	1.6909610000	0.5813550000	0.9586880000
P	-1.4223530000	1.0611320000	0.0488600000
P	-0.1712370000	-1.9887100000	0.0866520000
P	-1.6658810000	0.3053860000	2.1438770000
P	-0.5740050000	-1.6243980000	2.2593300000
P	0.4553650000	0.2636360000	2.8006890000
Si	1.5162680000	4.5721110000	-0.7946620000
Si	-5.2016460000	-0.9955140000	-0.7170520000
Si	3.9225910000	-3.0558140000	-0.9725570000
O	-3.8051540000	-0.1356630000	-0.1301480000
O	1.5331840000	3.1445720000	1.8501870000
O	1.8659700000	-3.4131470000	1.1957920000
O	1.6450930000	2.8861020000	-0.3785190000
O	2.2715500000	-2.5236480000	-0.8268660000
O	-2.6069210000	-0.2157040000	-2.0287220000
C	1.5825520000	2.4497260000	0.8697320000
C	-2.7325670000	0.0882090000	-0.8713910000
C	1.5344980000	-2.7494780000	0.2491300000
C	-6.3011410000	-1.0038360000	0.7852790000
H	-5.8110840000	-1.5020720000	1.6263280000
H	-7.2361840000	-1.5336180000	0.5775640000
H	-6.5523570000	0.0141240000	1.0957540000

C	-0.1144960000	5.2022800000	-0.1519800000
H	-0.9386280000	4.5690010000	-0.4933240000
H	-0.2979010000	6.2206930000	-0.5095450000
H	-0.1237180000	5.2129270000	0.9403130000
C	1.5708760000	4.5077190000	-2.6548860000
H	2.5052480000	4.0611090000	-3.0060480000
H	1.4986100000	5.5144520000	-3.0783790000
H	0.7424070000	3.9143270000	-3.0514380000
C	2.9806830000	5.4705480000	-0.0725650000
H	2.9707760000	5.4067060000	1.0180150000
H	2.9560250000	6.5280000000	-0.3553810000
H	3.9226480000	5.0489460000	-0.4350840000
C	-4.6577680000	-2.7068970000	-1.2124100000
H	-3.9387020000	-2.6620910000	-2.0336700000
H	-5.5181240000	-3.3002420000	-1.5386640000
H	-4.1880500000	-3.2299920000	-0.3744330000
C	-5.9375310000	-0.0288020000	-2.1303130000
H	-6.1959450000	0.9880530000	-1.8209120000
H	-6.8529790000	-0.5134410000	-2.4850450000
H	-5.2353910000	0.0318360000	-2.9650170000
C	3.9464420000	-4.9191850000	-0.9576780000
H	3.5612930000	-5.2997450000	-0.0087440000
H	4.9695880000	-5.2876240000	-1.0851600000
H	3.3381340000	-5.3311290000	-1.7679950000
C	4.4012450000	-2.3515620000	-2.6286550000
H	3.7612770000	-2.7455360000	-3.4229900000
H	5.4375130000	-2.6057640000	-2.8727470000
H	4.3112280000	-1.2617910000	-2.6315190000
C	4.8920850000	-2.3051460000	0.4296320000
H	4.7408070000	-1.2224320000	0.4724980000
H	5.9625890000	-2.4946770000	0.3005620000
H	4.5792790000	-2.7293280000	1.3865510000

$(Me_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	1.0955870000	3.4155550000	0.2227350000

Ge	2.5231990000	-2.5948730000	-0.2547310000
P	-1.1831370000	-1.4737990000	-0.0463060000
P	1.9318280000	-0.3831620000	0.3172740000
P	-0.5948570000	1.7741630000	0.3207640000
P	0.1398460000	0.0776510000	-0.8709870000
P	-1.0477140000	-1.1148750000	2.1369970000
P	1.1107920000	-0.5990710000	2.3649640000
P	-0.4309290000	1.0126910000	2.3965690000
C	2.6146500000	3.0938010000	1.4073330000
H	3.2971060000	3.9466410000	1.3433320000
H	2.2865910000	2.9870810000	2.4435340000
C	0.1742250000	5.0664310000	0.7287590000
H	-0.2217170000	4.9949190000	1.7441790000
H	0.8752160000	5.9049810000	0.6883700000
C	1.4736270000	-3.9750920000	0.6442050000
H	1.8734960000	-4.9553590000	0.3678590000
H	1.5330380000	-3.8682400000	1.7294420000
C	1.6714900000	3.5087450000	-1.6441590000
H	2.1971820000	2.5962630000	-1.9320840000
H	0.8165580000	3.6466370000	-2.3093560000
C	2.3436920000	-2.7355140000	-2.1971350000
H	2.7451940000	-3.6980410000	-2.5267090000
H	1.2941260000	-2.6755550000	-2.4914710000
H	4.7844180000	-3.7238090000	0.0091720000
H	5.0021470000	-1.9834650000	-0.2695390000
C	-3.3380040000	-0.1810650000	-2.4285610000
H	-2.8971580000	-0.9422100000	-3.0756520000
H	-3.5189750000	1.5266570000	0.4907540000
C	4.4063060000	-2.7289690000	0.2609950000
Ge	-3.3766760000	-0.7836410000	-0.5681950000
C	-4.0945940000	0.6065740000	0.6012380000
H	-4.0657680000	0.2924160000	1.6468400000
C	-4.4370860000	-2.4209420000	-0.4104960000
H	-4.4018980000	-2.8100090000	0.6094700000
H	-5.4794630000	-2.2089070000	-0.6647880000
H	-2.7588520000	0.7393920000	-2.5241220000

H	0.4289380000	-3.9141100000	0.3366350000
H	2.8958770000	-1.9382840000	-2.6989650000
H	4.5274890000	-2.5738790000	1.3353080000
H	-4.0600520000	-3.1874050000	-1.0906700000
H	-4.3604520000	0.0122940000	-2.7655050000
H	-5.1356710000	0.7963810000	0.3231490000
H	-0.6522430000	5.2679640000	0.0442040000
H	2.3501750000	4.3572760000	-1.7694410000
H	3.1424560000	2.1877650000	1.1067890000

$(Me_3Ge–CO_2)_3P_7$

Charge = 0 Multiplicity = 1

P	0.3002470000	0.0079240000	-0.6212870000
P	1.7731180000	0.3554930000	0.9846670000
P	-1.2661140000	1.3463030000	0.1740860000
P	-0.5455400000	-1.8593260000	0.1981050000
P	-1.5393640000	0.6570640000	2.2877560000
P	-0.7970820000	-1.4318670000	2.3810270000
P	0.5651000000	0.2503480000	2.8679010000
Ge	2.0649760000	4.4981250000	-0.6689660000
Ge	-5.2275280000	-0.6178150000	-0.6093840000
Ge	3.4319480000	-3.6734990000	-0.7480340000
O	-3.7167350000	0.2514180000	0.1125500000
O	2.0279490000	2.9178910000	1.8640040000
O	1.1700990000	-3.7084730000	1.2057050000
O	2.0367940000	2.6374290000	-0.3614430000
O	1.7800820000	-2.7643850000	-0.7357840000
O	-2.7259970000	0.4011290000	-1.8945190000
C	1.9512930000	2.2233530000	0.8797670000
C	-2.7303570000	0.5492840000	-0.6962820000
C	0.9937660000	-2.9299840000	0.3001910000
C	-6.2269000000	-0.9071240000	1.0279020000
H	-5.6537680000	-1.5336190000	1.7140640000
H	-6.4363310000	0.0463960000	1.5165660000
C	0.4598470000	5.2034500000	0.1605660000
H	-0.3750730000	4.5259770000	-0.0342200000

H	0.5986980000	5.2881140000	1.2385450000
C	1.9983640000	4.4887740000	-2.6079830000
H	2.0198320000	5.5115300000	-2.9932480000
H	1.0810310000	4.0052500000	-2.9493900000
C	3.7402170000	5.1646940000	0.0499070000
H	3.7642840000	5.0070310000	1.1287420000
H	4.5840550000	4.6448610000	-0.4084120000
C	-4.5789990000	-2.2507700000	-1.4313110000
H	-5.4146140000	-2.9284680000	-1.6254900000
H	-3.8710870000	-2.7464910000	-0.7634520000
C	-6.0700160000	0.6407360000	-1.8235250000
H	-6.9873370000	0.2066170000	-2.2304230000
H	-5.3885330000	0.8709540000	-2.6431930000
C	3.0363810000	-5.5709600000	-0.8459620000
H	3.9660920000	-6.1403880000	-0.9295290000
H	2.4181710000	-5.7846020000	-1.7203540000
C	4.1707580000	-2.9478600000	-2.3889970000
H	5.1598780000	-3.3722520000	-2.5799620000
H	4.2646280000	-1.8630090000	-2.3107790000
C	4.3718480000	-3.0988880000	0.8481310000
H	4.3036720000	-2.0125410000	0.9409000000
H	3.9249830000	-3.5568040000	1.7309200000
H	3.5206030000	-3.1834370000	-3.2337770000
H	2.5047720000	-5.8815300000	0.0540380000
H	5.4258160000	-3.3823050000	0.7849470000
H	3.8350430000	6.2337420000	-0.1591250000
H	0.2226810000	6.1858500000	-0.2561590000
H	2.8535470000	3.9449720000	-3.0139570000
H	-7.1758190000	-1.4041010000	0.8100310000
H	-6.3253920000	1.5629870000	-1.2976480000
H	-4.0707450000	-2.0201100000	-2.3677270000

