Supporting Information

A Computational Study to Determine Whether Substituents Make E_{13}≡Nitrogen (E_{13} = B, Al, Ga, In, and Tl) Triple Bonds Synthetically Accessible?

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Theoretical Methods

Using the Gaussian 09 program package,[1] all geometries are fully optimized using hybrid density functional theory at the M06-2X,[2] B3LYP,[3,4] and B3PW91[4,5] levels, in conjunction with the Def2-TZVP[6] and LANL2DZ+dp[7] basis sets. These DFT calculations are signified as M06-2X/Def2-TZVP, B3PW91/Def2-TZVP and B3LYP/LANL2DZ+dp, respectively. In order to confirm that the reactants and products have no imaginary frequencies and that the transition states possess only one imaginary frequency, frequency calculations were performed for all structures. Thermodynamic corrections to 298 K, heat capacity corrections and entropy corrections (ΔS) are applied to the three levels of DFT. The relative free energy (ΔG) at 298 K is also computed at the same levels of theory.

Next, Si*i*PrDis$_2$–E$_{13}$≡N–Si*i*PrDis$_2$, Tbt–E$_{13}$≡N–Tbt, and Ar*–E$_{13}$≡N–Ar* are the model reactants for this study. It is known that the B3LYP functional fails to describe nonvalent interactions, such as the London dispersion correctly. As a result, for large ligands, calculations were performed using dispersion-corrected M06-2X method.[2] Because of the limitations of the available memory size and CPU time, frequencies are not computed at the M06-2X/Def2-TZVP level of theory for the triply bonded L′-Tl≡N-R′ systems that have bulky ligands (L′), so the zero-point energies and the Gibbs free energies that are derived using M06-2X/Def2-TZVP cannot be used for these systems.

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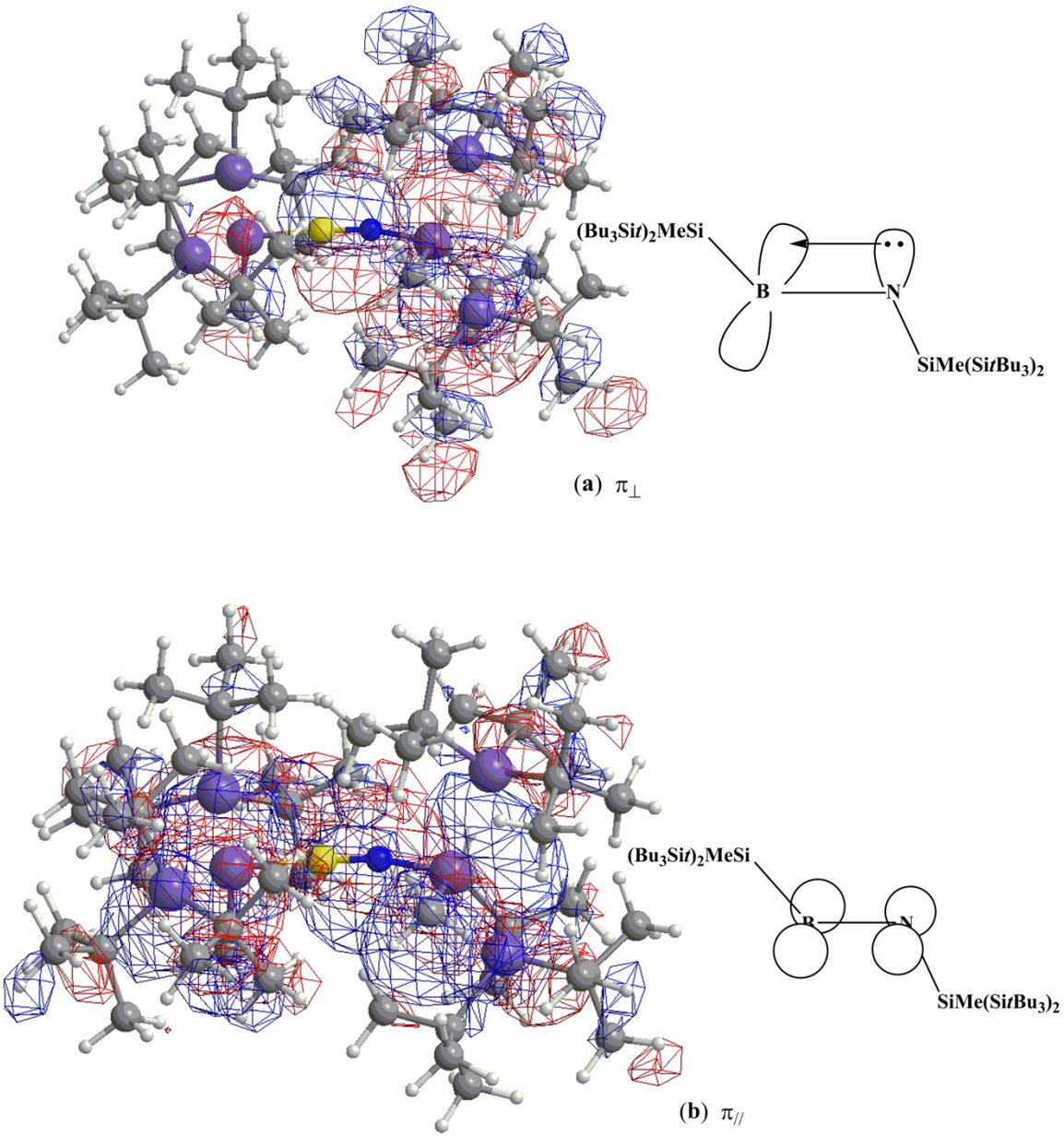


Figure S1: The natural B≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (SiMe(Si*t*Bu$_3$)$_2$)-Tl≡N-(SiMe(Si*t*Bu$_3$)$_2$. Also see Figure 1.

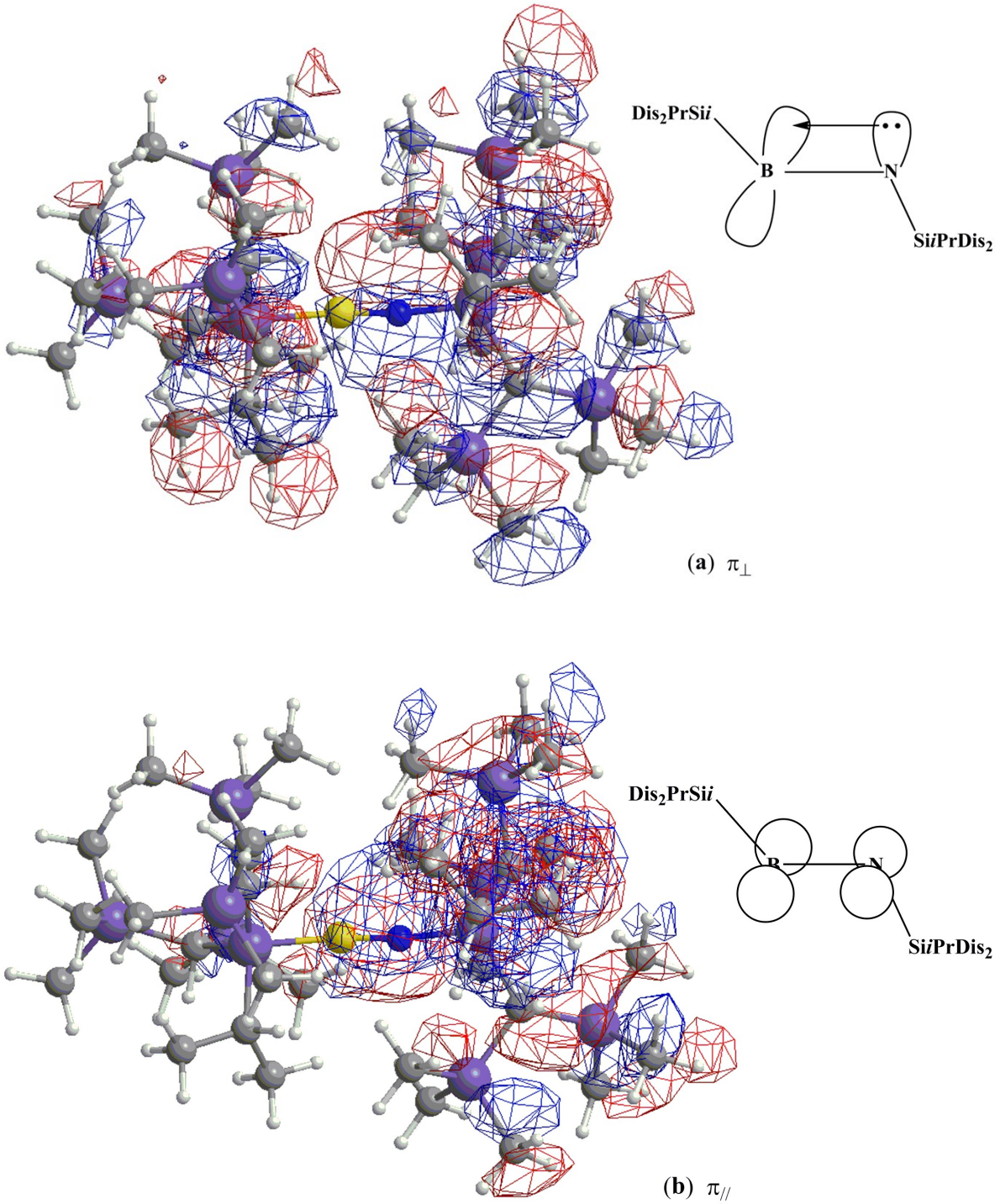


Figure S2: The natural B≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Si*i*PrDis$_2$)-B≡N-(Si*i*PrDis$_2$). Also see Figure 1.

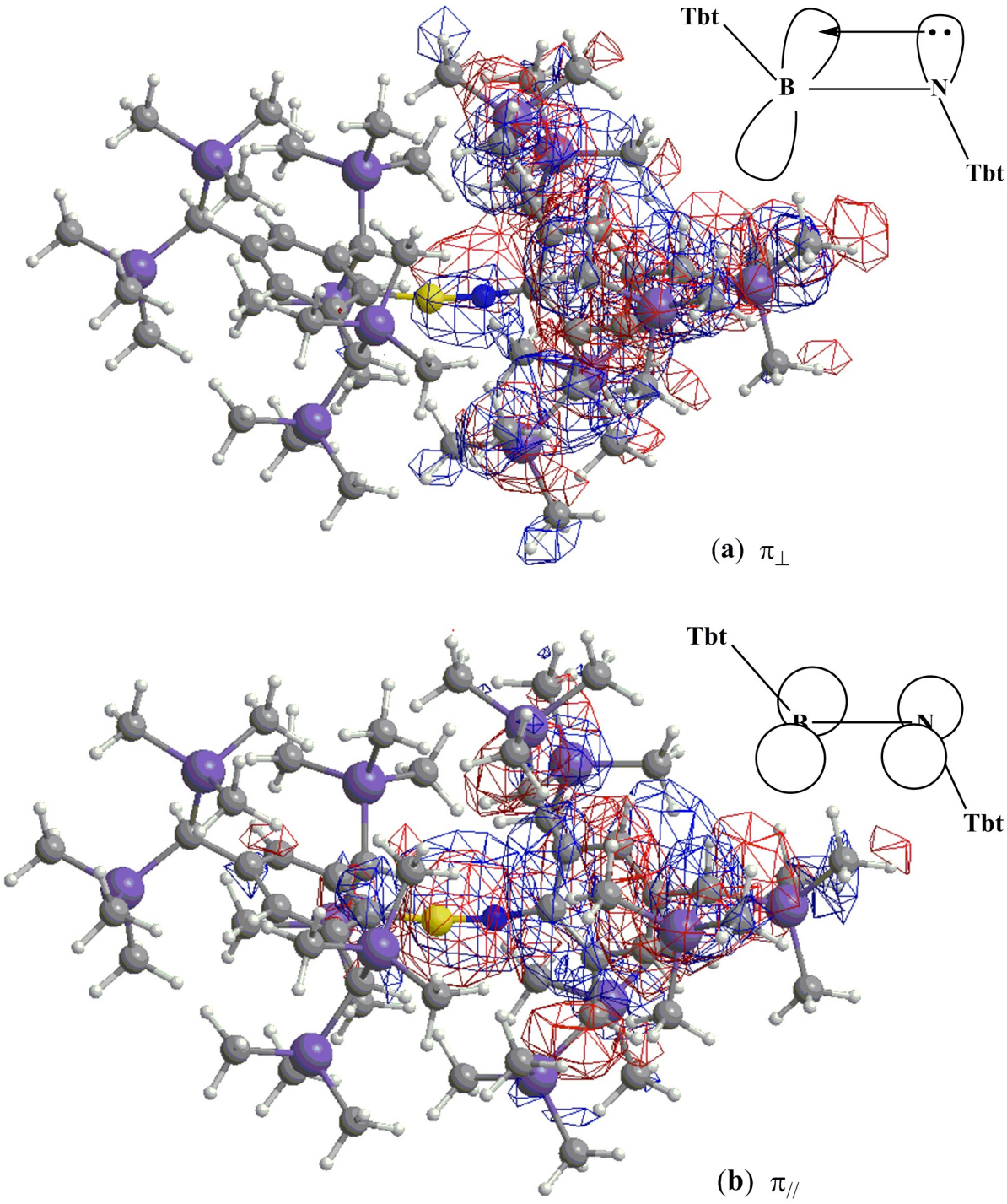


Figure S3: The natural B≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) of (Tbt)-B≡N-(Tbt). For comparison, also see Figure 1.

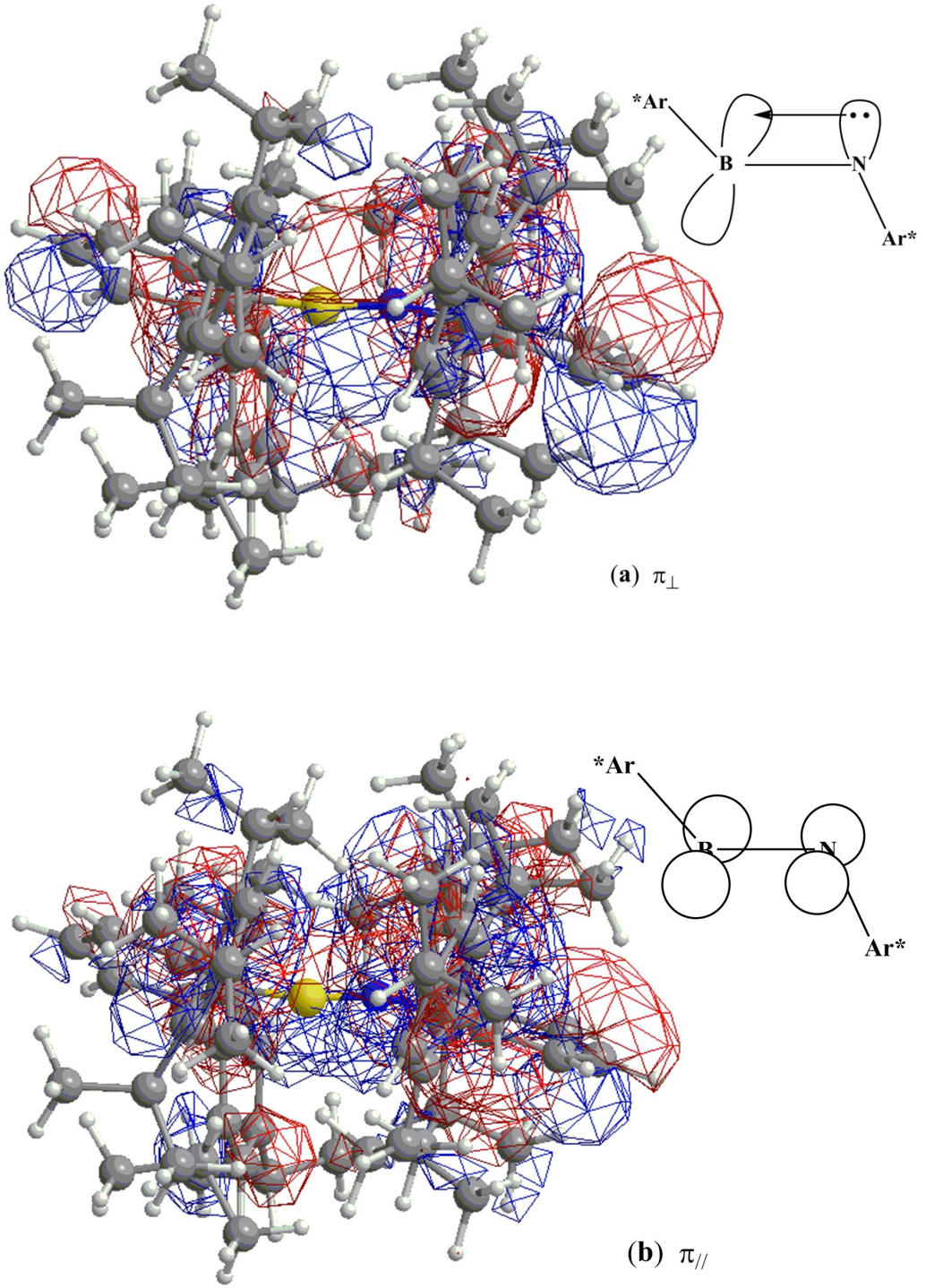


Figure S4: The natural B≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) of (Ar*)-B≡N-(Ar*). For comparison, also see Figure 1.

Table S1

The major geometrical parameters, the natural charge densities (Q_{Al} and Q_N), the singlet□triplet energy splitting (ΔE_{Al} and ΔE_N), the HOMO-LUMO energy gaps, the binding energies (BE), and the Wiberg bond index (WBI) for L-Al≡N-L using the M06-2X/Def2-TZVP, B3PW91/Def2-TZVP (in round brackets) and B3LYP/LANL2DZ+dp (in square brackets) levels of theory.