$(Et_3Ge)_3P_7$

Charge = 0 Multiplicity = 1

Ge	0.9799370000	3.3755630000	-0.0179720000
Ge	2.6833750000	-2.5263210000	-0.4231440000

P	-1.2654280000	-1.5430750000	0.1628510000
P	1.8656110000	-0.3949470000	0.1813160000
P	-0.6668150000	1.7111990000	0.3139770000
P	-0.0283320000	-0.0341130000	-0.8627040000
P	-0.9196080000	-1.0842930000	2.2994060000
P	1.2451590000	-0.5493210000	2.2981750000
P	-0.3028640000	1.0573580000	2.3967330000
C	2.5356970000	3.3084720000	1.1983070000
H	2.6488700000	4.3281400000	1.5846800000
H	2.2689460000	2.6853510000	2.0573030000
C	-0.0232060000	5.0369120000	0.3287740000
H	-0.3357120000	5.0196530000	1.3785830000
H	0.6946320000	5.8609310000	0.2362490000
C	1.3486630000	-3.8866880000	-0.9068820000
H	1.8707710000	-4.8481590000	-0.8205730000
H	0.5583830000	-3.8818980000	-0.1516520000
C	1.4819450000	3.2854720000	-1.9207800000
H	2.1358600000	2.4180910000	-2.0535130000
H	0.5738300000	3.0772570000	-2.4955540000
C	3.8442950000	-2.1206670000	-1.9635030000
H	4.1615170000	-3.0846960000	-2.3800070000
H	3.2350310000	-1.6372670000	-2.7343050000
H	4.5369840000	-3.8259990000	0.6332140000
H	4.3518740000	-2.3004680000	1.4783340000
C	-3.5806530000	-0.2560710000	-2.0623660000
H	-3.1316730000	-1.0498100000	-2.6682690000
H	-4.4123520000	-3.2815260000	-1.9089140000
C	3.8369130000	2.8241120000	0.5683910000
H	4.6499180000	2.8198780000	1.3018660000
H	3.7283380000	1.8056080000	0.1874290000
H	4.1505220000	3.4629590000	-0.2623250000
C	0.7561920000	-3.7252790000	-2.3022930000
H	0.0450300000	-4.5276620000	-2.5237760000
H	0.2172500000	-2.7786370000	-2.4025770000
H	1.5280450000	-3.7483070000	-3.0774740000
C	-1.2210740000	5.2545460000	-0.5884130000

H	-1.7450550000	6.1863230000	-0.3520100000
H	-0.9201700000	5.3066000000	-1.6395850000
H	-1.9433880000	4.4377400000	-0.4973830000
C	5.0550630000	-1.2614460000	-1.6145450000
H	5.6694100000	-1.0577330000	-2.4974740000
H	4.7515350000	-0.2972670000	-1.1954030000
H	5.6966020000	-1.7514790000	-0.8760240000
C	2.1532750000	4.5605480000	-2.4264220000
H	2.4189070000	4.4754140000	-3.4852330000
H	1.4966370000	5.4300580000	-2.3248830000
H	3.0742400000	4.7839770000	-1.8791100000
C	-5.0001100000	0.0455090000	-2.5377070000
H	-5.0152500000	0.3090500000	-3.6003840000
H	-5.6645530000	-0.8144850000	-2.4066540000
H	-5.4381330000	0.8855360000	-1.9905730000
C	3.0287800000	-3.8662210000	2.1899900000
H	3.7076560000	-4.2322050000	2.9669210000
H	2.3124320000	-3.1974990000	2.6765310000
H	2.4713260000	-4.7275230000	1.8101460000
H	-3.7228460000	1.5610760000	0.6286510000
C	-5.5919250000	0.6464450000	1.2786440000
H	-5.8694430000	1.4731020000	1.9408260000
H	-6.1496210000	0.7772200000	0.3464830000
H	-5.9486720000	-0.2760800000	1.7458510000
C	3.7938440000	-3.1535300000	1.0799100000
Ge	-3.4894990000	-0.8118770000	-0.1740740000
C	-4.0820850000	0.6174120000	1.0487410000
H	-3.5592580000	0.4884360000	2.0014540000
C	-4.5544990000	-2.4473180000	0.1002640000
H	-4.4057310000	-2.7712760000	1.1359930000
H	-5.6097560000	-2.1638120000	0.0152920000
C	-4.2204240000	-3.5741330000	-0.8717460000
H	-4.8191030000	-4.4680410000	-0.6692710000
H	-3.1664390000	-3.8599450000	-0.8031420000
H	-2.9394200000	0.6231260000	-2.1801560000

$(Et_3Ge–CO_2)_3P_7$

Charge = 0 Multiplicity = 1

P	0.2880030000	-0.0332110000	-0.4534340000
P	1.7550310000	0.2830030000	1.1641820000
P	-1.2995580000	1.2576350000	0.3792300000
P	-0.5434730000	-1.9327450000	0.3001730000
P	-1.5630780000	0.5016360000	2.4716750000
P	-0.8004310000	-1.5820860000	2.4970680000
P	0.5448280000	0.0980500000	3.0401600000
Ge	1.9077310000	4.4903610000	-0.3460210000
Ge	-5.2057930000	-0.8052880000	-0.4565060000
Ge	3.5518810000	-3.5327090000	-0.5925160000
O	-3.7343110000	0.1319380000	0.2823900000
O	1.9838590000	2.8171330000	2.1275840000
O	1.1223010000	-3.8717310000	1.2017400000
O	1.9570850000	2.6148850000	-0.1059740000
O	1.8359350000	-2.7331930000	-0.5966220000
O	-2.7271440000	0.3182970000	-1.7128700000
C	1.9030440000	2.1566950000	1.1201400000
C	-2.7475130000	0.4538780000	-0.5122470000
C	0.9961350000	-3.0073360000	0.3681610000
C	-6.1907940000	-1.1256640000	1.1984660000
H	-5.5722320000	-1.7688070000	1.8322300000
C	-7.5664820000	-1.7477940000	0.9673950000
H	-6.2775010000	-0.1678880000	1.7204970000
C	0.2899760000	5.1048850000	0.5626800000
H	-0.4170270000	4.2689710000	0.5230360000
C	-0.3269860000	6.3619150000	-0.0486860000
H	0.5369000000	5.2527750000	1.6171880000
C	1.7741640000	4.5362590000	-2.2942950000
C	2.9513700000	3.8718640000	-3.0035000000
H	1.6754690000	5.5839040000	-2.6013290000
H	0.8329100000	4.0452710000	-2.5626640000
C	3.6042880000	5.1843530000	0.3328220000
H	3.6326210000	4.9721940000	1.4046380000
C	3.7906640000	6.6755240000	0.0563050000

H	4.4081090000	4.6012570000	-0.1279590000
C	-4.4904550000	-2.4318180000	-1.2758710000
C	-4.3618240000	-2.3935150000	-2.7958440000
H	-5.1378810000	-3.2569100000	-0.9563200000
H	-3.5140790000	-2.6065360000	-0.8105360000
C	-6.1106050000	0.4325570000	-1.6679360000
C	-6.5447890000	1.7361820000	-1.0038910000
H	-6.9749670000	-0.1000820000	-2.0825920000
H	-5.4291600000	0.6226800000	-2.5012880000
C	3.3364020000	-5.4270880000	-1.0354650000
C	3.1465380000	-6.3619520000	0.1551960000
H	4.2231980000	-5.7083240000	-1.6166640000
H	2.4885490000	-5.4936370000	-1.7253790000
C	4.3331500000	-2.4999060000	-2.0539820000
C	3.5943050000	-2.6586870000	-3.3806390000
H	5.3818110000	-2.8038340000	-2.1532420000
H	4.3411290000	-1.4517940000	-1.7371380000
C	4.3271330000	-3.1324040000	1.1539010000
H	4.0731830000	-2.0910450000	1.3782440000
C	5.8390290000	-3.3487440000	1.2031500000
H	3.8129270000	-3.7485130000	1.8956860000
H	-8.2044420000	-1.1046010000	0.3527650000
H	-8.0910240000	-1.9151150000	1.9128220000
H	-7.4973840000	-2.7168740000	0.4627150000
H	-7.0426790000	2.3974720000	-1.7196050000
H	-5.6890840000	2.2809970000	-0.5954510000
H	-7.2439440000	1.5609150000	-0.1804200000
H	-5.3292170000	-2.2345560000	-3.2823860000
H	-3.9570350000	-3.3366380000	-3.1758070000
H	-3.6919650000	-1.5897480000	-3.1082780000
H	0.3524690000	7.2189380000	-0.0047890000
H	-1.2391110000	6.6468690000	0.4844090000
H	-0.5984970000	6.2119300000	-1.0978650000
H	3.8970430000	4.3724170000	-2.7729550000
H	2.8258050000	3.8971310000	-4.0902850000
H	3.0501100000	2.8246830000	-2.7058780000