L	**F**	**OH**	**H**	**CH_3**	**SiH_3**
Al≡N (Å)	1.752 (1.727) [1.702]	1.753 (1.727) [1.695]	1.649 (1.622) [1.608]	1.632 (1.618) [1.613]	1.655 (1.642) [1.636]
∠L-Al-N (°)	147.8 (146.6) [150.4]	138.0 (136.5) [143.5]	163.3 (168.5) [180]	179.4 (179.8) [179.1]	180.0 (180.0) [179.9]
∠Al-N-L (°)	123.6 (126.9) [128.0]	135.0 (138.6) [139.7]	149.5 (160.5) [179.1]	179.4 (179.9) [178.8]	180.0 (180.0) [179.2]
∠L-Al-N-L (°)	180.0 (179.3) [180.0]	160.7 (163.0) [164.7]	179.5 (180.0) [170.4]	179.0 (177.7) [179.7]	165.3 (171.7) [166.9]
Q_{Al}	0.9462 (0.6605) [0.6986]	0.6999 (0.5247) [0.5702]	0.6724 (0.3937) [0.3871]	0.3896 (0.3174) [0.3453]	0.2064 (0.3500) [0.3240]
Q_N	-0.4236 (-0.2307) [-0.2492]	-0.4914 (-0.3337) [-0.3384]	-0.7205 (-0.5978) [-0.6122]	-0.5466 (-0.3488) [-0.3633]	-0.5525 (-0.3794) [-0.4074]
ΔE_{Al} for Al (kcal/mol)	74.41 (72.09) [80.43]	68.50 (66.72) [73.47]	41.41 (39.34) [44.33]	45.59 (43.43) [48.82]	32.36 (29.17) [33.47]

ΔE_N for N (kcal/mol)	-46.00 (-48.48) [-45.47]	-21.39 (-21.68) [-19.91]	-50.89 (-55.08) [-49.44]	46.76 (48.23) [50.99]	44.87 (46.86) [48.02]
HOMO - LUMO (kcal/mol)	67.24 (68.61) [129.0]	68.32 (69.21) [119.5]	102.8 (109.5) [170.1]	92.14 (96.92) [148.8]	104.4 (105.1) [156.3]
BE (kcal/mol)	85.36 (83.82) [90.69]	84.48 (84.71) [90.30]	117.0 (118.3) [124.9]	105.4 (107.6) [115.7]	127.2 (129.8) [137.7]
WBI	1.307 (1.378) [1.348]	1.283 (1.347) [1.354]	1.393 (1.470) [1.406]	1.315 (1.353) [1.311]	1.128 (1.174) [1.122]

(1) The natural charge density on the aluminum atom; (2) The natural charge density on the nitrogen atom; (3) ΔE_{Al} = E(triplet state for L□Al) – E(singlet state for L□Al); (4) ΔE_N = E(triplet state for L□N) – E(singlet state for L□N) and (5) BE = E(singlet state for L□Al) + E(triplet state for L□N) – E(singlet state for L-Al≡N-L). (6) The Wiberg bond index (WBI) for the Al≡N bond: see reference (69,70).

Table S2

The major geometrical parameters, the natural charge densities (Q_{Ga} and Q_N), the singlet□triplet energy splitting (ΔE_{Ga} and ΔE_N), the HOMO-LUMO energy gaps, the binding energies (BE), and the Wiberg bond index (WBI) for L-Ga≡N-L using the M06-2X/Def2-TZVP, B3PW91/Def2-TZVP (in round brackets) and B3LYP/LANL2DZ+dp (in square brackets) levels of theory.

L	**F**	**OH**	**H**	**CH_3**	**SiH_3**
Ga≡N (Å)	1.780 (1.793) [1.796]	1.792 (1.804) [1.799]	1.677 (1.694) [1.697]	1.669 (1.679) [1.680]	1.662 (1.672) [1.681]
∠L-Ga-N (°)	148.7 (158.0) [160.7]	138.4 (140.1) [143.9]	161.8 (164.1) [164.1]	157.4 (159.5) [161.7]	178.2 (175.9) [179.6]
∠Ga-N-L (°)	119.2 (114.7) [112.9]	129.4 (126.9) [125.9]	131.4 (122.0) [127.0]	151.3 (146.1) [151.2]	176.2 (168.1) [178.7]
∠L-Ga-N-L (°)	180.0 (180.0) [180.0]	159.1 (158.6) [155.2]	179.7 (180.0) [180.0]	179.8 (179.9) [178.6]	175.8 (166.4) [175.0]
Q_{Ga}	0.9674 (0.6484) [0.8312]	0.6360 (0.4678) [0.6558]	0.6475 (0.2801) [0.4004]	0.4227 (0.2604) [0.4983]	0.1796 (0.2568) [0.4004]
Q_N	-0.4077 (-0.1937) [-0.2952]	-0.4268 (-0.2894) [-0.3764]	-0.6746 (-0.5308) [-0.6604]	-0.5541 (-0.3776) [-0.4815]	-0.4913 (-0.4463) [-0.5829]
ΔE_{Ga} for Ga (kcal/mol)	85.05 (89.46) [89.33]	76.30 (77.73) [78.14]	46.07 (46.80) [46.66]	49.28 (48.32) [49.54]	35.68 (33.92) [32.77]

ΔE_N for N (kcal/mol)	-46.00 (-48.48) [-45.47]	-21.39 (-21.68) [-19.91]	-50.89 (-55.08) [-49.44]	46.76 (48.23) [50.99]	44.87 (46.86) [48.02]
HOMO - LUMO (kcal/mol)	72.16 (76.70) [136.4]	74.45 (79.19) [130.5]	106.0 (111.2) [170.1]	91.47 (101.7) [152.9]	108.1 (110.0) [158.5]
BE (kcal/mol)	84.97 (84.43) [84.86]	82.21 (81.24) [80.50]	112.38 (111.25) [111.53]	97.82 (95.47) [98.49]	120.19 (118.59) [121.57]
WBI	1.307 (1.323) [1.287]	1.265 (1.283) [1.284]	1.448 (1.525) [1.455]	1.384 (1.434) [1.371]	1.205 (1.287) [1.201]

(1) The natural charge density on the gallium atom; (2) The natural charge density on the nitrogen atom; (3) ΔE_{Ga} = E(triplet state for L□Ga) – E(singlet state for L□Ga); (4) ΔE_N = E(triplet state for L□N) – E(singlet state for L□N) and (5) BE = E(singlet state for L□Ga) + E(triplet state for L□N) – E(singlet state for L-Ga≡N-L). (6) The Wiberg bond index (WBI) for the Ga≡N bond: see reference (69,70).

Table S3

The major geometrical parameters, the natural charge densities (Q_{In} and Q_N), the singlet□triplet energy splitting (ΔE_{In} and ΔE_N), the HOMO-LUMO energy gaps, the binding energies (BE), and the Wiberg bond index (WBI) for L-In≡N-L using the M06-2X/Def2-TZVP, B3PW91/Def2-TZVP (in round brackets) and B3LYP/LANL2DZ+dp (in square brackets) levels of theory.

L	**F**	**OH**	**H**	**CH_3**	**SiH_3**
In≡N (Å)	1.970 (2.009) [2.009]	2.018 (2.065) [2.073]	1.847 (1.887) [1.894]	1.848 (1.888) [1.894]	1.828 (1.875) [1.873]
∠L-In-N (°)	157.6 (160.8) [160.8]	132.7 (135.3) [140.4]	160.5 (165.9) [166.5]	151.7 (156.5) [157.2]	167.1 (170.0) [169.7]
∠In-N-L (°)	115.2 (112.7) [112.7]	127.3 (126.1) [123.1]	125.4 (114.1) [115.2]	142.1 (135.4) [136.2]	152.5 (148.3) [145.0]
∠L-In-N-L (°)	180.0 (180.0) [180.0]	155.8 (168.8) [157.5]	180.0 (180.0) [180.0]	178.1 (180.0) [178.0]	180.0 (171.7) [176.9]
Q_{In}	1.1782 (0.8271) [1.0077]	0.7438 (0.6360) [0.8227]	0.7966 (0.4233) [0.5836]	0.5921 (0.4646) [0.7215]	0.3959 (0.4503) [0.6325]
Q_N	-0.4874 (-0.2572) [-0.3418]	-0.4914 (-0.3337) [-0.3384]	-0.7205 (-0.5978) [-0.6122]	-0.5466 (-0.3488) [-0.3633]	-0.7186 (-0.5036) [-0.6757]
ΔE_{In} for In (kcal/mol)	80.04 (86.59) [84.22]	72.04 (73.84) [72.75]	45.31 (46.80) [44.75]	45.53 (46.02) [45.05]	36.66 (35.90) [33.35]

ΔE_N for N (kcal/mol)	-46.00 (-48.48) [-45.47]	-21.39 (-21.68) [-19.91]	-50.89 (-55.08) [-49.44]	46.76 (48.23) [50.99]	44.87 (46.86) [48.02]
HOMO - LUMO (kcal/mol)	67.20 (67.11) [127.4]	66.77 (70.95) [123.1]	90.72 (96.87) [142.4]	75.90 (83.97) [130.6]	89.98 (95.68) [140.3]
BE (kcal/mol)	71.73 (70.18) [67.51]	69.03 (66.36) [63.19]	93.81 (90.59) [88.79]	75.91 (71.33) [71.63]	100.3 (96.30) [97.58]
WBI	1.183 (1.165) [1.153]	1.084 (1.024) [1.024]	1.343 (1.406) [1.337]	1.294 (1.321) [1.270]	1.113 (1.182) [1.115]

(1) The natural charge density on the indium atom; (2) The natural charge density on the nitrogen atom; (3) ΔE_{In} = E(triplet state for L□In) – E(singlet state for L□In); (4) ΔE_N = E(triplet state for L□N) – E(singlet state for L□N) and (5) BE = E(singlet state for L□In) + E(triplet state for L□N) – E(singlet state for L-In≡N-L). (6) The Wiberg bond index (WBI) for the In≡N bond: see reference (69,70).

Table S4

The major geometrical parameters, the natural charge densities (Q_{Tl} and Q_N), the singlet□triplet energy splitting (ΔE_{Tl} and ΔE_N), the HOMO-LUMO energy gaps, the binding energies (BE), and the Wiberg bond index (WBI) for L-Tl≡N-L using the M06-2X/Def2-TZVP, B3PW91/Def2-TZVP (in round brackets) and B3LYP/LANL2DZ+dp (in square brackets) levels of theory.

L	**F**	**OH**	**H**	**CH_3**	**SiH_3**
Tl≡N (Å)	2.008 (2.068) [2.060]	2.087 (2.207) [2.300]	1.869 (1.923) [1.927]	1.873 (1.932) [1.940]	1.849 (1.917) [1.916]
∠L-Tl-N (°)	158.0 (167.6) [172.4]	127.3 (135.0) [134.5]	163.7 (169.8) [170.7]	152.0 (164.8) [162.4]	164.9 (169.0) [169.2]
∠Tl-N-L (°)	112.4 (109.5) [105.5]	126.5 (123.1) [119.9]	114.0 (109.4) [109.8]	134.6 (125.5) [126.5]	139.0 (132.0) [132.1]
∠L-Tl-N-L (°)	179.8 (178.1) [178.6]	171.1 (157.7) [144.3]	180.0 (179.9) [179.9]	177.8 (179.8) [179.7]	179.9 (179.0) [179.0]
Q_{Tl}	1.0732 (0.8345) [0.9394]	0.6773 (0.6205) [0.6721]	0.7244 (0.4702) [0.5126]	0.5257 (0.5899) [0.6613]	0.3866 (0.5192) [0.5049]
Q_N	-0.4013 (-0.2593) [-0.2628]	-0.3936 (-0.3503) [-0.3054]	-0.7202 (-0.6547) [-0.7401]	-0.6537 (-0.5300) [-0.5963]	-0.7169 (-0.5911) [-0.6825]
ΔE_{Tl} for Tl (kcal/mol)	102.2 (103.7) [102.1]	86.32 (80.73) [82.09]	54.67 (52.90) [51.15]	48.42 (44.70) [45.68]	42.19 (39.66) [37.29]

ΔE_N for N (kcal/mol)	-46.00 (-48.48) [-45.47]	-21.39 (-21.68) [-19.91]	-50.89 (-55.08) [-49.44]	46.76 (48.23) [50.99]	44.87 (46.86) [48.02]
HOMO - LUMO (kcal/mol)	69.89 (70.00) [140.6]	67.52 (68.21) [132.3]	95.56 (100.3) [147.5]	79.67 (88.81) [136.5]	92.87 (97.34) [144.3]
BE (kcal/mol)	81.13 (76.70) [72.38]	73.53 (65.39) [62.68]	91.74 (86.47) [82.67]	66.72 (59.12) [60.33]	92.26 (87.49) [86.81]
WBI	1.077 (0.999) [0.987]	0.892 (0.732) [0.580]	1.324 (1.341) [1.272]	1.266 (1.227) [1.230]	1.134 (1.150) [1.090]

(1) The natural charge density on the thallium atom; (2) The natural charge density on the nitrogen atom; (3) ΔE_{Tl} = E(triplet state for L□Tl) – E(singlet state for L□Tl); (4) ΔE_N = E(triplet state for L□N) – E(singlet state for L□N) and (5) BE = E(singlet state for L□Tl) + E(triplet state for L□N) – E(singlet state for L-Tl≡N-L). (6) The Wiberg bond index (WBI) for the Tl≡N bond: see reference (69,70).

Table S5

The Bond Lengths (Å), Bond Angles (°), Singlet□Triplet Energy Splitting ($\Delta E_{Al'}$ and $\Delta E_{N'}$), Natural Charge Densities ($Q_{Al'}$ and $Q_{N'}$), Binding Energies (BE), the Wiberg Bond Index (WBI), HOMO□LUMO Energy Gaps, and Some Reaction Enthalpies for L′-Al≡N-L′ at the M06-2X/Def2-TZVP Level of Theory. See also Scheme 2.

L'	SiMe(Si*t*Bu$_3$)$_2$	Si*i*PrDis$_2$	Tbt	Ar*
Al≡N(Å)	1.686	1.681	1.719	1.705
∠L'-Al-N (°)	163.4	169.2	161.3	164.2
∠Al-N-L' (°)	121.1	114.6	126.3	113.1
∠L'-Al-N-L' (°)	180.0	177.5	176.6	172.3
Q_{Al} (1)	1.0463	0.8104	0.8828	0.9514
Q_N (2)	-0.6761	-0.7543	-0.7445	-0.7324
ΔE_{ST} for L'-Al (kcal/mol) (3)	20.64	24.08	18.17	19.28
ΔE_{ST} for L'-N (kcal/mol) (4)	-22.30	-25.05	-25.52	-28.63
HOMO – LUMO (kcal / mol)	57.14	55.20	78.53	29.55
BE (kcal / mol) (5)	324.2	306.8	591.8	351.0
ΔH_1 (kcal / mol) (6)	154.2	83.52	96.15	28.30
ΔH_2 (kcal / mol) (6)	39.69	6.460	9.706	42.48
WBI (7)	2.111	2.145	2.117	2.182

(1) The natural charge density on aluminum. (2) The natural charge density on nitrogen. (3) $\Delta E_{Al'}$ (kcal mol^{-1}) = E(triplet state for L′–Al) –

E(singlet state for L′–Al). (4) $\Delta E_{N'}$ (kcal mol^{-1}) = E(triplet state for L′–N) – E(singlet state for L′–N). (5) BE (kcal mol^{-1}) = E(triplet state for L′–Al) + E(triplet state for L′–N) – E(singlet for L′-Al≡N-L′). (6) See Scheme 2. (7) The Wiberg bond index (WBI) for the Al≡N bond: see references (69,70).

Table S6

The Bond Lengths (Å), Bond Angles (°), Singlet□Triplet Energy Splitting ($\Delta E_{Ga'}$ and $\Delta E_{N'}$), Natural Charge Densities ($Q_{Ga'}$ and $Q_{N'}$), Binding Energies (BE), the Wiberg Bond Index (WBI), HOMO□LUMO Energy Gaps, and Some Reaction Enthalpies for L′-Ga≡N-L′ at the M06-2X/Def2-TZVP Level of Theory. See also Scheme 2.

L'	$SiMe(SitBu_3)_2$	$SiiPrDis_2$	Tbt	Ar*
Ga≡N(Å)	1.705	1.698	1.722	1.704
∠L'-Ga-N (°)	158.6	166.6	165.2	167.8
∠Ga-N-L' (°)	135.2	137.8	129.7	130.1
∠L'-Ga-N-L' (°)	176.4	178.3	180.0	175.9
Q_{Ga} (1)	0.6855	0.5227	0.6186	0.7607
Q_N (2)	-0.7526	-0.8662	-0.5930	-0.7281
ΔE_{ST} for L'-Ga (kcal/mol) (3)	22.17	18.81	17.13	15.36
ΔE_{ST} for L'-N (kcal/mol) (4)	-22.30	-25.05	-25.52	-28.63
HOMO – LUMO (kcal / mol)	56.75	61.82	36.53	40.28
BE (kcal / mol) (5)	596.7	484.4	836.1	589.5
ΔH_1 (kcal / mol) (6)	113.7	111.4	43.55	115.4
ΔH_2 (kcal / mol) (6)	38.79	1.843	9.015	25.12
WBI (7)	2.182	2.216	2.163	2.124

(1) The natural charge density on gallium. (2) The natural charge density on nitrogen. (3) $\Delta E_{Ga'}$ (kcal mol^{-1}) = E(triplet state for L′–Ga) – E(singlet state for L′–Ga). (4) $\Delta E_{N'}$ (kcal mol^{-1}) = E(triplet state for

L′–N) – E(singlet state for L′–N). (5) BE (kcal mol^{-1}) = E(triplet state for L′–Ga) + E(triplet state for L′–N) – E(singlet for L′-Ga≡N-L′). (6) See Scheme 2. (7) The Wiberg bond index (WBI) for the Ga≡N bond: see references (69,70).

Table S7

The Bond Lengths (Å), Bond Angles (°), Singlet□Triplet Energy Splitting ($\Delta E_{In'}$ and $\Delta E_{N'}$), Natural Charge Densities ($Q_{In'}$ and $Q_{N'}$), Binding Energies (BE), the Wiberg Bond Index (WBI), HOMO□LUMO Energy Gaps, and Some Reaction Enthalpies for L′-In≡N-L′ at the M06-2X/Def2-TZVP Level of Theory. See also Scheme 2.

L'	**SiMe(Si*t*Bu$_3$)$_2$**	**Si*i*PrDis$_2$**	**Tbt**	**Ar***
In≡N(Å)	1.879	1.866	1.902	1.876
∠L'-In-N (°)	149.7	146.0	142.9	142.0
∠In-N-L' (°)	123.3	121.4	124.3	115.8
∠L'-In-N-L' (°)	174.7	177.5	176.8	179.8
Q_{In} (1)	0.7760	0.8198	1.0330	1.5298
Q_N (2)	-0.8540	-0.9817	-0.6503	-0.7823
ΔE_{ST} for In (kcal/mol) (3)	21.94	20.99	16.71	18.94
ΔE_{ST} for N (kcal/mol) (4)	-22.30	-25.05	-25.52	-28.63
HOMO – LUMO (kcal / mol)	43.38	47.85	45.83	34.22
BE (kcal / mol) (5)	290.5	275.5	573.9	330.3
ΔH_1 (kcal / mol) (6)	140.3	96.26	116.1	43.63
ΔH_2 (kcal / mol) (6)	26.23	-13.17	-4.323	12.44
WBI (7)	2.206	2.105	2.152	2.213

(1) The natural charge density on indium. (2) The natural charge density on nitrogen. (3) $\Delta E_{In'}$ (kcal mol^{-1}) = E(triplet state for L′–In) – E(singlet state for L′–In). (4) $\Delta E_{N'}$ (kcal mol^{-1}) = E(triplet state for L′–N) – E(singlet state for L′–N). (5) BE (kcal mol^{-1}) = E(triplet

state for L′–In) + E(triplet state for L′–N) – E(singlet for L′-In≡N-L′). (6) See Scheme 2. (7) The Wiberg bond index (WBI) for the In≡N bond: see references (69,70).

Table S8

The Bond Lengths (Å), Bond Angles (°), Singlet□Triplet Energy Splitting ($\Delta E_{Tl'}$ and $\Delta E_{N'}$), Natural Charge Densities ($Q_{Tl'}$ and $Q_{N'}$), Binding Energies (BE), the Wiberg Bond Index (WBI), HOMO□LUMO Energy Gaps, and Some Reaction Enthalpies for L′-Tl≡N-L′ at the M06-2X/Def2-TZVP Level of Theory. See also Scheme 2.

L'	**SiMe(Si*t*Bu$_3$)$_2$**	**Si*i*PrDis$_2$**	**Tbt**	**Ar***
Tl≡N(Å)	1.891	1.877	1.930	1.894
∠R'-Tl-N (°)	150.8	153.2	150.9	151.2
∠Tl-N-R' (°)	121.1	123.1	122.4	113.7
∠R'-Tl-N-R' (°)	177.2	178.4	180.0	177.8
Q_{Tl}	0.7717	0.8554	1.1679	1.6085
Q_N	-0.8789	-0.9938	-0.7430	-0.8202
ΔE_{ST} for Tl (kcal/mol)	24.75	21.40	19.80	19.09
ΔE_{ST} for N (kcal/mol)	-22.30	-25.05	-25.52	-28.63
HOMO – LUMO (kcal/mol)	55.53	50.83	69.36	69.45
BE (kcal/mol)	310.5	311.8	307.5	310.3
ΔH_1 (kcal/mol)	110.0	117.5	90.48	48.15
ΔH_2 (kcal/mol)	76.14	81.28	88.33	76.34
WBI	2.106	2.115	2.201	2.136

(1) The natural charge density on thallium. (2) The natural charge density on nitrogen. (3) $\Delta E_{Tl'}$ (kcal mol^{-1}) = E(triplet state for L′–Tl) – E(singlet state for L′–Tl). (4) $\Delta E_{N'}$ (kcal mol^{-1}) = E(triplet state for

L′–N) – E(singlet state for L′–N). (5) BE (kcal mol^{-1}) = E(triplet state for L′–Tl) + E(triplet state for L′–N) – E(singlet for L′-Tl≡N-L′). (6) See Scheme 2. (7) The Wiberg bond index (WBI) for the Tl≡N bond: see references (69,70).

Table S9

The natural bond orbital (NBO) and natural resonance theory (NRT) analysis for L′-Al≡N-R′ molecules possessing bulky ligands (L′ = SiMe(Si*t*Bu$_3$)$_2$, Tbt, Si*i*PrDis$_2$, and Ar*) at the M06-2X/Def2-TZVP level of theory.[1,2]

L'-Al≡N-L'	WBI	NBO Analysis			NRT Analysis	
		Occupancy	Hybridization	Polarization	total / covalent / ionic	Resonance weight
L' = $SiMe(Si\textit{t}Bu_3)_2$	2.17	σ: 1.98	σ: 0.3429 Al ($sp^{1.19}$) + 0.9394 N ($sp^{0.99}$)	11.76% (Al) 88.24% (N)	2.57/0.49/2.08	Al–N :11.77 % Al=N : 79.06% Al≡N : 9.17%
		$\pi_{\perp}$: 1.93	$\pi_{\perp}$: 0.3425 Al ($sp^{16.45}$) + 0.9395 N ($sp^{97.50}$)	11.73% (Al) 88.27% (N)		
		$\pi_{\parallel}$: 1.93	$\pi_{\parallel}$: 0.3264 Al ($sp^{96.05}$) + 0.9452 N ($sp^{99.99}$)	10.65% (Al) 89.35% (N)		
L' = $Si\textit{i}PrDis_2$	2.14	σ: 1.98	σ: 0.3490 Al ($sp^{1.20}$) + 0.9371 N ($sp^{1.04}$)	12.18% (Al) 87.82% (N)	2.68/0.56/2.11	Al–N : 1.03% Al=N : 23.85% Al≡N : 75.12%
		$\pi_{\perp}$: 1.94	$\pi_{\perp}$: 0.3491Al ($sp^{46.67}$) + 0.9371 N ($sp^{99.99}$)	12.19% (Al) 87.81% (N)		
		$\pi_{\parallel}$: 1.93	$\pi_{\parallel}$: 0.3338 Al ($sp^{18.74}$) + 0.9427 N ($sp^{86.19}$)	11.14% (Al) 88.86% (N)		
L' = Tbt	2.11	σ: 1.88	σ: 0.4895 Al ($sp^{1.76}$) + 0.8720 N ($sp^{50.41}$)	23.96% (Al) 76.04% (N)	2.17/0.38/1.78	Al–N : 83.29% Al=N : 16.71% Al≡N : 0.00%
		$\pi_{\perp}$: 1.90	$\pi_{\perp}$: 0.362Al ($sp^{47.31}$) + 0.9528 N ($sp^{99.99}$)	0% (Al) 0% (N)		
		$\pi_{\parallel}$: 1.78	$\pi_{\parallel}$: 0.3491 Al ($sp^{18.74}$) + 0.9712 N ($sp^{87.38}$)	0% (Al) 0% (N)		
L' = Ar*	2.28	σ: 1.81	σ: 0.4818 Al ($sp^{1.29}$) + 0.8763 N ($sp^{84.71}$)	23.21% (Al) 76.79% (N)	2.16/0.33/1.83	Al–N :49.51 % Al=N : 49.83% Al≡N : 0.66%
		$\pi_{\perp}$: 1.89	$\pi_{\perp}$: 0.3211Al ($sp^{44.56}$) + 0.9153 N ($sp^{99.99}$)	0% (Al) 0% (N)		
		$\pi_{\parallel}$: 1.99	$\pi_{\perp}$: 0.3183 Al ($sp^{19.34}$) + 0.9280N ($sp^{88.19}$)	0% (Al) 0% (N)		

(1) The value of the Wiberg bond index (WBI) for the Al≡N bond and the occupancy of the corresponding σ and π bonding NBO (see references (69,70)). (2) NRT; see references (74-76).

Table S10

The natural bond orbital (NBO) and natural resonance theory (NRT) analysis for L′-Ga≡N-R′ molecules possessing bulky ligands (L′ = SiMe(Si*t*Bu$_3$)$_2$, Tbt, Si*i*PrDis$_2$, and Ar*) at the M06-2X/Def2-TZVP level of theory.[1,2]

L'-Ga≡N-L'	WBI	NBO Analysis			NRT Analysis	
		Occupancy	Hybridization	Polarization	total / covalent / ionic	Resonance weight
L' = SiMe(Si*t*Bu$_3$)$_2$	2.18	σ: 1.97	σ: 0.3736 Ga ($sp^{1.17}$) + 0.9276 N ($sp^{1.13}$)	13.96% (Ga) 86.04% (N)	2.17/0.55/1.62	Ga–N : 74.18% Ga=N : 14.12% Ga≡N : 11.70%
		$\pi_{\perp}$: 1.93	$\pi_{\perp}$: 0.3520 Ga ($sp^{9.66}$) + 0.9360 N ($sp^{33.25}$)	12.39% (Ga) 87.61% (N)		
		$\pi_{\parallel}$: 1.93	$\pi_{\parallel}$: 0.3329 Ga ($sp^{99.99}$) + 0.9429 N ($sp^{99.99}$)	11.08% (Ga) 88.92% (N)		
L' = Si*i*PrDis$_2$	2.21	σ: 1.97	σ: 0.3799 Ga ($sp^{1.19}$) + 0.9250 N ($sp^{1.20}$)	14.43% (Ga) 85.57% (N)	2.84/0.64/2.20	Ga–N : 3.08% Ga=N : 10.26% Ga≡N : 86.66%
		$\pi_{\perp}$: 1.93	$\pi_{\perp}$: 0.3696 Ga ($sp^{16.83}$) + 0.9292 N ($sp^{35.74}$)	13.66% (Ga) 86.34% (N)		
		$\pi_{\parallel}$: 1.93	$\pi_{\parallel}$: 0.3290 Ga ($sp^{21.83}$) + 0.9443 N ($sp^{79.29}$)	10.83% (Ga) 89.17% (N)		
L' = Tbt	2.16	σ: 1.86	σ: 0.4792 Ga ($sp^{1.36}$) + 0.8777 N ($sp^{22.83}$)	22.97% (Ga) 77.03% (N)	2.24/0.49/1.75	Ga–N : 0.00% Ga=N : 75.27% Ga≡N : 24.73%
		$\pi_{\perp}$: 1.90	$\pi_{\perp}$: 0.3439 Ga ($sp^{15.72}$) + 0.9190 N ($sp^{36.28}$)	0.00% (Ga) 0.00% (N)		
		$\pi_{\parallel}$: 1.92	$\pi_{\parallel}$: 0.3137 Ga ($sp^{20.88}$) + 0.9570 N ($sp^{79.33}$)	0.00% (Ga) 0.00% (N)		
L' = Ar*	2.24	σ: 1.83	σ: 0.4768 Ga ($sp^{1.22}$) + 0.8790 N ($sp^{30.55}$)	22.74% (Ga) 77.26% (N)	2.27/0.46/1.81	Ga–N : 56.53% Ga=N : 41.73% Ga≡N : 1.74%
		$\pi_{\perp}$: 1.93	$\pi_{\perp}$: 0.3539 Ga ($sp^{17.89}$) + 0.9391 N ($sp^{38.71}$)	0.00% (Ga) 0.00% (N)		
		$\pi_{\parallel}$: 1.92	$\pi_{\parallel}$: 0.3429 Ga ($sp^{20.83}$) + 0.9388 N ($sp^{78.92}$)	0.00% (Ga) 0.00% (N)		

(1) The value of the Wiberg bond index (WBI) for the Ga≡N bond and the occupancy of the corresponding σ and π bonding NBO (see references (69,70)). (2) NRT; see references (74-76).

Table S11

The natural bond orbital (NBO) and natural resonance theory (NRT) analysis for L′-In≡N-R′ molecules possessing bulky ligands (L′ = SiMe(Si*t*Bu$_3$)$_2$, Tbt, Si*i*PrDis$_2$, and Ar*) at the M06-2X/Def2-TZVP level of theory.[1,2]

L'-In≡N-L'	WBI	NBO Analysis			NRT Analysis	
		Occupancy	Hybridization	Polarization	total / covalent / ionic	Resonance weight
L' = SiMe(Si*t*Bu$_3$)$_2$	2.16	σ: 1.96	σ: 0.3570 In ($sp^{1.35}$) + 0.9341 N ($sp^{1.17}$)	12.75% (In) 87.25% (N)	1.89/0.53/1.36	In–N : 18.85% In=N : 72.99% In≡N : 8.16%
		$\pi_{\perp}$: 1.90	$\pi_{\perp}$: 0.3635 In ($sp^{5.24}$) + 0.9316 N ($sp^{99.99}$)	13.21% (In) 86.79% (N)		
		$\pi_{\parallel}$: 1.92	$\pi_{\parallel}$: 0.3038 In ($sp^{99.99}$) + 0.9527 N ($sp^{99.99}$)	9.23% (In) 90.77% (N)		
L' = Si*i*PrDis$_2$	2.10	σ: 1.96	σ: 0.3695 In ($sp^{1.31}$) + 0.9292 N ($sp^{1.29}$)	13.65% (In) 86.35% (N)	2.81/0.57/2.24	In–N : 1.64% In=N : 9.18% In≡N : 89.18%
		$\pi_{\perp}$: 1.90	$\pi_{\perp}$: 0.3744 In ($sp^{7.35}$) + 0.9273 N ($sp^{20.00}$)	14.01% (In) 85.99% (N)		
		$\pi_{\parallel}$: 1.92	$\pi_{\parallel}$: 0.3025 In ($sp^{29.43}$) + 0.9531 N ($sp^{99.99}$)	9.15% (In) 90.85% (N)		
L' = Tbt	2.15	σ: 1.80	σ: 0.5359 In ($sp^{1.48}$) + 0.8443 N ($sp^{78.75}$)	28.72% (In) 71.28% (N)	2.18/0.48/1.70	In–N : 0.77% In=N : 79.39% In≡N : 19.84%
		$\pi_{\perp}$: 1.89	$\pi_{\perp}$: 0.3822 In ($sp^{7.62}$) + 0.9417 N ($sp^{20.00}$)	0.00% (In) 0.00% (N)		
		$\pi_{\parallel}$:1.93	$\pi_{\parallel}$: 0.3211In ($sp^{29.43}$) + 0.9531 N ($sp^{99.99}$)	0.00% (In) 0.00% (N)		
L' = Ar*	2.13	σ: 1.78	σ: 0.5104 In ($sp^{1.09}$) + 0.8600 N ($sp^{53.66}$)	26.05% (In) 73.95% (N)	2.20/0.50/1.70	In–N : 41.12% In=N : 58.47% In≡N : 41.12%
		$\pi_{\perp}$: 1.90	$\pi_{\perp}$: 0.3521 In ($sp^{7.05}$) + 0.8974 N ($sp^{20.00}$)	0.00% (In) 0.00% (N)		
		$\pi_{\parallel}$: 1.91	$\pi_{\parallel}$: 0.3122 In ($sp^{29.43}$) + 0.9041 N ($sp^{99.99}$)	0.00% (In) 0.00% (N)		

(1) The value of the Wiberg bond index (WBI) for the In≡N bond and the occupancy of the corresponding σ and π bonding NBO (see references (69,70)). (2) NRT; see references (74-76).

Table S12

The natural bond orbital (NBO) and natural resonance theory (NRT) analysis for L′-Tl≡N-R′ molecules possessing bulky ligands (L′ = SiMe(Si*t*Bu$_3$)$_2$, Tbt, Si*i*PrDis$_2$, and Ar*) at the M06-2X/Def2-TZVP level of theory.[1,2]

L'-Tl≡N-L'	WBI	NBO Analysis			NRT Analysis	
		Occupancy	Hybridization	Polarization	total / covalent / ionic	Resonance weight
L' = SiMe(Si*t*Bu$_3$)$_2$	2.16	σ: 1.92	σ: 0.4042 Tl ($sp^{1.23}$) + 0.9147 N ($sp^{1.49}$)	16.34% (Tl) 83.66% (N)	2.14/0.58/1.56	Tl–N : 23.78% Tl=N : 68.39% Tl≡N : 7.83%
		$\pi_{\perp}$: 1.88	$\pi_{\perp}$: 0.3571 Tl ($sp^{4.91}$) + 0.9341 N ($sp^{10.62}$)	12.75% (Tl) 87.25% (N)		
		$\pi_{\parallel}$: 1.91	$\pi_{\parallel}$: 0.2986 Tl ($sp^{99.99}$) + 0.9544 N ($sp^{99.99}$)	8.91% (Tl) 91.09% (N)		
L' = Si*i*PrDis$_2$	2.11	σ: 1.93	σ: 0.4162 Tl ($sp^{1.19}$) + 0.9093 N ($sp^{1.62}$)	17.33% (Tl) 82.67% (N)	2.45/0.50/1.96	Tl–N : 54.83% Tl=N : 45.17% Tl≡N : 0.00%
		$\pi_{\perp}$: 1.89	$\pi_{\perp}$: 0.3703 Tl ($sp^{6.16}$) + 0.9289 N ($sp^{10.13}$)	13.71% (Tl) 86.29% (N)		
		$\pi_{\parallel}$: 1.92	$\pi_{\parallel}$: 0.2979 Tl ($sp^{58.41}$) + 0.9546 N ($sp^{99.99}$)	8.87% (Tl) 91.13% (N)		
L' = Tbt	2.21	σ: 1.75	σ: 0.5401 Tl ($sp^{0.97}$) + 0.8416 N ($sp^{29.07}$)	29.17% (Tl) 70.83% (N)	2.25/0.55/1.70	Tl–N : 74.46% Tl=N : 25.54% Tl≡N : 0.00%
		$\pi_{\perp}$: 0.00	$\pi_{\perp}$: 0.3853 Tl ($sp^{23.17}$) + 0.9344 N ($sp^{12.53}$)	0.00% (Tl) 0.00% (N)		
		$\pi_{\parallel}$: 0.00	$\pi_{\parallel}$: 0.3126 Tl ($sp^{66.71}$) + 0.9648 N ($sp^{99.99}$)	0.00% (Tl) 0.00% (N)		
L' = Ar*	2.13	σ: 1.75	σ: 0.5577 Tl ($sp^{0.97}$) + 0.8301 N ($sp^{43.29}$)	31.10% (Tl) 68.90% (N)	2.07/0.67/1.40	Tl–N : 58.00% Tl=N : 42.00% Tl≡N : 1.89%
		$\pi_{\perp}$: 0.00	$\pi_{\perp}$: 0.3811 Tl ($sp^{11.13}$) + 0.9186 N ($sp^{12.47}$)	0.00% (Tl) 0.00% (N)		
		$\pi_{\parallel}$: 0.00	$\pi_{\parallel}$: 0.3068 Tl ($sp^{63.75}$) + 0.9489 N ($sp^{99.99}$)	0.00% (Tl) 0.00% (N)		

(1) The value of the Wiberg bond index (WBI) for the Tl≡N bond and the occupancy of the corresponding σ and π bonding NBO (see references (69,70)). (2) NRT; see references (74-76).