H	4.7583620000	7.0278960000	0.4260890000
H	3.0205800000	7.2784870000	0.5473320000
H	3.7516760000	6.9009150000	-1.0142850000
H	6.2365700000	-3.1056250000	2.1930590000
H	6.3650590000	-2.7183740000	0.4796230000
H	6.1123000000	-4.3881930000	0.9937840000
H	4.0563340000	-2.0541070000	-4.1671370000
H	2.5515560000	-2.3435930000	-3.2904830000
H	3.5983120000	-3.6978690000	-3.7239610000
H	3.0234730000	-7.3977840000	-0.1760820000
H	2.2672280000	-6.0831450000	0.7391450000
H	4.0092280000	-6.3358310000	0.8279560000

($^{n}Bu_3Sn)_3P_7$

Charge = 0 Multiplicity = 1

Sn	-3.3690750000	-0.8758170000	-0.1585650000
Sn	2.7914750000	-2.2937890000	-0.1442050000
P	1.6453470000	1.3748840000	-0.6754660000
P	0.3377740000	-1.7006130000	-0.6023260000
P	-1.6494020000	0.9653850000	-0.6472410000
P	0.1245660000	0.2312050000	0.4245090000
P	1.0595250000	1.0301690000	-2.7820470000
P	0.3809870000	-1.0959770000	-2.7308860000
P	-1.1244440000	0.5546050000	-2.7596590000
Sn	0.8595390000	3.7879130000	-0.2956010000
C	5.1908570000	-7.3169930000	0.9453150000
H	5.1605150000	-8.4050280000	0.8396750000
H	5.1939260000	-7.0879270000	2.0160160000
C	4.0134780000	-6.6536710000	0.2443420000
H	6.1437180000	-6.9703970000	0.5319740000
H	4.0134730000	-6.9253130000	-0.8187300000
C	4.0212680000	-5.1320640000	0.3671250000
H	3.0717700000	-7.0391150000	0.6549510000
H	4.9667030000	-4.7510600000	-0.0414980000
H	4.0288320000	-4.8637240000	1.4322780000
C	2.8368740000	-4.4663500000	-0.3305880000

H	2.8320220000	-4.7083650000	-1.3991960000
H	1.8919530000	-4.8421010000	0.0772350000
C	1.3591710000	-2.5058670000	5.3243570000
H	1.5612470000	-2.2021190000	6.3553400000
H	1.3753750000	-3.6003190000	5.2918870000
C	2.3725660000	-1.9117610000	4.3559690000
H	0.3421670000	-2.1838290000	5.0771030000
H	2.3568000000	-0.8171870000	4.4284140000
C	2.1197300000	-2.3139780000	2.9058470000
H	3.3856770000	-2.2210330000	4.6431710000
H	1.1044870000	-2.0024030000	2.6271600000
H	2.1280290000	-3.4101950000	2.8345400000
C	3.1266070000	-1.7151810000	1.9280930000
H	3.1011070000	-0.6209100000	1.9663080000
H	4.1474540000	-2.0179580000	2.1912370000
C	8.0340730000	-1.4886680000	-2.1123460000
H	8.6990680000	-0.9576930000	-2.7991530000
H	8.1486000000	-2.5608510000	-2.3030030000
C	6.5864830000	-1.0503300000	-2.2848090000
H	8.3868490000	-1.2958160000	-1.0938350000
H	6.5030320000	0.0310060000	-2.1202280000
C	5.6259220000	-1.7690310000	-1.3402930000
H	6.2656350000	-1.2248100000	-3.3192390000
H	5.9560280000	-1.5969510000	-0.3066720000
H	5.7118900000	-2.8510930000	-1.5070420000
C	4.1762270000	-1.3213760000	-1.5124880000
H	4.0741930000	-0.2457260000	-1.3393240000
H	3.8310640000	-1.5149580000	-2.5339660000
C	-5.5843360000	-5.4543050000	-2.6413760000
H	-5.4544920000	-6.2958930000	-3.3274930000
H	-6.4250410000	-4.8556260000	-3.0071240000
C	-4.3169420000	-4.6175180000	-2.5374970000
H	-5.8702350000	-5.8626370000	-1.6663810000
H	-3.4828080000	-5.2461520000	-2.2019790000
C	-4.4578960000	-3.4316560000	-1.5860970000
H	-4.0348720000	-4.2453380000	-3.5301660000

H	-4.7461530000	-3.8083840000	-0.5953180000
H	-5.2949370000	-2.8062550000	-1.9243590000
C	-3.1849320000	-2.5952320000	-1.4827990000
H	-2.3437230000	-3.1898100000	-1.1144160000
H	-2.8926980000	-2.2178600000	-2.4689580000
C	-3.8547920000	-4.5075970000	4.1662310000
H	-3.6718560000	-4.7266770000	5.2219030000
H	-3.3524140000	-5.2803230000	3.5751690000
C	-3.3586290000	-3.1187230000	3.7887930000
H	-4.9309170000	-4.6052580000	3.9891970000
H	-3.8546830000	-2.3648370000	4.4129690000
C	-3.5898450000	-2.7777850000	2.3189250000
H	-2.2864610000	-3.0356170000	4.0074190000
H	-4.6629080000	-2.8653290000	2.1009450000
H	-3.0945860000	-3.5365930000	1.6987740000
C	-3.0841560000	-1.3870980000	1.9419570000
H	-3.5901830000	-0.6167550000	2.5348100000
H	-2.0146650000	-1.2983700000	2.1594760000
C	-8.9236600000	-0.4556160000	0.9008180000
H	-9.8612870000	0.0878210000	0.7544780000
H	-8.7240570000	-0.4883110000	1.9769710000
C	-7.7738560000	0.1990420000	0.1478030000
H	-9.0814040000	-1.4854460000	0.5639260000
H	-8.0118480000	0.2488630000	-0.9220790000
C	-6.4458370000	-0.5325500000	0.3265060000
H	-7.6558500000	1.2380250000	0.4802080000
H	-6.5713060000	-1.5730130000	-0.0016250000
H	-6.2130050000	-0.5840390000	1.3987710000
C	-5.2903310000	0.1235570000	-0.4268020000
H	-5.5023070000	0.1627060000	-1.5012090000
H	-5.1592710000	1.1601600000	-0.0967110000
C	-4.3479370000	5.5172520000	-1.7099030000
H	-5.0390340000	5.8535550000	-2.4879560000
H	-4.3240120000	6.2876340000	-0.9319020000
C	-2.9563030000	5.2572060000	-2.2700080000
H	-4.7673640000	4.6101870000	-1.2623080000

H	-3.0127810000	4.5068320000	-3.0684630000
C	-1.9695810000	4.7751480000	-1.2102650000
H	-2.5677390000	6.1704520000	-2.7383830000
H	-2.3614310000	3.8585570000	-0.7521700000
H	-1.9185260000	5.5224390000	-0.4067130000
C	-0.5769710000	4.5053020000	-1.7715610000
H	-0.6257040000	3.7642950000	-2.5758830000
H	-0.1480080000	5.4150070000	-2.2076920000
C	6.1797880000	4.6079980000	1.4173080000
H	7.1210520000	5.1563090000	1.3203310000
H	6.3907290000	3.5498000000	1.2315530000
C	5.1229770000	5.1327030000	0.4552600000
H	5.8483050000	4.6993600000	2.4569560000
H	4.9473820000	6.1996110000	0.6428280000
C	3.7976960000	4.3824840000	0.5562120000
H	5.4931510000	5.0634230000	-0.5753210000
H	3.4322470000	4.4473760000	1.5904980000
H	3.9773810000	3.3148390000	0.3717560000
C	2.7318720000	4.8978750000	-0.4063870000
H	2.5027360000	5.9514400000	-0.2060590000
H	3.0892200000	4.8462890000	-1.4410260000
C	-0.3535220000	6.7662720000	4.3446240000
H	-0.7298720000	6.7862660000	5.3711900000
H	-0.9661810000	7.4549650000	3.7535970000
C	-0.3898020000	5.3601690000	3.7625490000
H	0.6671900000	7.1625650000	4.3578040000
H	0.2024680000	4.6825840000	4.3901840000
C	0.1334160000	5.2913000000	2.3297190000
H	-1.4166080000	4.9746790000	3.7856480000
H	1.1590660000	5.6837290000	2.3088930000
H	-0.4588780000	5.9752140000	1.7065840000
C	0.1000460000	3.8816810000	1.7438750000
H	0.6977830000	3.1957840000	2.3535330000
H	-0.9208080000	3.4855660000	1.7347520000