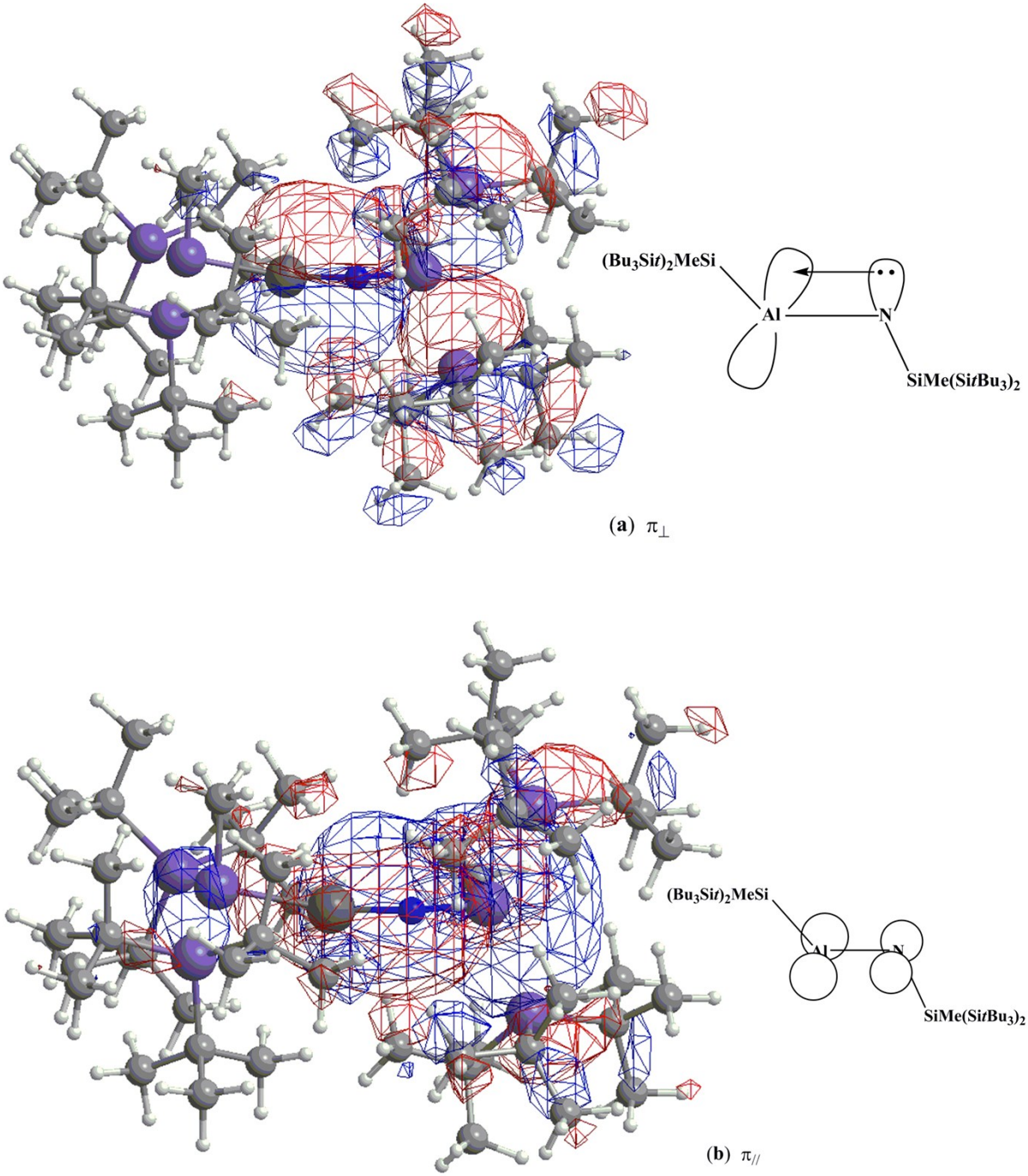


Figure S5: The natural Al≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (SiMe(Si*t*Bu$_3$)$_2$)-Al≡N-(SiMe(Si*t*Bu$_3$)$_2$. Also see Figure 1.

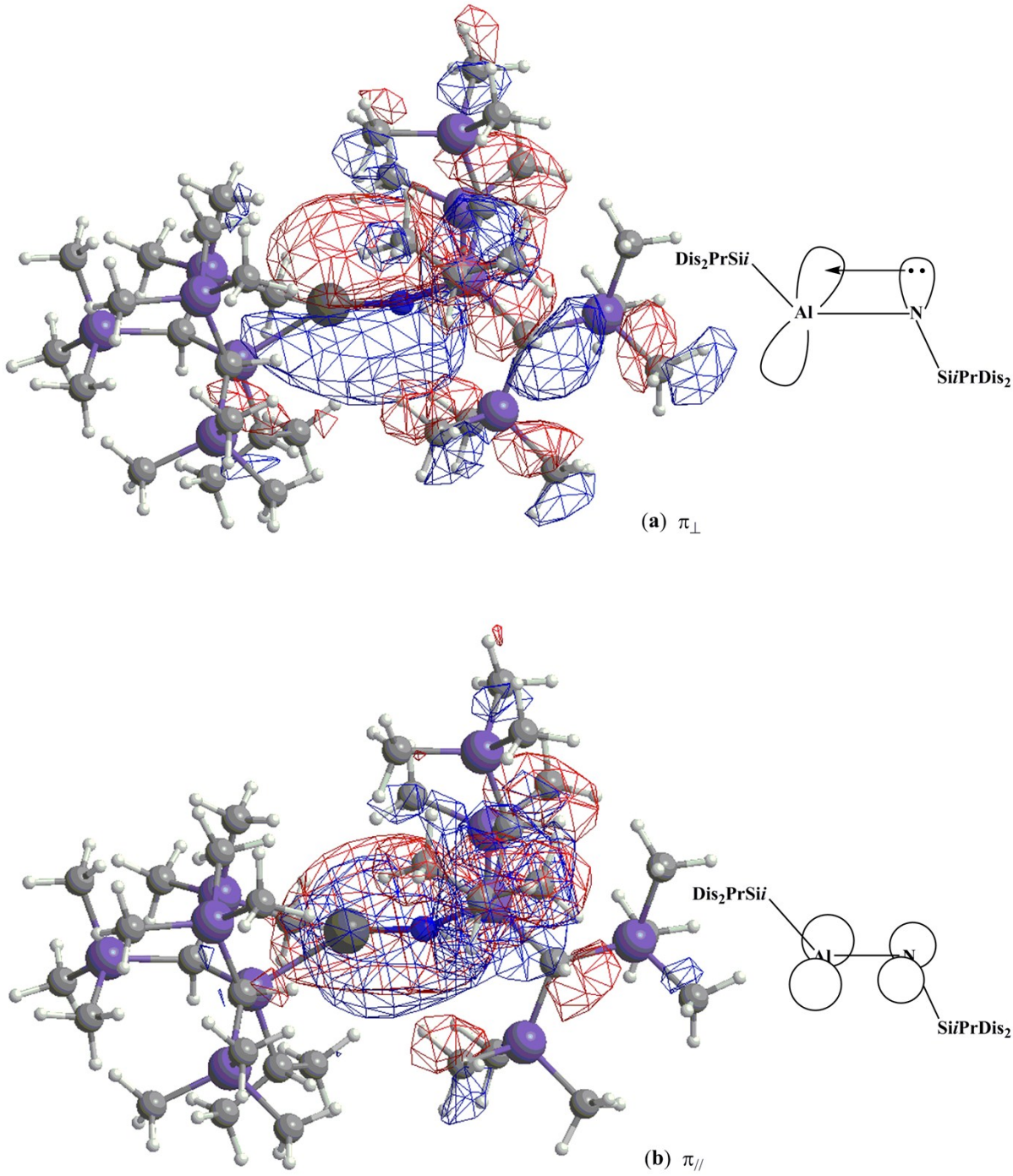


Figure S6: The natural Al≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Si*i*PrDis$_2$)-Al≡N-(Si*i*PrDis$_2$). Also see Figure 1.

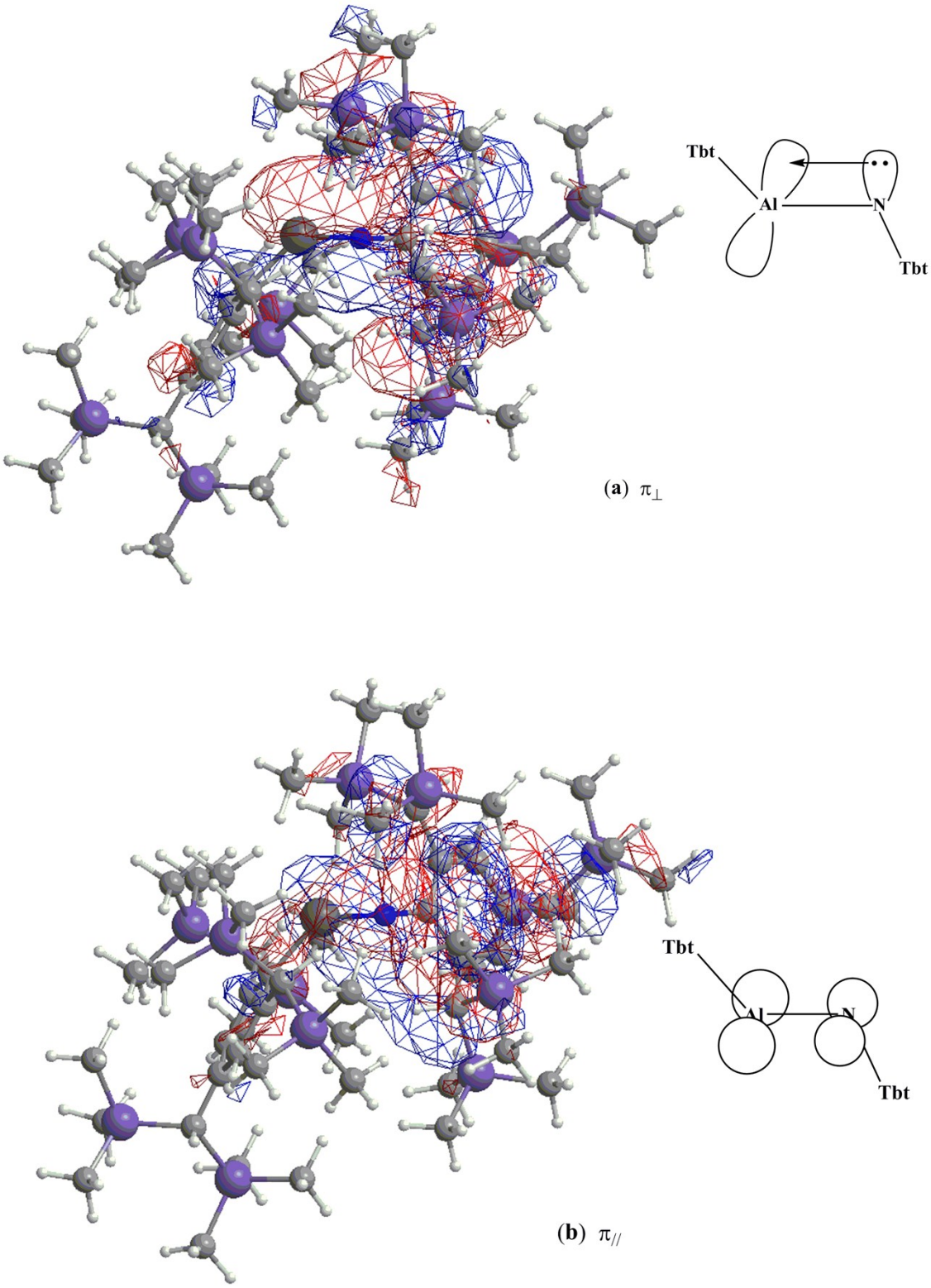
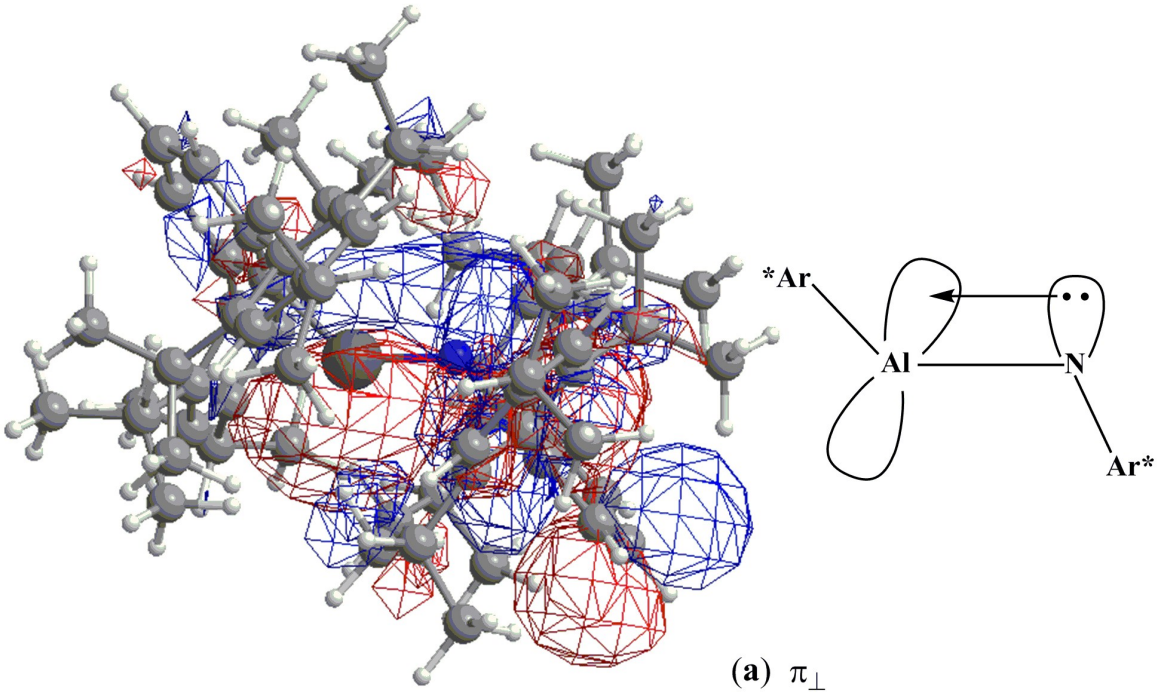
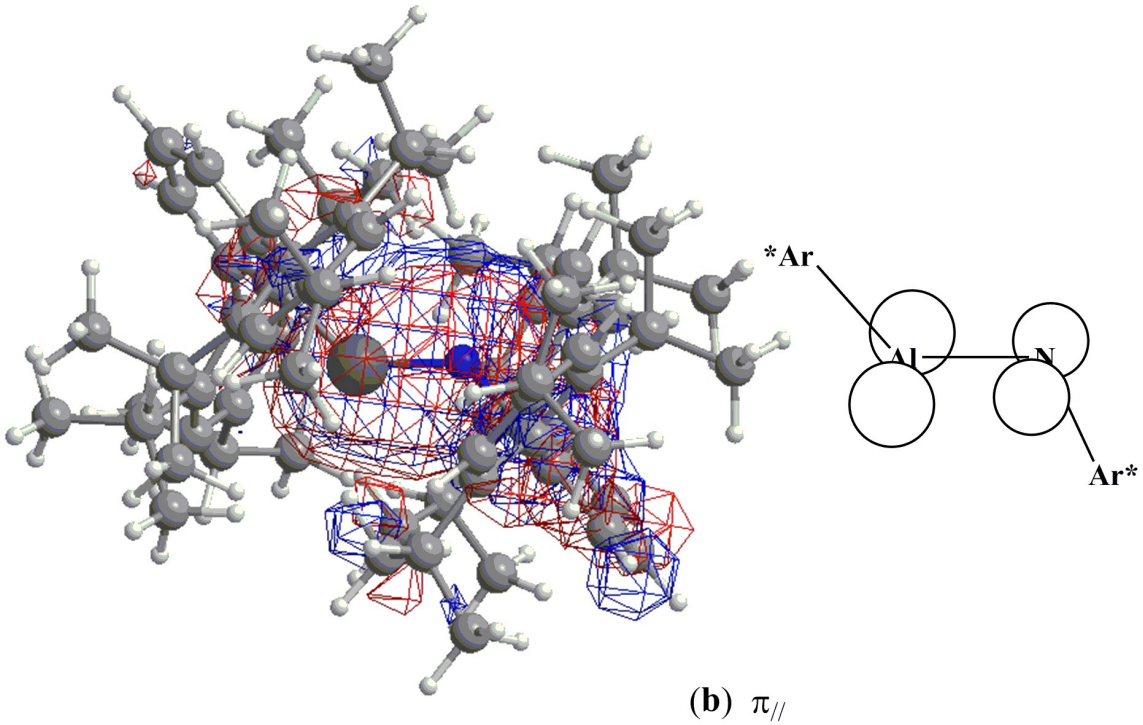


Figure S7: The natural Al≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Tbt)-Al≡N-(Tbt). Also see Figure 1.



(a) $\pi_{\perp}$



(b) $\pi_{//}$

Figure S8: The natural Al≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Ar*)-Al≡N-(Ar*). Also see Figure 1.

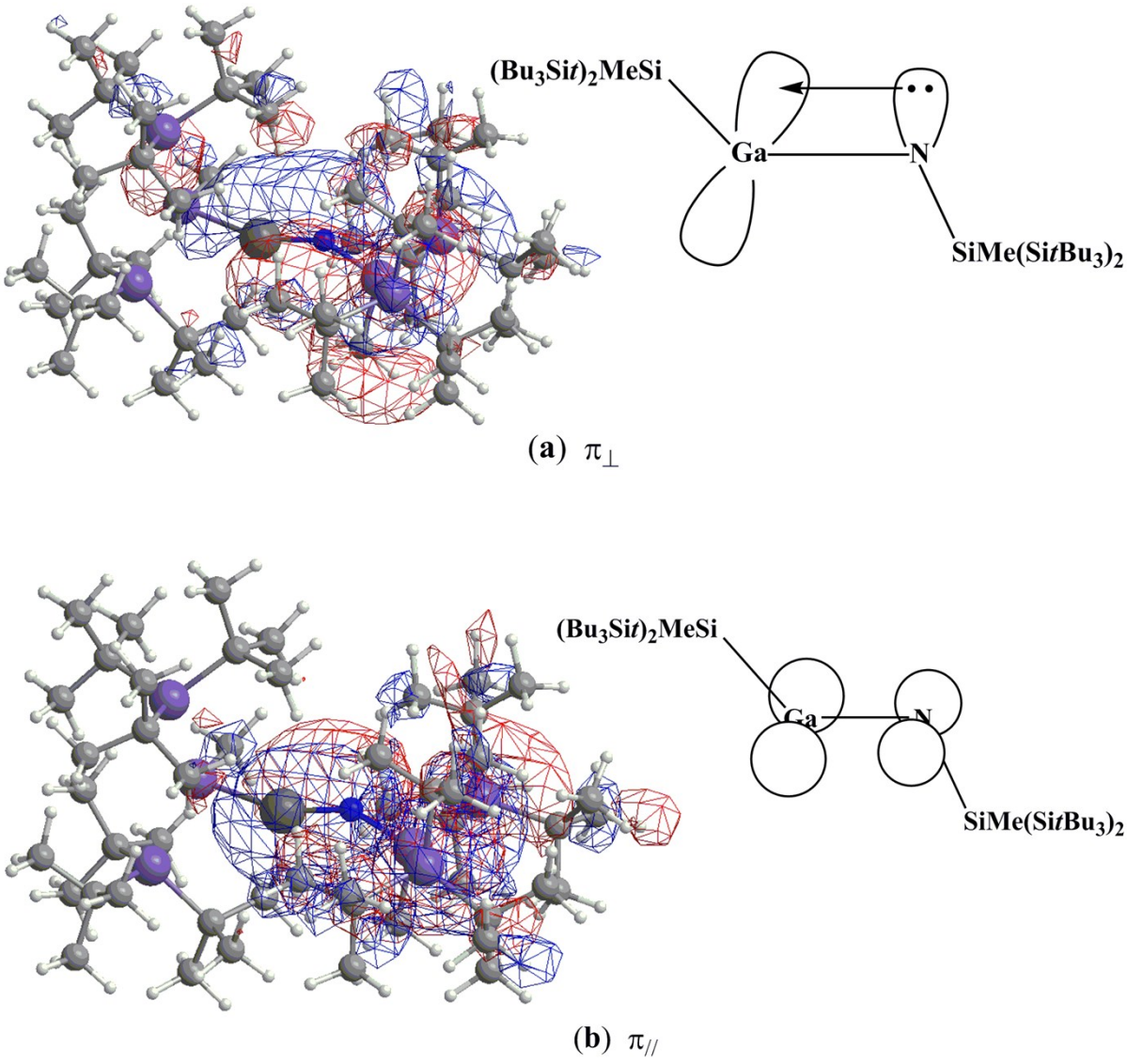


Figure S9: The natural Ga≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (SiMe(Si*t*Bu$_3$)$_2$)-Ga≡N-(SiMe(Si*t*Bu$_3$)$_2$. Also see Figure 1.

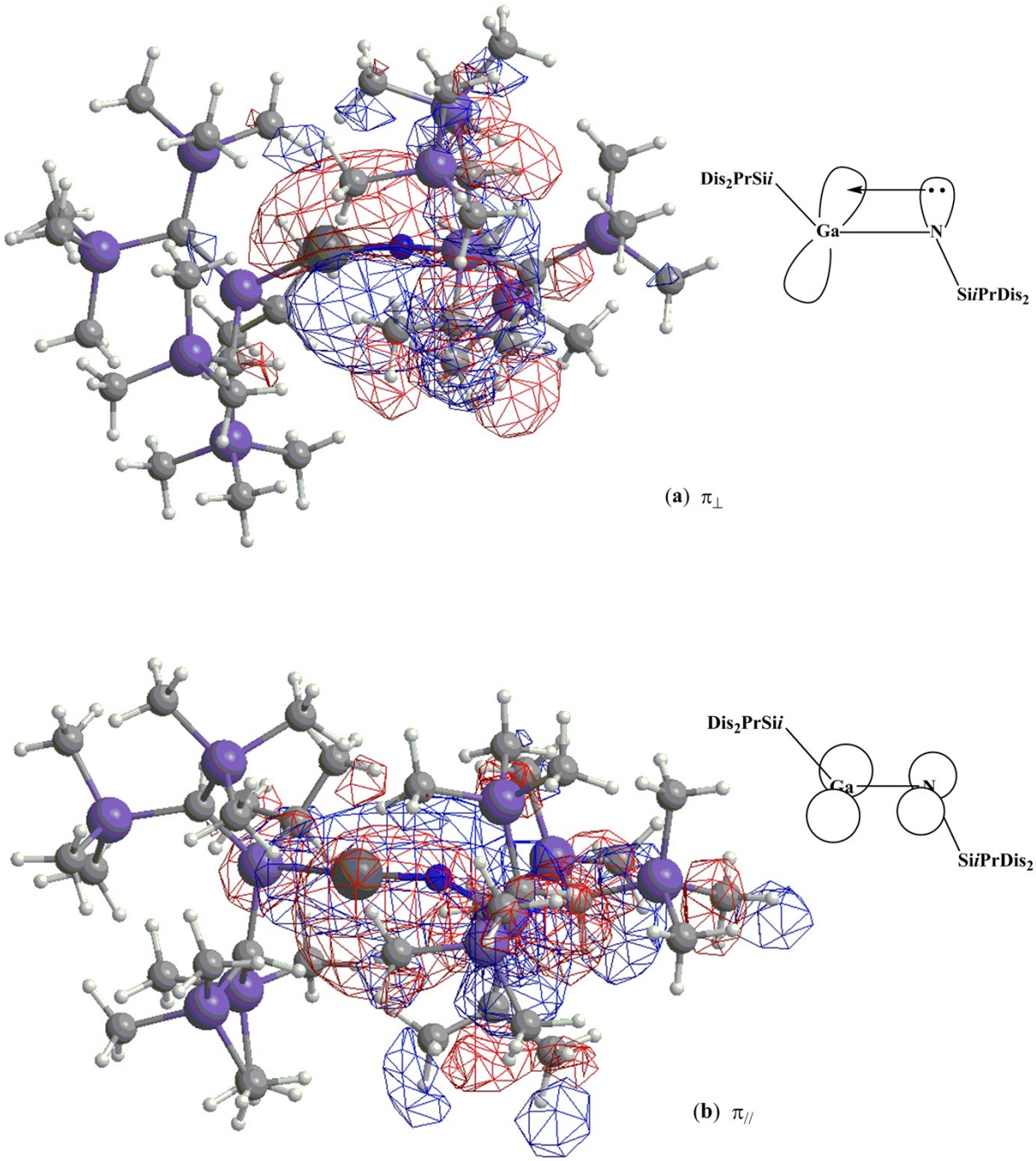


Figure S10: The natural Ga≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Si*i*PrDis$_2$)-Ga≡N-(Si*i*PrDis$_2$). Also see Figure 1.

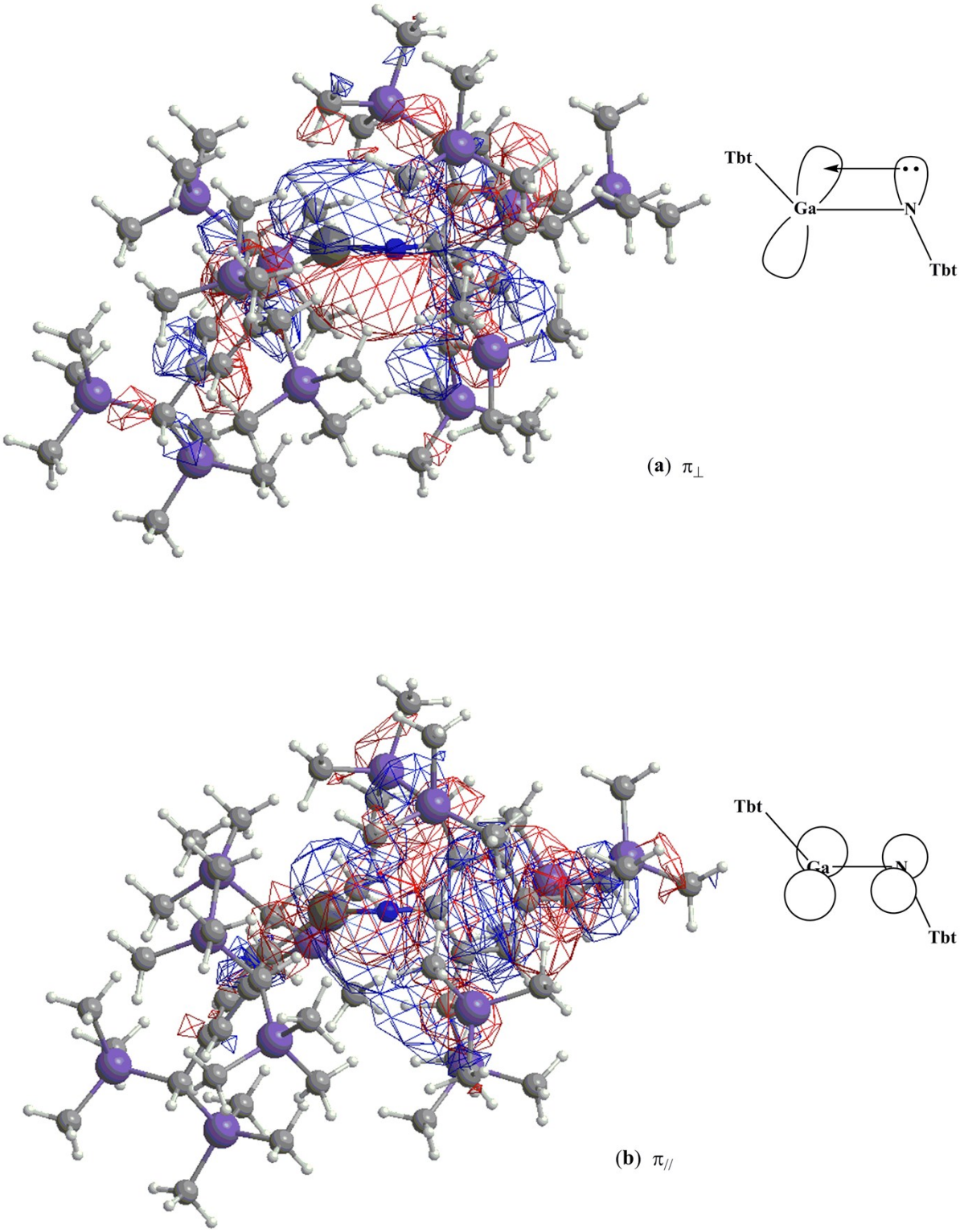


Figure S11: The natural Ga≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Tbt)-Ga≡N-(Tbt). Also see Figure 1.

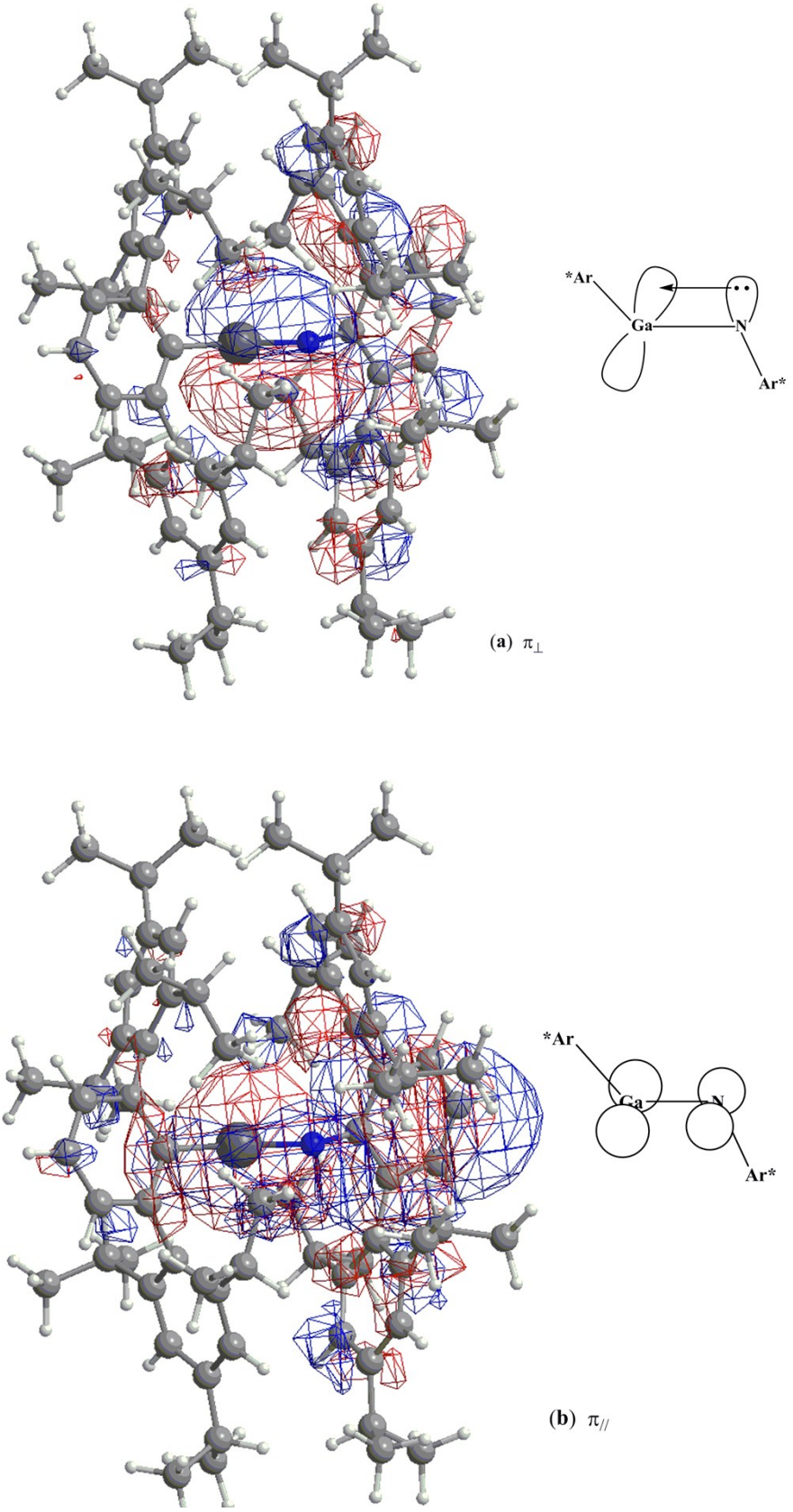
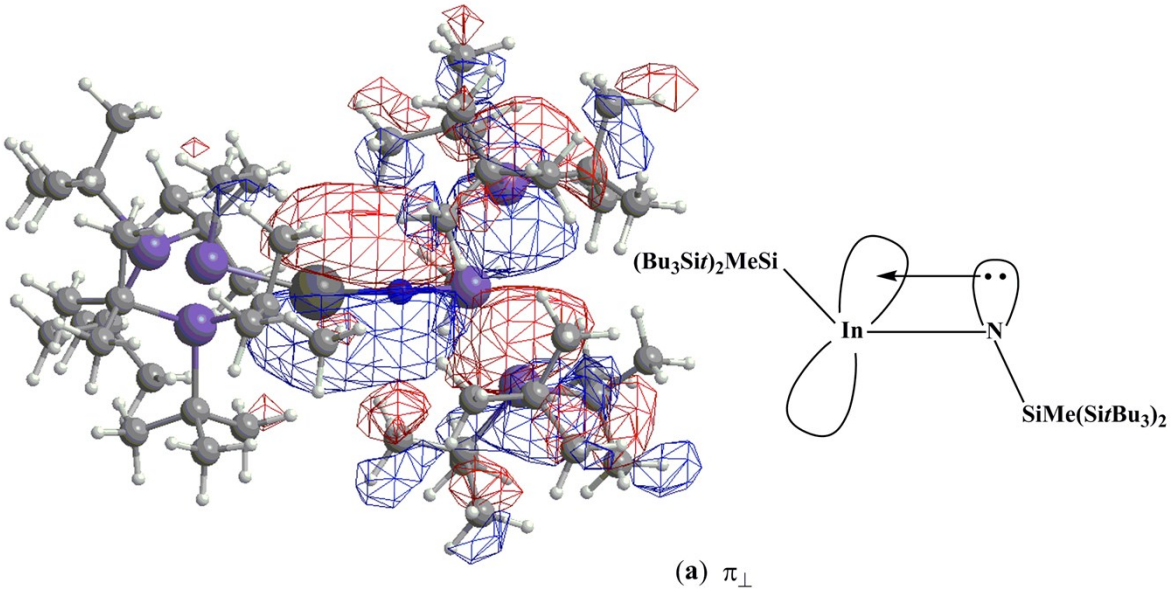
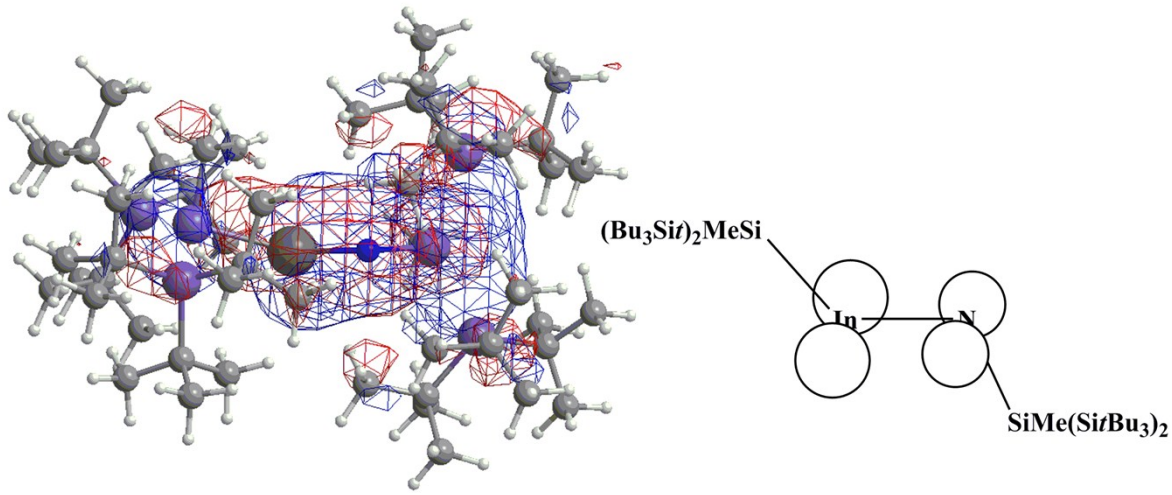


Figure S12: The natural Ga≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Ar*)-Ga≡N-(Ar*). Also see Figure 1.