(^{n}Bu$_3$Sn–CO$_2$)$_3$P$_7$

Charge = 0 Multiplicity = 1

P	-0.4021660000	0.1008280000	0.1553040000
P	-1.4348630000	1.4892810000	-1.2130090000
P	1.6310610000	0.4230090000	-0.6413820000
P	-0.8204770000	-1.7431750000	-0.9856920000
P	1.4173270000	0.0591970000	-2.8403820000
P	-0.4048310000	-1.1784030000	-3.1120620000
P	-0.5442200000	1.0332300000	-3.2209080000
O	3.1009400000	-1.8102650000	-0.9460290000
O	-0.3344720000	3.9305270000	-1.6812080000
O	-3.3280070000	-1.9566710000	-2.0240820000
O	-0.0691750000	3.1334070000	0.3882330000
O	-3.2185270000	-1.3217090000	0.1076880000
O	2.2237440000	-1.5679480000	1.0861990000
C	-0.4878260000	3.0706900000	-0.8397240000
C	2.3867220000	-1.1914910000	-0.0610890000
C	-2.6944420000	-1.6667110000	-1.0279260000
Sn	-5.3144290000	-1.0812120000	-0.0923710000
C	-5.1340200000	-1.9943110000	5.4658920000
H	-5.2865220000	-1.6172740000	6.4810210000
H	-4.0850400000	-2.2946780000	5.3770470000
C	-5.4951050000	-0.9487320000	4.4200210000
H	-5.7453120000	-2.8956230000	5.3516070000
H	-6.5414240000	-0.6425720000	4.5467390000
C	-5.2883180000	-1.4391360000	2.9897180000
H	-4.8929850000	-0.0451160000	4.5765670000
H	-5.8849250000	-2.3494270000	2.8390840000
H	-4.2409810000	-1.7418900000	2.8654010000
C	-5.6514940000	-0.3950800000	1.9354380000
H	-6.7016880000	-0.0954290000	2.0325420000
H	-5.0537680000	0.5129750000	2.0717820000
C	-7.9268010000	3.5114430000	-2.1436890000
H	-7.9753430000	4.2762470000	-2.9236430000
H	-7.7898010000	4.0234770000	-1.1855580000
C	-6.8007880000	2.5205330000	-2.4030660000
H	-8.8987060000	3.0078080000	-2.1123070000

H	-6.9426420000	2.0439950000	-3.3809250000
C	-6.6982900000	1.4366720000	-1.3332020000
H	-5.8432140000	3.0521510000	-2.4617130000
H	-7.6598150000	0.9079670000	-1.2751280000
H	-6.5618660000	1.9177460000	-0.3556210000
C	-5.5623330000	0.4515180000	-1.5992060000
H	-5.6905820000	-0.0535240000	-2.5611020000
H	-4.5994200000	0.9733510000	-1.6455890000
C	-9.7590980000	-4.5571980000	-0.2467650000
H	-10.1478350000	-5.5650040000	-0.4164720000
H	-10.2805960000	-3.8812850000	-0.9323570000
C	-8.2525760000	-4.4973850000	-0.4559920000
H	-10.0293510000	-4.2649570000	0.7732480000
H	-7.7549130000	-5.2054370000	0.2183080000
C	-7.6710540000	-3.1044340000	-0.2277580000
H	-8.0050780000	-4.8230070000	-1.4737620000
H	-7.9193410000	-2.7817260000	0.7925950000
H	-8.1818350000	-2.3992360000	-0.8978040000
C	-6.1606020000	-3.0428530000	-0.4481100000
H	-5.6453030000	-3.7429130000	0.2186860000
H	-5.8947310000	-3.3242920000	-1.4708070000
Sn	1.2614280000	4.7370390000	0.7388310000
C	0.7579890000	10.3397210000	1.2925880000
H	0.1112330000	11.2211030000	1.2717180000
H	1.5551320000	10.4963000000	0.5585630000
C	-0.0222370000	9.0673890000	0.9933900000
H	1.2249940000	10.2946280000	2.2819420000
H	-0.8331930000	8.9480710000	1.7226120000
C	0.8477490000	7.8132080000	1.0121610000
H	-0.5057850000	9.1494430000	0.0122690000
H	1.3321380000	7.7367730000	1.9952320000
H	1.6611190000	7.9396120000	0.2849710000
C	0.0618390000	6.5388440000	0.7062050000
H	-0.7522920000	6.4064160000	1.4269240000
H	-0.3932170000	6.5864680000	-0.2877470000
C	3.8316920000	0.8581600000	3.8594700000

H	4.0145820000	0.4135720000	4.8419400000
H	4.8058520000	1.0520910000	3.3978140000
C	3.0139850000	2.1383380000	3.9695810000
H	3.3158970000	0.1140740000	3.2440580000
H	2.0660640000	1.9278830000	4.4804020000
C	2.7117230000	2.7604690000	2.6099960000
H	3.5422710000	2.8697140000	4.5949040000
H	2.1950670000	2.0147300000	1.9932830000
H	3.6588240000	2.9647290000	2.0926090000
C	1.8807580000	4.0408220000	2.6942920000
H	0.9629070000	3.8670680000	3.2669930000
H	2.4315370000	4.8334160000	3.2128850000
C	6.5125020000	5.7163110000	-1.1443040000
H	7.2682420000	5.5368090000	-1.9139170000
H	6.9209000000	5.3658360000	-0.1906520000
C	5.2028770000	5.0137760000	-1.4732110000
H	6.3719750000	6.7993380000	-1.0644140000
H	4.8301440000	5.3574070000	-2.4459340000
C	4.1207700000	5.2395490000	-0.4203390000
H	5.3750320000	3.9355970000	-1.5788400000
H	3.9543700000	6.3204120000	-0.3149730000
H	4.5004770000	4.8988970000	0.5524660000
C	2.8108430000	4.5296050000	-0.7576040000
H	2.3980140000	4.8855320000	-1.7055820000
H	2.9724340000	3.4511830000	-0.8675420000
Sn	3.7079600000	-3.7141350000	-0.2246880000
C	7.8672850000	-5.5393850000	3.1244980000
H	8.5567120000	-5.3351850000	3.9482510000
H	8.4680050000	-5.7875250000	2.2433030000
C	6.9554220000	-4.3513240000	2.8525480000
H	7.2885270000	-6.4300360000	3.3902190000
H	6.3871200000	-4.1037780000	3.7575310000
C	5.9781920000	-4.5959680000	1.7056320000
H	7.5588930000	-3.4646880000	2.6215130000
H	5.3825880000	-5.4895760000	1.9377730000
H	6.5508770000	-4.8443990000	0.8016060000

C	5.0597530000	-3.4050180000	1.4386730000
H	4.4503560000	-3.1666170000	2.3148280000
H	5.6461830000	-2.5084990000	1.2093510000
C	-0.4728660000	-5.4869700000	3.1736590000
H	-1.4805810000	-5.9045680000	3.2530930000
H	-0.4862040000	-4.4945780000	3.6356140000
C	-0.0123710000	-5.4079210000	1.7248940000
H	0.1955940000	-6.1185380000	3.7684030000
H	-0.0331560000	-6.4079740000	1.2730470000
C	1.3859000000	-4.8141410000	1.5760880000
H	-0.7143000000	-4.7952710000	1.1455570000
H	2.0952270000	-5.4131370000	2.1633070000
H	1.3944330000	-3.8096290000	2.0129430000
C	1.8345620000	-4.7407200000	0.1192700000
H	1.9037180000	-5.7395010000	-0.3263590000
H	1.0991220000	-4.1810540000	-0.4706860000
C	7.7843570000	-2.8123830000	-4.0088850000
H	8.2764330000	-3.1052250000	-4.9404810000
H	8.5402690000	-2.8228690000	-3.2167060000
C	6.6242660000	-3.7393850000	-3.6735340000
H	7.4424140000	-1.7789130000	-4.1245980000
H	5.8979920000	-3.7362670000	-4.4956230000
C	5.9094960000	-3.3566600000	-2.3805390000
H	6.9863270000	-4.7722020000	-3.5914580000
H	5.5414340000	-2.3267910000	-2.4680710000
H	6.6420830000	-3.3466460000	-1.5617620000
C	4.7502780000	-4.2894340000	-2.0347640000
H	4.0113800000	-4.3000000000	-2.8433820000
H	5.1030010000	-5.3212020000	-1.9199370000

$(Me_3Si)_3As_7$

Charge = 0 Multiplicity = 1

As	0.8939160000	0.1150580000	-0.9128230000
As	2.8027210000	1.0463970000	0.2499980000
As	2.1198270000	0.8964180000	2.5834390000
Si	2.5932900000	3.4144540000	-0.1436870000