(a) $\pi_{\perp}$



(b) $\pi_{//}$

Figure S13: The natural In≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (SiMe(Si*t*Bu$_3$)$_2$)-In≡N-(SiMe(Si*t*Bu$_3$)$_2$. Also see Figure 1.

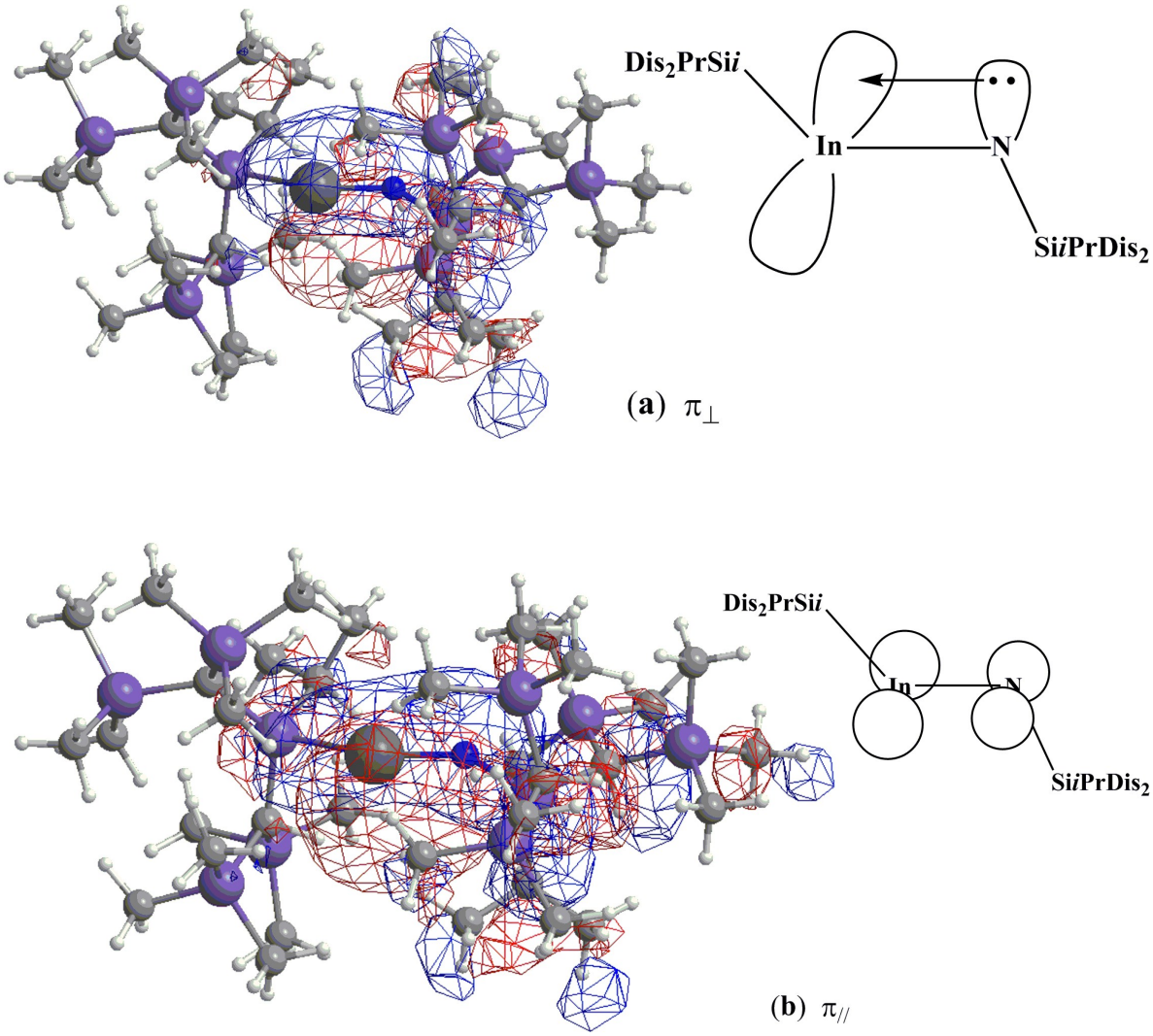


Figure S14: The natural In≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Si*i*PrDis$_2$)-In≡N-(Si*i*PrDis$_2$). Also see Figure 1.

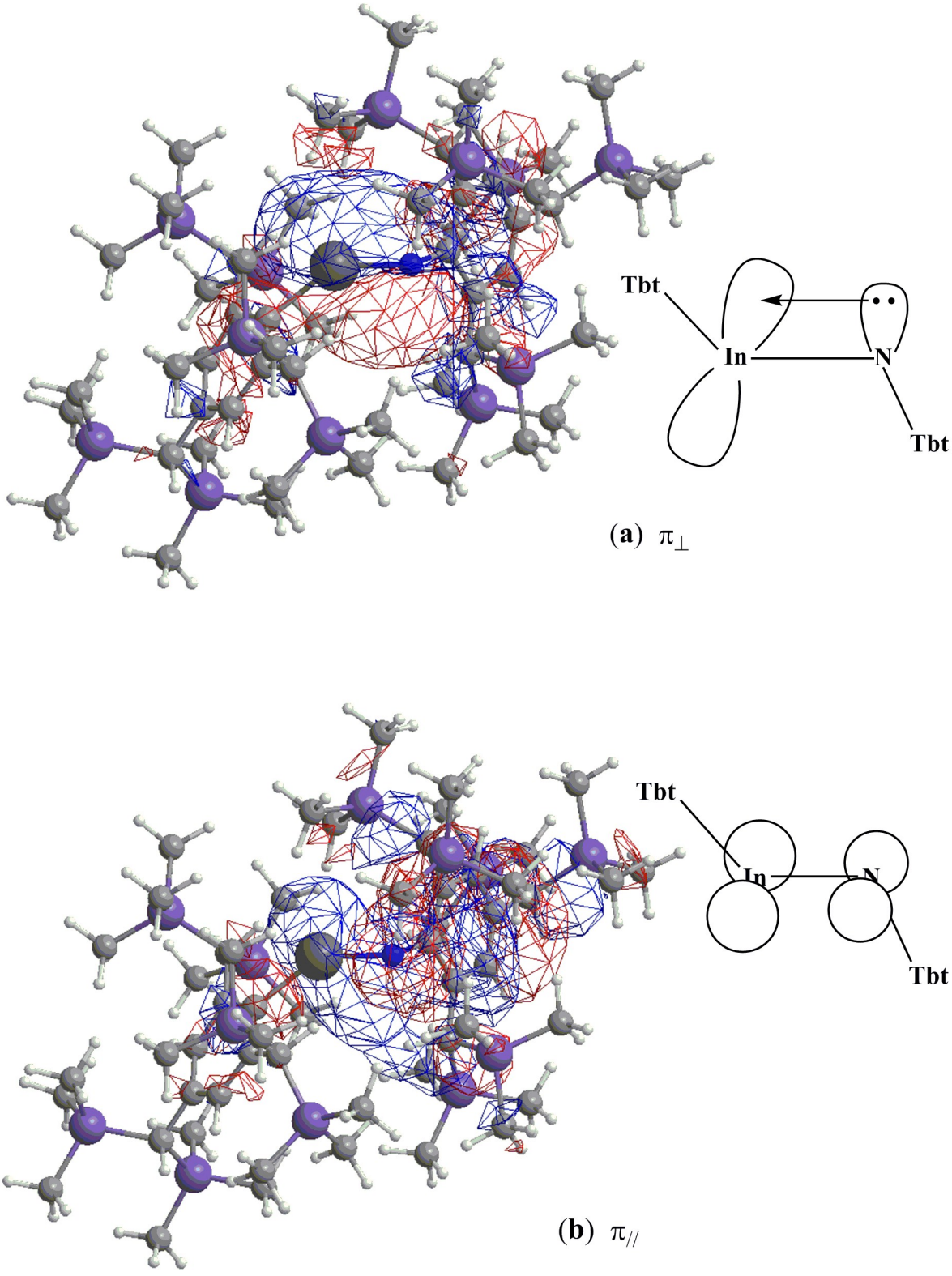
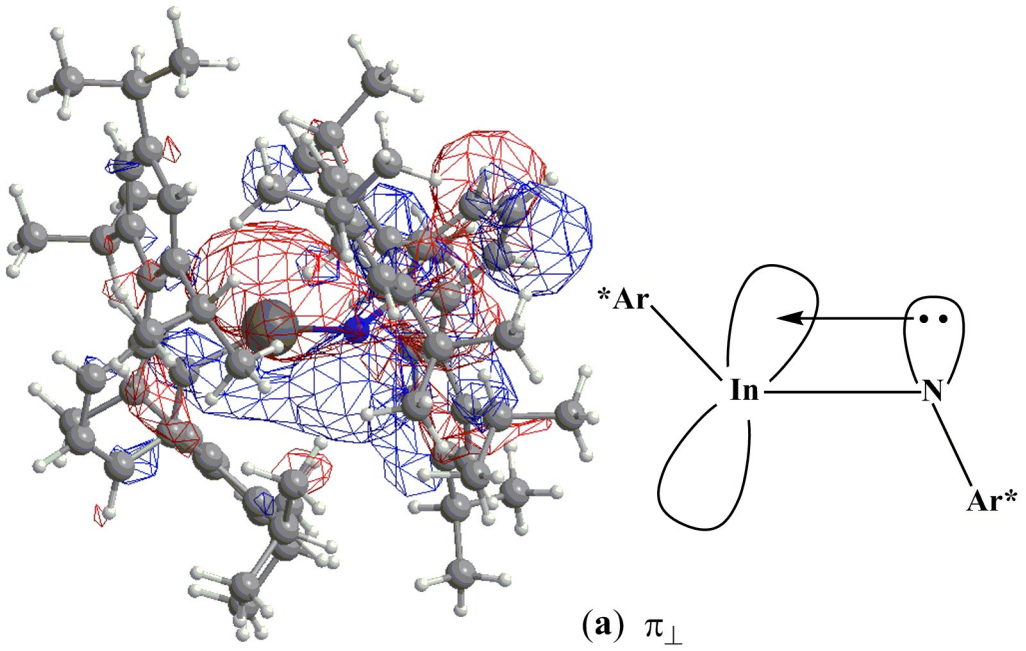
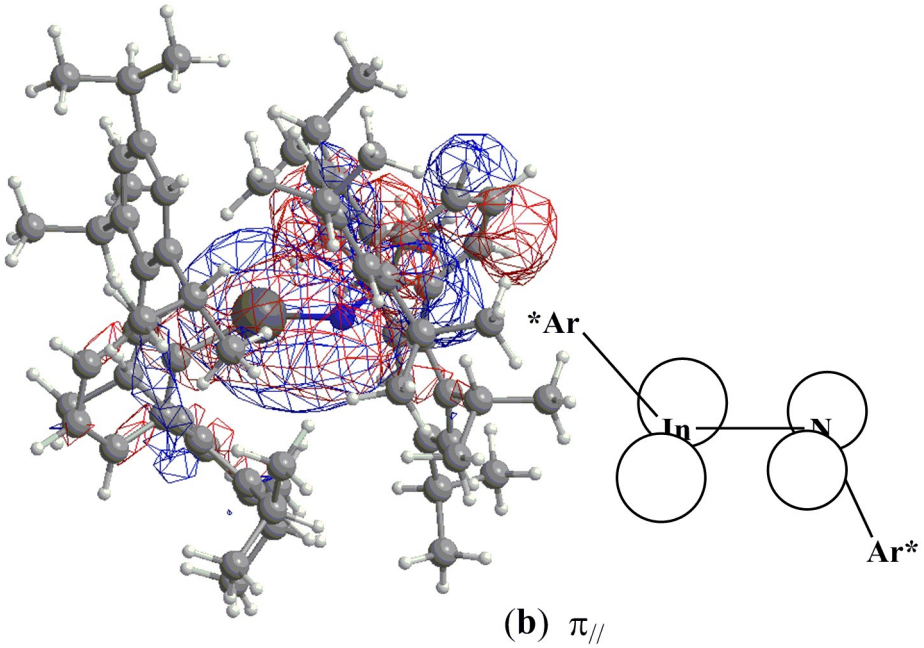


Figure S15: The natural In≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Tbt)-In≡N-(Tbt). Also see Figure 1.

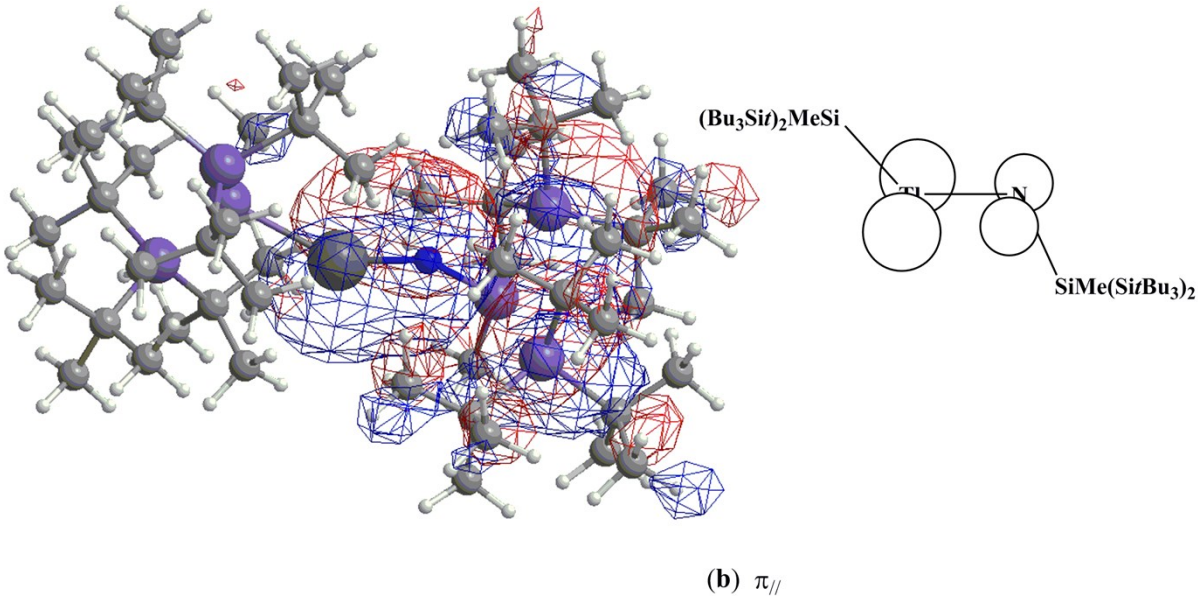


(a) $\pi_{\perp}$

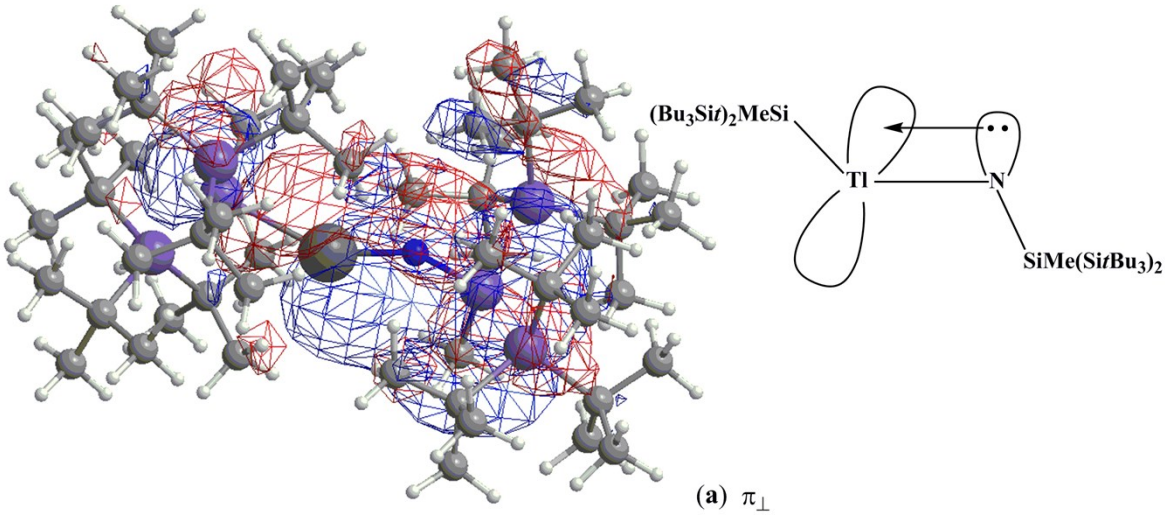


(b) $\pi_{//}$

Figure S16: The natural In≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Ar*)-In≡N-(Ar*). Also see Figure 1.



(**b**) $\pi_{//}$



(**a**) $\pi_{\perp}$

Figure S17: The natural Tl≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (SiMe(Si*t*Bu$_3$)$_2$)-Tl≡N-(SiMe(Si*t*Bu$_3$)$_2$. Also see Figure 1.

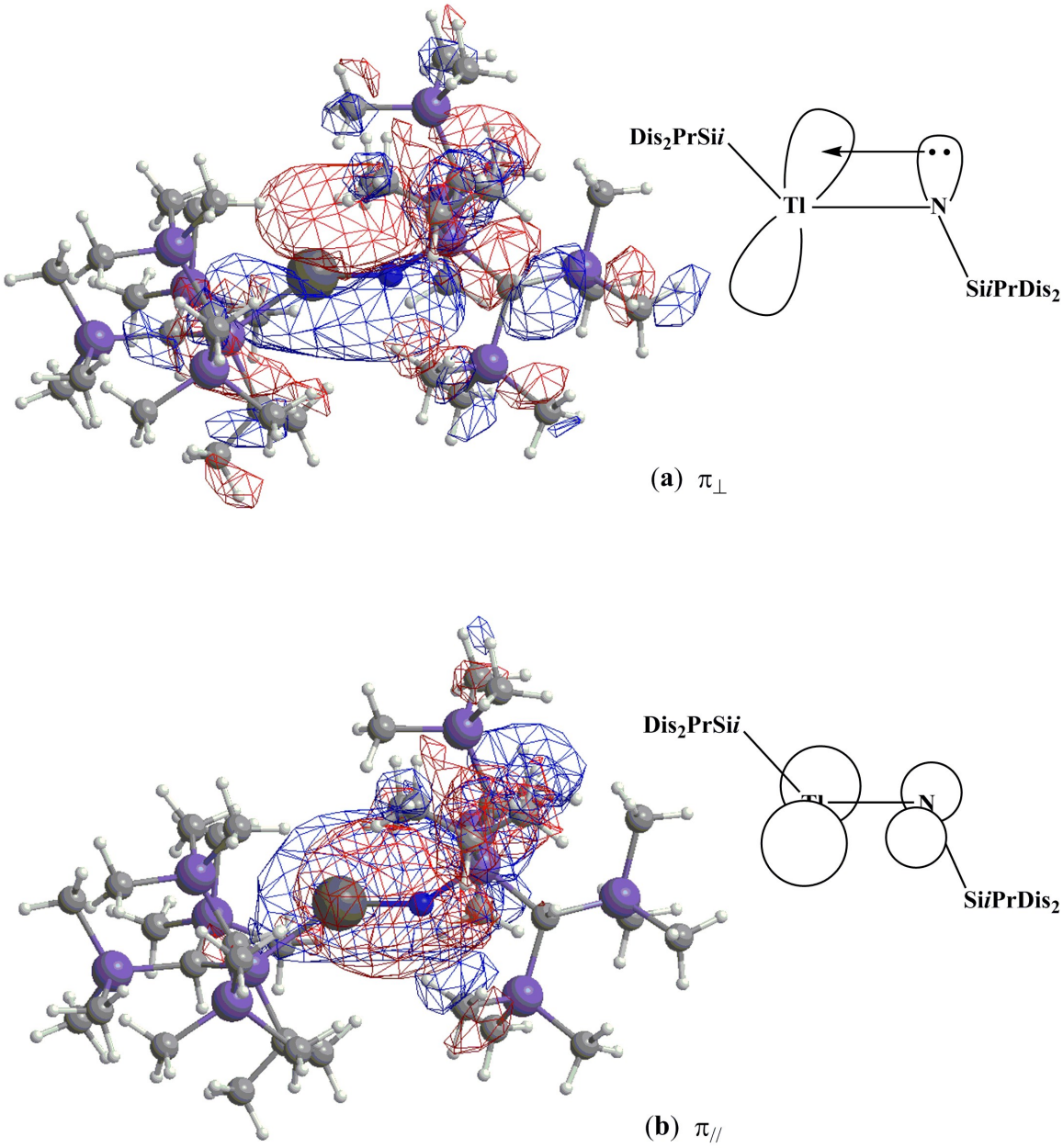


Figure S18: The natural Tl≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Si*i*PrDis$_2$)-Tl≡N-(Si*i*PrDis$_2$). Also see Figure 1.

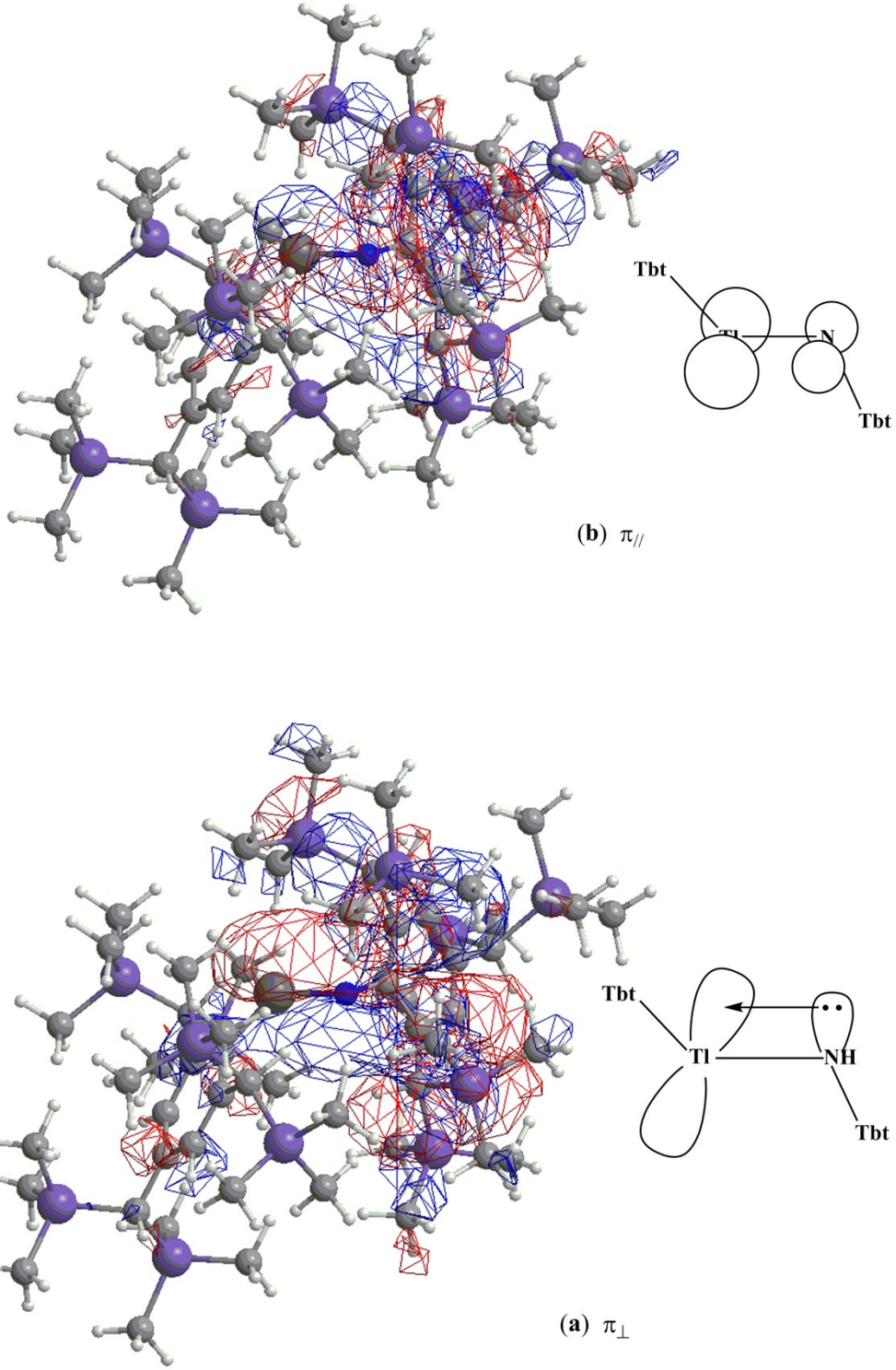


Figure S19: The natural Tl≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Tbt)-Tl≡N-(Tbt). Also see Figure 1.

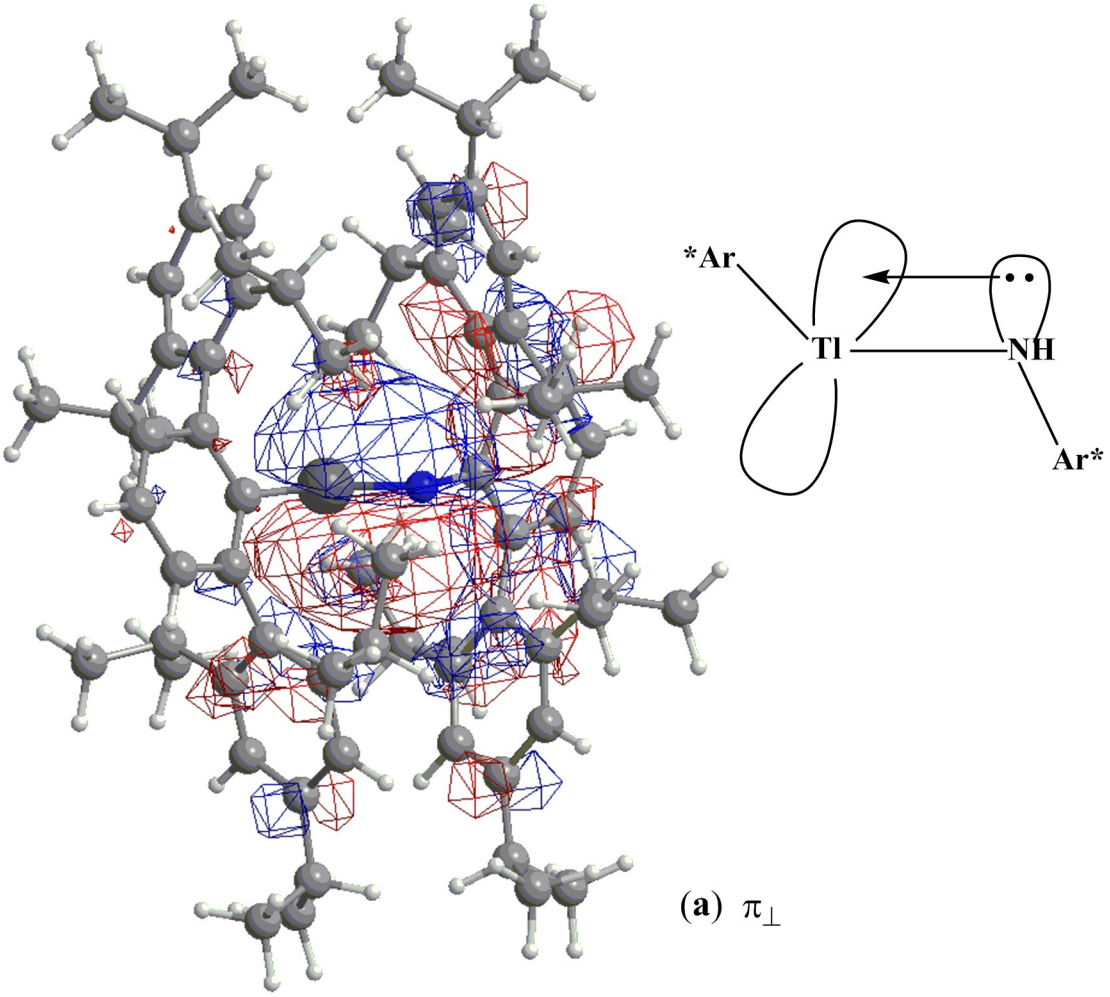


Figure S20: The natural Tl≡N π bonding orbitals ($\pi_{\perp}$ (a) and $\pi_{||}$ (b)) for (Ar*)-Tl≡N-(Ar*). Also see Figure 1.

b97d3/LANL2DZ+dp

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SiMe(SitBu3)2-B≡N-SiMe(SitBu3)2

--

Atomic Number	Coordinates (Angstroms) X	Y	Z
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[SiMe(SitBu3)2]2-B=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
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C	-4.743258	3.114860	1.379360
H	-5.656305	3.375652	0.827111
H	-4.743877	3.717186	2.306449
H	-4.809578	2.062200	1.675167
C	-2.261254	3.268404	1.539330
H	-2.022364	2.220728	1.769211
H	-2.481677	3.780548	2.494231
H	-1.355670	3.724930	1.129098
C	-3.541500	4.932229	0.195594
H	-4.382384	5.159666	-0.474686
H	-2.621290	5.300465	-0.277693
H	-3.690590	5.525830	1.117177
C	-0.695560	3.464591	-1.444522
H	-0.285117	2.651887	-0.829965
H	-0.899432	4.317185	-0.786370
H	0.088388	3.779790	-2.156388
C	-2.480545	4.213054	-3.028643
H	-3.232215	3.911281	-3.772357
H	-1.642262	4.671769	-3.586563
H	-2.920547	4.996623	-2.398047
C	-1.435265	1.968511	-3.257448
H	-2.240483	1.484783	-3.823888

H	-0.845350	1.188205	-2.766157
H	-0.770302	2.473050	-3.982281
C	-5.987136	1.279645	-1.076288
H	-6.838652	0.952188	-1.700827
H	-6.399441	1.850109	-0.235757
H	-5.512666	0.384908	-0.672898
C	-4.841662	1.410476	-3.285710
H	-5.842774	1.253309	-3.728309
H	-4.360595	0.425523	-3.209049
H	-4.263382	2.016081	-3.997138
C	-5.686900	3.474259	-2.174385
H	-6.639306	3.284498	-2.706267
H	-5.097152	4.157069	-2.797991
H	-5.942339	3.994383	-1.241010
C	2.284189	-4.721018	0.125287
H	1.301450	-4.554271	-0.329665
H	2.122099	-5.313659	1.044414
H	2.887262	-5.335403	-0.558780
C	4.321346	-3.848362	1.182210
H	4.072015	-4.517834	2.026026
H	4.899841	-3.013579	1.594120
H	4.967036	-4.419096	0.497382
C	2.143833	-2.714115	1.592244
H	1.181925	-2.357598	1.214765
H	2.652027	-1.847046	2.033850
H	1.939056	-3.424227	2.413921
C	5.500629	-3.323737	-2.472812
H	4.952087	-3.418622	-3.418322
H	5.360035	-4.251529	-1.895456
H	6.576280	-3.258607	-2.725353
C	6.158387	-1.946806	-0.533744
H	6.347515	-2.910233	-0.047576
H	5.873176	-1.232540	0.239956
H	7.118091	-1.608769	-0.965469
C	5.296577	-0.831954	-2.584558

H	4.731308	-0.902208	-3.520108
H	6.365030	-0.733471	-2.851979
H	5.005471	0.099488	-2.086215
C	2.277011	-4.249554	-2.984495
H	1.666183	-4.901513	-2.350691
H	3.306680	-4.627104	-2.962245
H	1.906697	-4.372160	-4.018957
C	0.665252	-2.491072	-2.274039
H	0.034513	-2.816008	-3.121443
H	0.461759	-1.428416	-2.098441
H	0.333834	-3.039055	-1.385363
C	2.481283	-1.946793	-3.873981
H	1.706590	-2.161667	-4.633374
H	3.442694	-2.250559	-4.310243
H	2.498277	-0.861596	-3.722009
C	5.018913	-0.291973	2.397001
H	4.393938	-0.949978	1.783577
H	5.219067	-0.818467	3.348310
H	5.983390	-0.163348	1.891668
C	5.380850	1.928461	3.421066
H	5.669545	1.414954	4.357482
H	5.007193	2.922449	3.695102
H	6.300751	2.061282	2.833956
C	3.166890	0.780641	3.663009
H	2.344325	0.211851	3.204621
H	2.746269	1.709578	4.072447
H	3.552223	0.192906	4.516929
C	6.382480	1.610985	-0.081919
H	6.111026	0.618586	-0.446874
H	6.858650	1.494798	0.901326
H	7.150818	2.013449	-0.768493
C	5.733479	3.907211	0.550714
H	5.023668	4.740122	0.473775
H	6.630540	4.194644	-0.030016
H	6.043417	3.813928	1.600029

C	4.795426	2.881945	-1.508877
H	4.539065	1.973519	-2.065471
H	5.661563	3.340003	-2.022507
H	3.952227	3.577610	-1.597884
C	3.047380	4.272077	2.602356
H	3.056430	3.747860	3.567663
H	2.379498	5.146010	2.717002
H	4.057062	4.653078	2.407285
C	2.233552	4.292590	0.243036
H	1.892816	3.727597	-0.632537
H	3.120761	4.869450	-0.049373
H	1.437718	5.017624	0.491771
C	1.103674	2.891658	1.939544
H	0.532015	2.438027	1.126243
H	0.529069	3.753862	2.320601
H	1.145926	2.139302	2.733097

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B=N-[SiMe(SitBu3)2]2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.111613	0.679817	-1.180442
N	-0.001097	0.097656	0.058149
Si	-1.905447	-0.372032	0.433569
Si	-2.933928	-1.858911	-1.614255
Si	-3.226103	1.684874	1.621730
C	-1.840553	-1.727437	1.750646
H	-1.601175	-2.700968	1.312807
H	-2.826238	-1.809920	2.226676
H	-1.120145	-1.516799	2.537871
C	-4.383600	-3.065575	-0.971816

C	-4.687954	-4.161002	-2.029562
H	-4.947447	-3.748774	-3.013409
H	-5.558503	-4.746969	-1.679239
H	-3.860482	-4.868898	-2.160811
C	-5.717762	-2.337398	-0.706325
H	-5.635693	-1.640419	0.132340
H	-6.485098	-3.084447	-0.428974
H	-6.099081	-1.790585	-1.579263
C	-4.045549	-3.797316	0.350238
H	-4.835496	-4.544083	0.555760
H	-4.030189	-3.104896	1.200547
H	-3.087250	-4.330275	0.327486
C	-3.607543	-0.645040	-2.998910
C	-4.421286	0.485931	-2.343644
H	-3.856930	0.959677	-1.532754
H	-5.378326	0.137117	-1.934258
H	-4.648539	1.266849	-3.092284
C	-4.526412	-1.321203	-4.046734
H	-4.837523	-0.560800	-4.787731
H	-5.444454	-1.728798	-3.599354
H	-4.028090	-2.129144	-4.598540
C	-2.439735	0.033805	-3.754799
H	-1.863312	-0.676605	-4.363384
H	-1.739145	0.538835	-3.069465
H	-2.852849	0.794000	-4.444195
C	-1.510971	-3.007360	-2.355578
C	-1.862860	-3.524103	-3.775808
H	-1.062234	-4.214035	-4.103113
H	-1.904060	-2.709225	-4.510978
H	-2.809995	-4.075138	-3.822530
C	-0.185333	-2.237803	-2.486055
H	0.553949	-2.873026	-3.006800
H	0.226629	-1.976180	-1.506705
H	-0.285195	-1.306892	-3.053165
C	-1.213732	-4.242290	-1.473233

H	-1.011424	-3.971341	-0.430414
H	-0.309386	-4.748313	-1.859058
H	-2.024589	-4.982754	-1.480026
C	-2.139587	2.078412	3.227940
C	-3.393756	3.279955	0.447794
C	-5.021590	1.096155	2.177485
C	-5.800987	2.197130	2.946731
H	-5.729441	3.186607	2.471031
H	-5.474276	2.298883	3.988859
H	-6.871897	1.919452	2.967282
C	-4.963952	-0.157645	3.077191
H	-5.988352	-0.425962	3.395601
H	-4.365315	-0.006081	3.986520
H	-4.556609	-1.022165	2.535164
C	-5.876959	0.729280	0.943068
H	-6.710552	0.072410	1.250756
H	-5.295686	0.204043	0.181232
H	-6.320174	1.611576	0.470487
C	-2.295809	3.228931	-0.629566
H	-2.416980	2.382650	-1.319083
H	-1.297346	3.141474	-0.191811
H	-2.314242	4.154879	-1.232792
C	-4.747773	3.409210	-0.290992
H	-4.997175	2.533844	-0.897279
H	-4.677191	4.272681	-0.977992
H	-5.583995	3.611797	0.393782
C	-3.227432	4.616002	1.221960
H	-2.189173	4.799551	1.520867
H	-3.866497	4.683362	2.116189
H	-3.514679	5.446737	0.551717
C	-0.921837	2.966572	2.883548
H	-0.448681	2.666533	1.941422
H	-0.163377	2.873587	3.681295
H	-1.185281	4.028880	2.815726
C	-2.927930	2.784907	4.356978