C	1.9867110000	3.6582520000	-1.9063660000
H	2.6007720000	3.1076200000	-2.6244740000
H	2.0338300000	4.7211550000	-2.1684940000
H	0.9504130000	3.3287180000	-2.0203630000
C	4.3552080000	4.0547140000	0.0241830000
H	4.7461470000	3.8877200000	1.0322930000
H	4.3864180000	5.1322730000	-0.1720580000
H	5.0285000000	3.5617190000	-0.6825600000
C	1.4854420000	4.3190600000	1.0715670000
H	0.4502090000	3.9779510000	0.9984940000
H	1.5098380000	5.3925000000	0.8503330000
H	1.8203500000	4.1810670000	2.1034440000
As	-0.8459430000	1.3069530000	0.2778760000
As	-0.3316200000	0.7986920000	2.6042140000
Si	-2.7972350000	-0.0608740000	-0.0779840000
C	-2.7342670000	-0.7164870000	-1.8386150000
H	-2.5760070000	0.0866440000	-2.5637480000
H	-3.6822860000	-1.2087380000	-2.0829980000
H	-1.9325810000	-1.4498330000	-1.9610710000
C	-4.2309000000	1.1441360000	0.1087020000
H	-4.2656280000	1.5704030000	1.1156910000
H	-5.1822210000	0.6305280000	-0.0697190000
H	-4.1531770000	1.9708980000	-0.6028740000
C	-3.0049030000	-1.4678180000	1.1469270000
H	-2.1939770000	-2.1949640000	1.0612090000
H	-3.9509110000	-1.9836570000	0.9450490000
H	-3.0335040000	-1.1050800000	2.1781800000
As	0.7523070000	-1.9829120000	0.2888050000
As	0.9787860000	-1.2755910000	2.6086610000
Si	2.9036100000	-2.9931520000	-0.1005700000
C	3.3986240000	-2.6311390000	-1.8775490000
H	2.6080300000	-2.9056660000	-2.5814400000
H	4.2941820000	-3.2074080000	-2.1355820000
H	3.6277180000	-1.5713330000	-2.0182790000
C	2.5806840000	-4.8346850000	0.1154720000
H	2.2520340000	-5.0652450000	1.1332050000

H	3.4967620000	-5.4042360000	-0.0770330000
H	1.8097470000	-5.1892220000	-0.5743790000
C	4.2547930000	-2.4563570000	1.0869400000
H	4.4809200000	-1.3926310000	0.9810730000
H	5.1677260000	-3.0241620000	0.8724970000
H	3.9778540000	-2.6464910000	2.1276700000

$(Me_3Si–CO_2)_3As_7$

Charge = 0 Multiplicity = 1

As	-0.2331750000	0.5083160000	-1.4662100000
As	0.4961370000	2.1904470000	0.1263520000
As	0.5541960000	0.9890130000	2.2703730000
C	-1.2644820000	3.0840480000	0.4543980000
As	-2.0189440000	-0.3915250000	-0.0946580000
As	-0.9168110000	-0.9468570000	2.0327940000
C	-2.0383880000	-2.2225470000	-0.9022370000
As	1.4209710000	-1.1776290000	-0.9120680000
As	1.4720400000	-1.1596520000	1.5471160000
C	3.0305040000	-0.0250020000	-1.2067740000
O	-1.6085660000	3.4644760000	1.5416750000
O	-2.4641280000	-3.1311410000	-0.0346360000
O	3.0585440000	0.9058190000	-1.9676590000
O	-1.9365770000	3.2830750000	-0.6721950000
O	4.0692720000	-0.4745040000	-0.5137660000
O	-1.7637920000	-2.4409480000	-2.0524720000
Si	-2.6406790000	-4.8131340000	-0.4406910000
C	-3.9173470000	-4.9657990000	-1.7908750000
H	-4.8744430000	-4.5368040000	-1.4802690000
H	-4.0870260000	-6.0188710000	-2.0378370000
H	-3.5853370000	-4.4500740000	-2.6949720000
C	-3.2281320000	-5.5384860000	1.1716150000
H	-2.4941340000	-5.3753400000	1.9656290000
H	-3.3869750000	-6.6172180000	1.0755370000
H	-4.1724990000	-5.0859140000	1.4864700000
C	-0.9727410000	-5.4744550000	-0.9460130000
H	-0.6188960000	-4.9796450000	-1.8533580000

H	-1.0313820000	-6.5504330000	-1.1398980000
H	-0.2310530000	-5.3164310000	-0.1574640000
Si	5.6448520000	0.2575760000	-0.5848240000
C	6.6173350000	-0.8057810000	0.5962960000
H	6.1899450000	-0.7681410000	1.6021420000
H	7.6556660000	-0.4649250000	0.6585260000
H	6.6249770000	-1.8498320000	0.2711320000
C	5.5039540000	2.0202240000	0.0043630000
H	4.8583110000	2.5993610000	-0.6599120000
H	6.4904550000	2.4947240000	0.0259020000
H	5.0883020000	2.0672220000	1.0151580000
C	6.2782390000	0.1314690000	-2.3337430000
H	6.3105510000	-0.9093580000	-2.6686030000
H	7.2929310000	0.5370960000	-2.4019780000
H	5.6368980000	0.6933680000	-3.0167150000
Si	-3.4402460000	4.1550290000	-0.7349890000
C	-3.1302830000	5.9002840000	-0.1561270000
H	-2.8091400000	5.9088800000	0.8880990000
H	-4.0447710000	6.4966610000	-0.2391500000
H	-2.3578780000	6.3864650000	-0.7590340000
C	-4.6967830000	3.2646250000	0.3147380000
H	-4.8156950000	2.2262370000	-0.0078540000
H	-5.6724620000	3.7556580000	0.2371010000
H	-4.3934370000	3.2651030000	1.3642150000
C	-3.8540660000	4.0757740000	-2.5497660000
H	-3.0701700000	4.5420510000	-3.1529240000
H	-4.7939380000	4.5976880000	-2.7557100000
H	-3.9642610000	3.0397750000	-2.8820600000

$(Et_3Ge)_3As_7$

Charge = 0 Multiplicity = 1

Ge	-2.1776230000	2.9861750000	0.3897510000
Ge	-1.6860310000	-3.4361760000	0.7121590000
As	1.8142140000	-1.1616190000	0.1029010000
As	-1.8511480000	-1.0208560000	0.1642570000
As	0.0843720000	2.0629250000	-0.0026150000

As	0.0414140000	0.0039730000	1.2710450000
As	1.2625630000	-0.7501260000	-2.2328540000
As	-1.1811080000	-0.9553700000	-2.1779410000
As	-0.1352110000	1.2620540000	-2.2937910000
C	-3.5216370000	2.3626130000	-0.9140710000
H	-3.0258370000	2.2847130000	-1.8870010000
H	-3.8000060000	1.3432880000	-0.6294320000
C	-1.9248820000	4.9374830000	0.2060810000
H	-1.6005780000	5.1380760000	-0.8208350000
H	-2.9125530000	5.4017120000	0.3116670000
C	-0.4155960000	-3.8055130000	2.1730180000
H	-0.3775520000	-4.8991500000	2.2579450000
H	0.5789260000	-3.4849570000	1.8482160000
C	-2.6630980000	2.5635720000	2.2570220000
H	-2.8463760000	1.4859440000	2.3148190000
H	-1.7826510000	2.7610780000	2.8775420000
C	-3.5192780000	-3.8581120000	1.3135570000
H	-3.4996620000	-4.8926570000	1.6786780000
H	-3.7499130000	-3.2274820000	2.1783250000
H	-1.7403330000	-5.5359840000	-0.6361440000
H	-1.8314550000	-4.1598970000	-1.7187920000
C	3.6339330000	1.0500670000	2.2510310000
H	3.3761780000	0.2094380000	2.9036710000
H	5.4070230000	-1.5388340000	2.3005130000
C	-4.7525060000	3.2603910000	-1.0226830000
H	-5.4562230000	2.8707090000	-1.7657490000
H	-5.2930340000	3.3358270000	-0.0747680000
H	-4.4876490000	4.2765210000	-1.3294010000
C	-0.7792540000	-3.1802910000	3.5153790000
H	-0.0493280000	-3.4468300000	4.2867730000
H	-0.8031430000	-2.0876120000	3.4575160000
H	-1.7604630000	-3.5133070000	3.8671110000
C	-0.9437610000	5.5360630000	1.2084010000
H	-0.8359210000	6.6166400000	1.0685770000
H	-1.2715990000	5.3725680000	2.2400060000
H	0.0515040000	5.0918590000	1.1087680000

C	-4.5814660000	-3.6908850000	0.2320010000
H	-5.5799710000	-3.9384880000	0.6067550000
H	-4.6184530000	-2.6595680000	-0.1340480000
H	-4.3875750000	-4.3374360000	-0.6294970000
C	-3.8674290000	3.3442980000	2.7789620000
H	-4.0618250000	3.1130360000	3.8316470000
H	-3.7145590000	4.4257340000	2.7075260000
H	-4.7785570000	3.1051340000	2.2232160000
C	4.9117840000	1.7302270000	2.7373030000
H	4.8155200000	2.0542850000	3.7789860000
H	5.7754790000	1.0597680000	2.6849070000
H	5.1500470000	2.6182170000	2.1445990000
C	0.1925690000	-4.7286710000	-1.1874270000
H	0.3341870000	-5.3903420000	-2.0482280000
H	0.6626450000	-3.7716150000	-1.4288730000
H	0.7469090000	-5.1582500000	-0.3479030000
H	3.1404770000	2.5741960000	-0.6420410000
C	5.2560690000	2.3833180000	-1.1134730000
H	5.2551800000	3.1860610000	-1.8583100000
H	5.6457280000	2.8063460000	-0.1828760000
H	5.9708790000	1.6280410000	-1.4531450000
C	-1.2862780000	-4.5619030000	-0.8590120000
Ge	3.7430650000	0.3581890000	0.4044830000
C	3.8549870000	1.8005290000	-0.9391470000
H	3.4919360000	1.3988530000	-1.8905380000
C	5.3075670000	-0.8370620000	0.2389960000
H	5.3004930000	-1.2584540000	-0.7721320000
H	6.2030560000	-0.2077050000	0.3014720000
C	5.3587310000	-1.9452040000	1.2852540000
H	6.2362990000	-2.5855230000	1.1489190000
H	4.4734300000	-2.5865020000	1.2333000000
H	2.7872350000	1.7426060000	2.2934900000

$(Et_3Ge–CO_2)_3As_7$

Charge = 0 Multiplicity = 1

As	-0.3676570000	0.0182020000	0.9365430000

As	-1.8848890000	0.6812660000	-0.8355140000
As	1.6223720000	0.9975590000	-0.0419920000
As	0.0032380000	-2.2570780000	0.1787920000
As	1.7004110000	0.0265500000	-2.2989540000
As	0.3406960000	-2.0059220000	-2.2436890000
As	-0.6674670000	0.1238250000	-2.8957520000
Ge	-1.0888990000	5.0035640000	0.5195570000
Ge	5.4502780000	-1.4137200000	0.7811360000
Ge	-4.5151920000	-2.7738540000	0.9867420000
O	4.0353350000	-0.3496890000	0.1153110000
O	-1.4490310000	3.2795280000	-1.8896750000
O	-2.2453170000	-3.6705480000	-0.7906200000
O	-1.3756140000	3.1434580000	0.3471850000
O	-2.6731620000	-2.3420620000	0.9644400000
O	2.7609610000	-0.7182460000	1.9227720000
C	-1.4907110000	2.6480850000	-0.8626070000
C	2.9472180000	-0.2268510000	0.8354240000
C	-1.9059320000	-2.8608540000	0.0377760000
C	6.6903390000	-1.2066680000	-0.7142200000
H	6.2089690000	-1.6272150000	-1.6027610000
C	8.0466720000	-1.8644760000	-0.4673570000
H	6.8048250000	-0.1347480000	-0.9027180000
C	0.5794110000	5.4125790000	-0.4155030000
H	1.2223850000	4.5339960000	-0.2966500000
C	1.2849280000	6.6677530000	0.0959680000
H	0.3504660000	5.4866900000	-1.4816560000
C	-0.9299010000	5.1122960000	2.4643430000
C	-2.1618730000	4.6040090000	3.2087830000
H	-0.7194610000	6.1557090000	2.7263410000
H	-0.0417070000	4.5380160000	2.7480010000
C	-2.7029750000	5.8601430000	-0.1764090000
H	-2.7637430000	5.6072210000	-1.2378950000
C	-2.7293250000	7.3731830000	0.0348320000
H	-3.5610460000	5.3865530000	0.3117000000
C	4.7963360000	-3.2473020000	0.9867050000
C	4.3577350000	-3.6321060000	2.3965260000

H	5.6018880000	-3.9034180000	0.6353450000
H	3.9727760000	-3.3695910000	0.2751960000
C	6.0690100000	-0.5610240000	2.4269070000
C	6.4664430000	0.9020570000	2.2537900000
H	6.9152340000	-1.1530640000	2.7959880000
H	5.2662870000	-0.6660350000	3.1613400000
C	-4.6810110000	-4.6725700000	1.4400450000
C	-4.7724440000	-5.6250890000	0.2512250000
H	-5.5667450000	-4.7609830000	2.0809610000
H	-3.8229280000	-4.9207660000	2.0734400000
C	-5.0568960000	-1.6005940000	2.4513180000
C	-4.3590800000	-1.9081740000	3.7740640000
H	-6.1450190000	-1.6817540000	2.5577260000
H	-4.8508090000	-0.5730870000	2.1337580000
C	-5.2384570000	-2.2474310000	-0.7491900000
H	-4.8364840000	-1.2540370000	-0.9740130000
C	-6.7661330000	-2.2370200000	-0.7861940000
H	-4.8266810000	-2.9307780000	-1.4960170000
H	8.5550810000	-1.4346610000	0.4016170000
H	8.7125650000	-1.7379020000	-1.3262440000
H	7.9520680000	-2.9406610000	-0.2901480000
H	6.8002210000	1.3354620000	3.2015550000
H	5.6267130000	1.5046610000	1.8965460000
H	7.2830650000	1.0210000000	1.5350130000
H	5.1807260000	-3.5443950000	3.1124760000
H	4.0075870000	-4.6684730000	2.4268440000
H	3.5448830000	-2.9900800000	2.7411390000
H	0.6716930000	7.5655340000	-0.0291550000
H	2.2198460000	6.8393150000	-0.4463440000
H	1.5368570000	6.5889270000	1.1578240000
H	-3.0531310000	5.1894440000	2.9621170000
H	-2.0236730000	4.6623720000	4.2928210000
H	-2.3717250000	3.5612310000	2.9568060000
H	-3.6559520000	7.8087920000	-0.3513280000
H	-1.9020590000	7.8690400000	-0.4821180000
H	-2.6632850000	7.6413160000	1.0942280000

H	-7.1324150000	-1.9386390000	-1.7731590000
H	-7.1880080000	-1.5359070000	-0.0594210000
H	-7.1876850000	-3.2245730000	-0.5724740000
H	-4.6807480000	-1.2206850000	4.5624920000
H	-3.2741120000	-1.8169200000	3.6774740000
H	-4.5760360000	-2.9238360000	4.1192720000
H	-4.8538590000	-6.6635720000	0.5873210000
H	-3.8913430000	-5.5414980000	-0.3879080000
H	-5.6502300000	-5.4141540000	-0.3671970000

$(^{n}Bu_3Sn)_3As_7$

Charge = 0 Multiplicity = 1

Sn	-3.5786010000	-0.8460740000	0.1936460000
Sn	2.7682600000	-2.5975040000	0.0751250000
As	1.8498520000	1.2988990000	-0.3874680000
As	0.1977400000	-1.9880600000	-0.2693400000
As	-1.7952050000	1.0738680000	-0.2847260000
As	0.1248260000	0.1493820000	0.8640510000
As	1.1262180000	0.9694970000	-2.6865220000
As	0.2610260000	-1.3270570000	-2.6101760000
As	-1.2972170000	0.5711920000	-2.6131960000
Sn	1.0262020000	3.8073570000	-0.0250410000
C	5.3515500000	-7.4636300000	1.4317720000
H	5.3086880000	-8.5541730000	1.5012240000
H	5.5541920000	-7.0749800000	2.4351570000
C	4.0593420000	-6.8864870000	0.8704680000
H	6.2076460000	-7.2051520000	0.7998860000
H	3.8618250000	-7.3121250000	-0.1213130000
C	4.0803460000	-5.3637290000	0.7616660000
H	3.2137850000	-7.1862090000	1.5023110000
H	4.9291990000	-5.0682870000	0.1306050000
H	4.2881150000	-4.9428860000	1.7549160000
C	2.7830190000	-4.7800940000	0.2055790000
H	2.5821730000	-5.1760350000	-0.7962910000
H	1.9331340000	-5.0752500000	0.8312010000
C	2.2334810000	-2.1562240000	5.6994670000

H	2.6034950000	-1.7416770000	6.6414400000
H	2.2437640000	-3.2473770000	5.7909100000
C	3.0733770000	-1.6953930000	4.5163290000
H	1.1898130000	-1.8450000000	5.5871230000
H	3.0727900000	-0.5994210000	4.4657990000
C	2.5834180000	-2.2512410000	3.1818320000
H	4.1193880000	-1.9920010000	4.6655940000
H	1.5359180000	-1.9527280000	3.0407300000
H	2.5775570000	-3.3484950000	3.2359610000
C	3.4196270000	-1.7875790000	1.9926730000
H	3.4113910000	-0.6955410000	1.9125660000
H	4.4677840000	-2.0846910000	2.1217710000
C	7.8846060000	-1.7509290000	-2.1973060000
H	8.4811400000	-1.3988780000	-3.0435640000
H	8.1492270000	-2.7983110000	-2.0181870000
C	6.3932720000	-1.5977240000	-2.4620300000
H	8.1905950000	-1.1787720000	-1.3152840000
H	6.1580980000	-0.5463880000	-2.6686850000
C	5.5257240000	-2.0791220000	-1.3014400000
H	6.1177940000	-2.1532140000	-3.3671960000
H	5.8049240000	-1.5216470000	-0.3973930000
H	5.7692070000	-3.1296680000	-1.0931760000
C	4.0302150000	-1.9232600000	-1.5702640000
H	3.7841370000	-0.8746790000	-1.7641270000
H	3.7359720000	-2.4881820000	-2.4618370000
C	-6.3032440000	-4.9019410000	-2.6665970000
H	-6.2720880000	-5.6912740000	-3.4228320000
H	-7.0678040000	-4.1801040000	-2.9723450000
C	-4.9469810000	-4.2299790000	-2.5031800000
H	-6.6358940000	-5.3557430000	-1.7271920000
H	-4.1930210000	-4.9773240000	-2.2264280000
C	-4.9513790000	-3.1181800000	-1.4564920000
H	-4.6210060000	-3.8124330000	-3.4639060000
H	-5.2803570000	-3.5396910000	-0.4970720000
H	-5.7123240000	-2.3767730000	-1.7342710000
C	-3.5920470000	-2.4415390000	-1.2971850000

H	-2.8259740000	-3.1659070000	-1.0016460000
H	-3.2623020000	-2.0121940000	-2.2492970000
C	-4.2977160000	-4.9042320000	4.0635250000
H	-4.0966230000	-5.2845640000	5.0689290000
H	-3.9377690000	-5.6510310000	3.3482370000
C	-3.6313530000	-3.5552750000	3.8316050000
H	-5.3841640000	-4.8334310000	3.9468000000
H	-3.9838200000	-2.8338330000	4.5794540000
C	-3.8912170000	-2.9922180000	2.4361480000
H	-2.5483910000	-3.6447050000	3.9831330000
H	-4.9763170000	-2.9134540000	2.2853210000
H	-3.5371440000	-3.7182210000	1.6924030000
C	-3.2246380000	-1.6392060000	2.1981800000
H	-3.5849190000	-0.8960550000	2.9184540000
H	-2.1417770000	-1.7183350000	2.3398080000
C	-9.0395720000	-0.3359890000	1.6934460000
H	-9.9624050000	0.2498540000	1.6594790000
H	-8.7647280000	-0.4608080000	2.7460200000
C	-7.9206160000	0.3352470000	0.9091110000
H	-9.2630660000	-1.3297530000	1.2916410000
H	-8.2298860000	0.4725780000	-0.1346370000
C	-6.6116760000	-0.4504540000	0.9395590000
H	-7.7408530000	1.3421220000	1.3064400000
H	-6.7988880000	-1.4596560000	0.5495620000
H	-6.3081680000	-0.5863960000	1.9864630000
C	-5.4883330000	0.2201760000	0.1512430000
H	-5.7776370000	0.3432350000	-0.8988280000
H	-5.3009760000	1.2272520000	0.5406110000
C	-3.9261540000	6.1243470000	-1.5554630000
H	-4.5958070000	6.4382980000	-2.3611360000
H	-3.7464190000	6.9949810000	-0.9160130000
C	-2.6206180000	5.5613500000	-2.0999600000
H	-4.4566330000	5.3783870000	-0.9546810000
H	-2.8312310000	4.7137010000	-2.7641560000
C	-1.6641830000	5.1009590000	-1.0030690000
H	-2.1207540000	6.3158870000	-2.7204280000

H	-2.1688080000	4.3430790000	-0.3898880000
H	-1.4604440000	5.9472700000	-0.3332360000
C	-0.3574230000	4.5356740000	-1.5517170000
H	-0.5591670000	3.7082230000	-2.2393010000
H	0.1840590000	5.2970020000	-2.1251300000
C	6.2629720000	4.9274990000	1.8497660000
H	7.1667040000	5.5397490000	1.7827540000
H	6.5547260000	3.8853940000	1.6833060000
C	5.2097580000	5.3697320000	0.8432610000
H	5.8860820000	5.0034570000	2.8750790000
H	4.9571690000	6.4245570000	1.0101140000
C	3.9326230000	4.5359560000	0.9065990000
H	5.6212850000	5.3142220000	-0.1723970000
H	3.5271850000	4.5884900000	1.9265360000
H	4.1890500000	3.4804870000	0.7439830000
C	2.8730340000	4.9718650000	-0.1006770000
H	2.5944360000	6.0203770000	0.0626660000
H	3.2653270000	4.9107340000	-1.1220970000
C	-0.3289660000	6.8921590000	4.5201690000
H	-0.7216340000	6.9295040000	5.5401450000
H	-0.9431180000	7.5571580000	3.9040790000
C	-0.3337700000	5.4727370000	3.9699740000
H	0.6850160000	7.3051480000	4.5397750000
H	0.2585300000	4.8192820000	4.6227010000
C	0.2135660000	5.3797220000	2.5473140000
H	-1.3547730000	5.0717610000	3.9856370000
H	1.2338450000	5.7861260000	2.5344170000
H	-0.3789020000	6.0404990000	1.9004700000
C	0.2083240000	3.9564790000	1.9939600000
H	0.7971660000	3.2933510000	2.6371840000
H	-0.8085870000	3.5506740000	1.9725900000

($^{n}Bu_3Sn–CO_2)_3As_7$

Charge = 0 Multiplicity = 1

As	-0.2577170000	-0.0394600000	0.7078430000
As	-1.9634510000	0.5085280000	-0.9278520000

As	1.5266570000	1.2446200000	-0.3169240000
As	0.3565740000	-2.1942220000	-0.2254770000
As	1.5730360000	0.4359750000	-2.6370130000
As	0.5011550000	-1.7624350000	-2.6411100000
As	-0.8209810000	0.2440540000	-3.0869780000
O	4.0406790000	0.0439410000	-0.4285420000
O	-1.8726340000	3.1944460000	-1.8408890000
O	-1.8193420000	-3.7472300000	-1.1703290000
O	-1.7063230000	2.9621960000	0.3688690000
O	-2.2006860000	-2.7172220000	0.7660740000
O	3.0110220000	-0.3472450000	1.5057200000
C	-1.8095560000	2.5051340000	-0.8431060000
C	3.0371500000	0.1355040000	0.3905570000
C	-1.4741330000	-3.0068040000	-0.2711360000
Sn	5.5725110000	-1.1615900000	0.3999040000
C	9.6796260000	-0.1469230000	4.1467300000
H	10.0092860000	0.3832980000	5.0444180000
H	10.3560620000	0.1297610000	3.3313490000
C	8.2351290000	0.1857560000	3.8006180000
H	9.8058870000	-1.2189910000	4.3300540000
H	7.5821590000	-0.0706160000	4.6439700000
C	7.7362160000	-0.5351980000	2.5509580000
H	8.1282480000	1.2676760000	3.6529720000
H	7.8520160000	-1.6173310000	2.7009890000
H	8.3942410000	-0.2778130000	1.7098040000
C	6.2856830000	-0.2024450000	2.2069770000
H	5.6069170000	-0.4842230000	3.0168700000
H	6.1633490000	0.8762900000	2.0582250000
C	5.8149520000	-6.3776980000	2.5444910000
H	5.3573260000	-7.3659890000	2.6422070000
H	5.9195650000	-5.9601020000	3.5512610000
C	4.9851770000	-5.4638140000	1.6537900000
H	6.8225660000	-6.5178020000	2.1392500000
H	4.8701820000	-5.9166470000	0.6611680000
C	5.5899340000	-4.0712010000	1.4962450000
H	3.9716850000	-5.3657820000	2.0613440000

H	6.6069130000	-4.1734250000	1.0929650000
H	5.7046190000	-3.6228200000	2.4921490000
C	4.7512140000	-3.1556550000	0.6050500000
H	4.6453420000	-3.5835400000	-0.3977170000
H	3.7434650000	-3.0350230000	1.0134190000
C	9.9430980000	-3.0760900000	-2.6641640000
H	10.6007250000	-2.9407850000	-3.5272280000
H	9.4492340000	-4.0472120000	-2.7732670000
C	8.9245190000	-1.9500900000	-2.5553960000
H	10.5744590000	-3.1260830000	-1.7708980000
H	9.4433210000	-0.9861810000	-2.4807640000
C	7.9871100000	-2.1017990000	-1.3603440000
H	8.3251050000	-1.9009730000	-3.4729030000
H	8.5924490000	-2.1572910000	-0.4450870000
H	7.4733300000	-3.0695610000	-1.4372750000
C	6.9644130000	-0.9713020000	-1.2541780000
H	7.4704160000	-0.0040940000	-1.1600910000
H	6.3566930000	-0.9171470000	-2.1641870000
Sn	-4.1038560000	-3.6340050000	0.6247750000
C	-7.9383430000	-3.5690820000	4.8054690000
H	-8.2938620000	-3.1069170000	5.7305360000
H	-7.7355970000	-4.6237760000	5.0188560000
C	-6.6977360000	-2.8676950000	4.2704880000
H	-8.7577330000	-3.5316020000	4.0800870000
H	-6.9170030000	-1.8070440000	4.0954290000
C	-6.1701400000	-3.4839940000	2.9775140000
H	-5.9022920000	-2.8916000000	5.0257120000
H	-6.9718100000	-3.4628920000	2.2265520000
H	-5.9567410000	-4.5465300000	3.1570160000
C	-4.9238270000	-2.7796800000	2.4430370000
H	-5.1343010000	-1.7227180000	2.2461920000
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C	-8.6972480000	-2.1321140000	-2.3249500000
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H	-9.0308190000	-1.5048250000	-1.4917080000
C	-7.1781260000	-2.2112500000	-2.3800560000

H	-9.1406210000	-3.1240880000	-2.1886050000
H	-6.8683230000	-2.8170310000	-3.2405340000
C	-6.5623230000	-2.7990680000	-1.1128120000
H	-6.7587580000	-1.2115670000	-2.5471320000
H	-6.9893700000	-3.7976080000	-0.9462240000
H	-6.8778170000	-2.1911980000	-0.2539730000
C	-5.0379090000	-2.8748120000	-1.1742890000
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H	-4.6101230000	-1.8795490000	-1.3403690000
C	-6.0392550000	-8.9017000000	0.0097150000
H	-5.8431680000	-9.9766190000	0.0519530000
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C	-4.8101390000	-8.0935360000	0.4012040000
H	-6.8807090000	-8.6916600000	0.6781860000
H	-4.4893540000	-8.3710030000	1.4131260000
C	-5.0440120000	-6.5858500000	0.3513270000
H	-3.9731630000	-8.3443560000	-0.2619200000
H	-5.8868050000	-6.3393400000	1.0115250000
H	-5.3671930000	-6.3138320000	-0.6624720000
C	-3.8061930000	-5.7775180000	0.7400100000
H	-3.4861000000	-6.0254710000	1.7576380000
H	-2.9718610000	-6.0053480000	0.0702520000
Sn	-1.5609320000	5.0733240000	0.3862480000
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H	-1.6817890000	8.1850560000	6.2377180000
H	-2.8036160000	8.4715810000	4.9040150000
C	-1.4947340000	6.7639650000	4.6002350000
H	-1.0982620000	8.8962890000	4.7301590000
H	-0.4802830000	6.4569840000	4.8835610000
C	-1.6324390000	6.6768420000	3.0826090000
H	-2.1713140000	6.0333070000	5.0607440000
H	-0.9611290000	7.4172200000	2.6265520000
H	-2.6494960000	6.9847690000	2.8041630000
C	-1.3358700000	5.2821530000	2.5337060000
H	-0.3164330000	4.9757770000	2.7924090000
H	-2.0050690000	4.5415480000	2.9856770000

C	2.8757470000	8.4357760000	-0.6899510000
H	3.7836560000	8.6100400000	-1.2739520000
H	3.1613340000	8.4105640000	0.3668660000
C	2.1845470000	7.1442610000	-1.1040930000
H	2.2189830000	9.3001890000	-0.8332290000
H	1.9353770000	7.1818090000	-2.1716960000
C	0.9125950000	6.8627270000	-0.3085970000
H	2.8728810000	6.2986810000	-0.9837280000
H	0.2289480000	7.7144640000	-0.4275170000
H	1.1659410000	6.8281370000	0.7596090000
C	0.2258020000	5.5656730000	-0.7318270000
H	-0.0505310000	5.5881260000	-1.7899480000
H	0.9011880000	4.7120650000	-0.6035780000
C	-4.7137450000	9.3603860000	-1.5207680000
H	-5.6721670000	9.7026200000	-1.9207780000
H	-3.9420250000	9.6006860000	-2.2593130000
C	-4.7368640000	7.8693040000	-1.2155320000
H	-4.5023640000	9.9464330000	-0.6202930000
H	-5.5367620000	7.6494820000	-0.4973870000
C	-3.4139340000	7.3502290000	-0.6583090000
H	-4.9828610000	7.3074050000	-2.1249210000
H	-3.1686990000	7.9166320000	0.2505580000
H	-2.6165700000	7.5776570000	-1.3784740000
C	-3.4398140000	5.8508570000	-0.3627030000
H	-4.2210700000	5.6143020000	0.3676610000
H	-3.6576560000	5.2808850000	-1.2705570000

7. Crystallography Tables

Table S8. Crystallography data for molecules **6**-**8**.

Identification code	**6**	**7**	**8**
Empirical formula	$C_{32.5}H_{44.5}Ge_3N_{3.5}O_3P_7$	$C_{39}H_{60}Ge_3N_3O_3P_7$	$C_{35}H_{53}Ge_3N_3O_{9.5}P_7S_3$
Formula weight / g mol^{-1}	966.77	1053.46	1198.54
Temperature / K	100.00(10)	100.0(3)	100.0(3)
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/n$	$P2_1/n$	P-1
a/ Å	10.93920(10)	14.6729(2)	13.2603(3)
b/ Å	20.9710(2)	20.5725(3)	13.7420(3)
c/ Å	18.2317(2)	15.8849(2)	14.7414(3)
□/□°	90	90	73.987(2)
□/□°	89.9510(10)	94.2470(10)	87.041(2)
□/□°	90	90	89.564(2)
Volume / Å^3	4182.46(7)	4781.82(11)	2578.49(10)
Z	4	4	2
□$_{calc}$ g cm^{-3}	1.535	1.463	1.544
□□/ mm^{-1}	5.375	4.743	5.680
F(000)	1956.0	2160.0	2160.01218.0
Crystal size / mm^3	0.186 x 0.155 x 0.06	0.18 x 0.1 x 0.03	0.26 x 0.12 x 0.03
Radiation	Cu K□ (□□= 1.54184)	Cu K□ (□□= 1.54184)	Cu K□ (□□= 1.54184)
2□□range for data collection / °	6.424 to 151.768	7.042 to 152.48	6.246 to 152.818
Index ranges	-13 ≤ h ≤ 13, -25 ≤ k ≤ 26, -15 ≤ l ≤ 22	-18 ≤ h ≤ 18, -22 ≤ k ≤ 25, -19 ≤ l ≤ 17	-15 ≤ h ≤ 16, -17 ≤ k ≤ 17, -17 ≤ l ≤ 18
Reflections collected	19585	29680	32445
Independent reflections	7766 [R_{int} = 0.0176, R_{sigma} = 0.0200]	9613 [R_{int} = 0.0233, R_{sigma} = 0.0219]	10226 [R_{int} = 0.0208, R_{sigma} = 0.0202]
Data/restraints/parameters	7766/0/451	9613/159/580	10226/163/617
Goodness-of-fit on F^2	1.058	1.181	1.047
Final R indices [I>=2□□(I)]	R_1 = 0.0311, wR_2 = 0.0819	R_1 = 0.0475, wR_2 = 0.1086	R_1 = 0.0300, wR_2 = 0.0765
Final R indices [all data]	R_1 = 0.0328, wR_2 = 0.0829	R_1 = 0.0489, wR_2 = 0.1094	R_1 = 0.0314, wR_2 = 0.0774
Largest diff. peak/hole/ e Å^{-3}	1.22/-0.80	0.79/-0.64	1.13/-0.65
CCDC	2202019	2202020	2202022

Table S9. Crystallography data for **11** and **5**.

Identification code	**11**	**5**
Empirical formula	$C_{33}H_{51}As_7N_3O_9S_3Si_3$	$C_{30}H_{75}As_{11}Ge_5$
Formula weight / g mol^{-1}	1338.66	1622.97
Temperature / K	99.99(10)	100.00(10)
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a/ Å	13.8023(3)	7.6695(3)
b/ Å	13.5652(3)	14.0092(6)
c/ Å	14.0438(3)	24.6674(7)
□/□°	94.859(2)	85.802(3)
□/□°	93.493(2)	84.724(3)
□/□°	91.697(2)	84.724(3)
Volume / Å^3	2477.18(11)	2608.60(17)
Z	2	2
□$_{calc}$ g cm^{-3}	1.795	2.066
□□/ mm^{-1}	7.678	11.185
F(000)	1326.0	1156.0
Crystal size / mm^3	0.092 x 0.053 x 0.024	0.12 x 0.1 x 0.08
Radiation	Cu K□ (□□= 1.54184)	Cu Kα (λ = 1.54184)
2□□range for data collection / °	6.33 to 151.664	3.604 to 152.726
Index ranges	-16 ≤ h ≤ 16, -17 ≤ k ≤ 16, -17 ≤ l ≤ 11	-9 ≤ h ≤ 8, -17 ≤ k ≤ 16, -27 ≤ l ≤ 30
Reflections collected	32941	27987
Independent reflections	9935 [R_{int} = 0.0209, R_{sigma} = 0.0196]	10433 [R_{int} = 0.0572, R_{sigma} = 0.0695]
Data/restraints/parameters	9935/0/535	10433/203/504
Goodness-of-fit on F^2	1.044	1.042
Final R indices [I>=2□□(I)]	R_1 = 0.0224, wR_2 = 0.0598	R_1 = 0.0564, wR_2 = 0.1504
Final R indices [all data]	R_1 = 0.0237, wR_2 = 0.0606	R_1 = 0.0809, wR_2 = 0.1672
Largest diff. peak/hole/ e Å^{-3}	0.74/-0.84	1.57/-1.06
CCDC	2202021	2202018

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