H	-2.214501	3.098639	5.142407
H	-3.459642	3.684093	4.015898
H	-3.655431	2.113028	4.834477
C	-1.560987	0.779318	3.830380
H	-0.801540	0.350690	3.167980
H	-2.316331	0.006809	4.025527
H	-1.063575	1.013486	4.789820
Si	1.881923	0.281316	0.517942
Si	3.214093	-1.873516	1.413956
Si	2.881909	2.051137	-1.462145
C	1.934935	1.316213	2.110831
H	1.293255	0.887161	2.893495
H	1.638728	2.359383	1.962811
H	2.965621	1.309294	2.494617
C	1.902432	-3.008532	2.319078
C	2.478741	-4.223638	3.086894
H	1.634308	-4.826803	3.471446
H	3.075500	-3.918444	3.957313
H	3.093514	-4.885271	2.463893
C	0.944296	-3.553186	1.243101
H	0.537648	-2.751587	0.613615
H	0.096515	-4.072331	1.724235
H	1.435446	-4.281686	0.585527
C	1.078388	-2.203902	3.350970
H	0.180671	-2.780982	3.632868
H	0.749398	-1.233220	2.960838
H	1.637748	-2.012383	4.273713
C	4.008643	-2.828431	-0.106593
C	3.047104	-2.771996	-1.313725
H	2.126912	-3.340424	-1.141562
H	3.540691	-3.203379	-2.204130
H	2.757692	-1.742756	-1.564485
C	4.311508	-4.321153	0.177915
H	3.403816	-4.910997	0.367015
H	4.996775	-4.461770	1.025568

H	4.797911	-4.757324	-0.714700
C	5.337604	-2.182855	-0.555053
H	6.124066	-2.250091	0.209051
H	5.214488	-1.130253	-0.821445
H	5.708684	-2.707677	-1.454881
C	4.590047	-1.393222	2.763969
C	5.530799	-2.607691	2.993102
H	6.214611	-2.368976	3.829319
H	6.156587	-2.819391	2.115781
H	4.996740	-3.528225	3.258569
C	5.505984	-0.211011	2.392364
H	6.233907	-0.056382	3.210783
H	4.956930	0.732170	2.269758
H	6.080642	-0.394746	1.478362
C	3.969084	-1.039902	4.138997
H	3.536353	-1.917001	4.637075
H	3.195295	-0.262217	4.076170
H	4.768351	-0.658891	4.801215
C	1.741150	3.672550	-1.558495
C	4.649403	2.602998	-0.760455
C	3.114058	1.263006	-3.255146
C	3.374892	2.366411	-4.314636
H	4.237569	3.000956	-4.071273
H	2.506156	3.018009	-4.472041
H	3.590038	1.876236	-5.282881
C	1.871452	0.466725	-3.702551
H	2.020872	0.116150	-4.741839
H	0.945359	1.051076	-3.658768
H	1.723965	-0.419420	-3.073292
C	4.308735	0.285214	-3.330029
H	5.277350	0.795684	-3.239747
H	4.297646	-0.217752	-4.314749
H	4.255822	-0.497231	-2.564239
C	5.478285	1.349055	-0.441751
H	4.880931	0.604768	0.091315

H	6.338171	1.612508	0.199363
H	5.879156	0.877017	-1.345559
C	5.511980	3.446785	-1.733506
H	5.760667	2.891538	-2.649036
H	6.470274	3.683223	-1.232433
H	5.052021	4.397882	-2.024376
C	4.509970	3.398876	0.559185
H	3.940697	2.849526	1.320239
H	4.027842	4.375131	0.417862
H	5.517150	3.589424	0.974561
C	2.540458	4.927998	-1.994040
H	1.833695	5.774627	-2.079106
H	3.021818	4.806265	-2.974455
H	3.306956	5.223514	-1.265738
C	0.559687	3.554707	-2.549736
H	0.900087	3.503110	-3.592651
H	-0.071368	4.457512	-2.457321
H	-0.059183	2.670515	-2.345894
C	1.160316	3.964554	-0.160131
H	0.568927	3.117352	0.203431
H	1.939327	4.176068	0.584092
H	0.492565	4.843943	-0.204387

SiiPrDis2-B≡N-SiiPrDis2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

B	0.305208	-0.349683	-0.003104
N	-0.949006	-0.143949	-0.120650

Si	-2.538439	0.421345	-0.545958
Si	2.248365	-0.716085	-0.332304
C	-3.166239	1.484862	0.901881
H	-4.258262	1.560384	0.754752
C	-3.698157	-1.019350	-1.089125
H	-3.939956	-0.646690	-2.105526
C	-2.313384	1.302971	-2.237153
H	-2.043305	0.445834	-2.882407
C	-1.142548	2.292819	-2.350308
H	-0.963900	2.567532	-3.405297
H	-0.216217	1.847677	-1.959709
H	-1.318083	3.224423	-1.796890
C	-3.624076	1.889153	-2.806651
H	-3.448398	2.352406	-3.793878
H	-4.053374	2.660236	-2.152776
H	-4.396737	1.116033	-2.945172
C	2.148420	-2.264433	-1.465704
H	1.558659	-1.955712	-2.341133
C	1.377474	-3.411064	-0.786904
H	1.215093	-4.241013	-1.496838
H	0.396566	-3.085531	-0.421833
H	1.933134	-3.825462	0.070854
C	3.510718	-2.782451	-1.960001
H	3.370248	-3.631514	-2.652781
H	4.126867	-3.149889	-1.122773
H	4.091786	-2.015692	-2.488067
C	2.678578	0.885830	-1.336555
H	1.631398	1.182843	-1.566252
C	3.229628	-1.350333	1.193922
H	3.226216	-2.427197	0.918811
Si	-2.793278	-2.617002	-1.603478
Si	-5.486607	-1.323277	-0.503485
Si	-2.611769	3.303977	1.023586
Si	-2.955803	0.607731	2.586532
C	-3.909509	-3.715829	-2.670573

H	-3.323175	-4.587968	-3.011054
H	-4.252354	-3.182840	-3.573524
H	-4.798558	-4.101359	-2.150599
C	-1.353587	-2.218983	-2.760993
H	-0.813593	-3.144513	-3.023256
H	-0.635142	-1.517266	-2.321384
H	-1.728866	-1.780876	-3.701839
C	-2.216344	-3.659669	-0.146623
H	-1.703412	-4.564946	-0.513936
H	-3.066426	-3.984952	0.471988
H	-1.515935	-3.120722	0.505473
C	-6.562809	-1.373437	-2.060954
H	-6.260049	-2.163717	-2.764443
H	-6.519934	-0.411142	-2.600892
H	-7.618860	-1.551543	-1.792922
C	-6.265296	0.036432	0.552516
H	-7.336267	-0.203561	0.676339
H	-6.209114	1.026379	0.070408
H	-5.830137	0.115816	1.557634
C	-5.781776	-2.943957	0.428280
H	-5.176435	-3.041732	1.341144
H	-5.587286	-3.830316	-0.194591
H	-6.843294	-2.984710	0.730433
C	-3.186647	4.109412	2.639213
H	-2.932227	5.183517	2.597898
H	-2.707980	3.694540	3.538460
H	-4.278507	4.035489	2.772369
C	-3.425453	4.405880	-0.282334
H	-3.268931	5.460005	0.007487
H	-4.515794	4.238112	-0.319662
H	-3.031226	4.284863	-1.299461
C	-0.735465	3.478952	0.954306
H	-0.445073	4.450659	0.523482
H	-0.268334	2.690438	0.351254
H	-0.299682	3.422320	1.963427

C	-1.256330	0.965493	3.311787
H	-0.473664	0.738744	2.575940
H	-1.077071	0.334992	4.198026
H	-1.137121	2.015443	3.618701
C	-4.279663	1.153824	3.828786
H	-4.023295	2.091395	4.342669
H	-4.394897	0.372483	4.600464
H	-5.265461	1.295361	3.356267
C	-3.135684	-1.260663	2.466042
H	-2.561575	-1.699076	1.642904
H	-4.189076	-1.546122	2.340344
H	-2.780725	-1.721679	3.403683
Si	3.283549	0.870753	-3.151424
Si	3.194862	2.439930	-0.346816
Si	2.336432	-1.529337	2.876907
Si	5.119755	-1.103261	1.314490
C	2.210288	-0.250391	-4.233792
H	2.346944	0.043633	-5.289147
H	1.138817	-0.139957	-3.998349
H	2.464757	-1.317236	-4.156577
C	3.036693	2.598265	-3.882284
H	3.231020	2.547774	-4.968011
H	3.727582	3.344162	-3.460783
H	2.009726	2.971511	-3.745105
C	5.096383	0.460049	-3.485862
H	5.274717	0.605331	-4.566520
H	5.381065	-0.573099	-3.243055
H	5.784283	1.130104	-2.947136
C	2.274119	3.975724	-0.960979
H	2.788000	4.470651	-1.797935
H	2.210346	4.703050	-0.133382
H	1.245960	3.755397	-1.281340
C	2.711516	2.215255	1.452249
H	2.950487	3.118322	2.039151
H	3.233657	1.369713	1.911449

H	1.631626	2.033658	1.551764
C	5.033722	2.861038	-0.425275
H	5.391803	2.969558	-1.461850
H	5.675364	2.124859	0.078326
H	5.187790	3.832514	0.077084
C	5.658734	0.159347	2.609280
H	5.319892	1.182942	2.392323
H	6.762155	0.177887	2.647842
H	5.299458	-0.108887	3.615228
C	5.878846	-0.628753	-0.340299
H	5.961708	-1.506434	-0.998696
H	6.897689	-0.231895	-0.191153
H	5.300929	0.131990	-0.873289
C	5.934169	-2.751269	1.764192
H	7.023056	-2.675805	1.596580
H	5.561364	-3.569742	1.124300
H	5.779171	-3.048560	2.811163
C	3.270914	-2.786220	3.940299
H	4.226963	-2.394447	4.322639
H	3.480471	-3.722414	3.397406
H	2.649572	-3.042524	4.816297
C	0.614061	-2.265415	2.649321
H	-0.059320	-1.639163	2.049027
H	0.143100	-2.392685	3.639358
H	0.660703	-3.257954	2.173706
C	2.187081	0.013756	3.947800
H	1.557186	0.797859	3.511934
H	3.166095	0.457088	4.184308
H	1.721387	-0.289241	4.902463

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[SiiPrDis2]-B=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.386447	-0.172387	1.444456
B	-0.149286	-0.273350	0.265302
Si	-1.963683	0.391506	-0.382886
Si	1.849684	-0.357364	-0.505824
C	-2.787737	1.077239	1.208030
H	-3.843499	1.221613	0.911263
C	-3.133488	-0.835092	-1.285924
H	-2.790704	-0.659184	-2.321068
C	-1.338019	1.624789	-1.787929
H	-0.246399	1.544826	-1.669227
C	-1.642674	3.128823	-1.700303
H	-1.092358	3.662494	-2.496305
H	-1.327821	3.563785	-0.745559
H	-2.709044	3.348743	-1.842084
C	-1.639898	1.136700	-3.222197
H	-1.160692	1.805942	-3.956034
H	-2.717054	1.143539	-3.443639
H	-1.260529	0.122491	-3.416852
C	1.430470	-0.879006	-2.319358
H	0.914764	-0.005124	-2.739911
C	0.481262	-2.071278	-2.450045
H	0.296627	-2.297073	-3.514858
H	-0.483212	-1.865758	-1.977450
H	0.890977	-2.985446	-1.991986
C	2.690572	-1.142099	-3.165932
H	2.396080	-1.321182	-4.215951
H	3.223322	-2.041781	-2.822593
H	3.399214	-0.306381	-3.159555
C	2.428449	1.492588	-0.540582
H	1.438322	1.957373	-0.341835

C	2.790161	-1.839942	0.265650
H	2.448369	-2.623542	-0.447741
Si	-3.125342	-2.758741	-1.396577
Si	-4.904383	-0.136798	-1.430055
Si	-2.323153	2.793609	1.917311
Si	-2.994146	-0.163521	2.659623
C	-4.689416	-3.661597	-0.833873
H	-4.550495	-4.724900	-1.100807
H	-5.611121	-3.319524	-1.326206
H	-4.840766	-3.620697	0.254747
C	-2.968404	-3.150548	-3.244608
H	-2.865681	-4.240585	-3.387979
H	-2.086086	-2.673342	-3.699945
H	-3.852660	-2.823815	-3.812814
C	-1.710868	-3.650277	-0.519531
H	-1.249973	-4.381286	-1.204946
H	-2.074953	-4.202364	0.359827
H	-0.918484	-2.977171	-0.178463
C	-5.689336	-0.789403	-3.020754
H	-5.877100	-1.872935	-3.008976
H	-5.045179	-0.571433	-3.889511
H	-6.655317	-0.283453	-3.189592
C	-4.960610	1.744113	-1.624144
H	-6.020223	2.054546	-1.622954
H	-4.526988	2.078078	-2.578901
H	-4.460031	2.295493	-0.817812
C	-6.022738	-0.538676	0.031650
H	-6.128263	-1.616715	0.213715
H	-7.029190	-0.134147	-0.173578
H	-5.669819	-0.075758	0.963868
C	-2.746955	3.038668	3.750196
H	-2.375159	4.041923	4.026498
H	-2.285832	2.319909	4.440295
H	-3.833462	3.036134	3.926448
C	-3.388737	4.139215	1.117836

H	-3.211214	4.316413	0.050434
H	-3.226368	5.093676	1.648985
H	-4.455308	3.880030	1.242232
C	-0.483054	3.149809	1.791327
H	-0.278170	4.190603	2.093717
H	-0.070604	3.001921	0.785252
H	0.081988	2.483782	2.460370
C	-1.590152	-0.231388	3.929813
H	-0.945567	0.657072	3.959790
H	-0.935207	-1.094515	3.741935
H	-2.040956	-0.358066	4.931817
C	-4.610661	0.323600	3.544471
H	-4.423828	0.778263	4.529493
H	-5.240416	-0.568006	3.705852
H	-5.207828	1.044004	2.961725
C	-3.231101	-1.930568	2.078058
H	-2.377688	-2.284154	1.490094
H	-4.141170	-2.041375	1.476326
H	-3.322510	-2.593254	2.956357
Si	2.894779	2.458596	-2.150534
Si	3.388772	2.194016	0.980745
Si	2.297246	-2.743502	1.908143
Si	4.686763	-1.929710	-0.006679
C	1.807441	2.211961	-3.680063
H	2.177601	2.932659	-4.431379
H	0.755576	2.462493	-3.491243
H	1.850600	1.217210	-4.141067
C	2.664954	4.305996	-1.806197
H	2.758174	4.845540	-2.764914
H	3.413604	4.723132	-1.118357
H	1.667130	4.532585	-1.397223
C	4.659992	2.273862	-2.805813
H	4.805145	3.084027	-3.542976
H	4.832540	1.324008	-3.333088
H	5.442271	2.378447	-2.042516

C	2.842006	3.960490	1.417210
H	3.611771	4.696085	1.133262
H	2.708852	4.026926	2.510077
H	1.896856	4.273671	0.957666
C	3.093493	1.150069	2.498940
H	3.578947	1.620360	3.371526
H	3.518229	0.148059	2.379780
H	2.023693	1.020668	2.708909
C	5.259713	2.316362	0.749914
H	5.541458	3.072206	0.000161
H	5.746627	1.369340	0.483658
H	5.682940	2.645506	1.715785
C	5.670710	-1.660025	1.581383
H	5.518208	-0.645826	1.981526
H	6.745148	-1.762554	1.349554
H	5.431534	-2.375498	2.380544
C	5.362662	-0.665661	-1.232636
H	5.334855	-1.047622	-2.262732
H	6.417939	-0.455767	-0.989916
H	4.829412	0.288824	-1.215144
C	5.123460	-3.604964	-0.770889
H	6.133264	-3.555566	-1.213732
H	4.421339	-3.852783	-1.586390
H	5.108340	-4.439831	-0.056738
C	3.250668	-4.387315	1.945188
H	4.337752	-4.297858	2.082016
H	3.070990	-4.979645	1.032456
H	2.859606	-4.975090	2.794178
C	0.522166	-3.362981	2.019423
H	-0.224460	-2.571562	1.912075
H	0.407564	-3.802959	3.026800
H	0.313771	-4.161391	1.292187
C	2.622443	-1.908849	3.565766
H	1.920203	-1.084198	3.748311
H	3.645852	-1.537172	3.710238

H	2.441043	-2.683598	4.332892

B=N-[SiiPrDis2]2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.081082	-0.212414	1.496489
N	-0.086748	-0.242690	0.132817
Si	-1.751433	0.395309	-0.388185
Si	1.679661	-0.350817	-0.557813
C	-2.616530	1.055423	1.202488
H	-3.653727	1.191250	0.836682
C	-2.979843	-0.791448	-1.289164
H	-2.646875	-0.618280	-2.327845
C	-1.191594	1.637578	-1.787899
H	-0.098144	1.554405	-1.710472
C	-1.491241	3.141514	-1.663708
H	-0.951841	3.690348	-2.456069
H	-1.167991	3.561389	-0.705407
H	-2.558866	3.361250	-1.791284
C	-1.546529	1.191019	-3.225241
H	-1.070201	1.865034	-3.955910
H	-2.628440	1.234158	-3.416061
H	-1.202825	0.172546	-3.457741
C	1.395737	-0.867190	-2.372892
H	0.911317	0.006911	-2.830441
C	0.435639	-2.048929	-2.529362
H	0.276521	-2.274981	-3.597965
H	-0.537842	-1.836227	-2.080985

H	0.823961	-2.966576	-2.059158
C	2.676426	-1.156765	-3.171907
H	2.422538	-1.352611	-4.228668
H	3.188111	-2.053293	-2.790894
H	3.392955	-0.328622	-3.151694
C	2.367723	1.472508	-0.513091
H	1.404744	1.989113	-0.317097
C	2.608557	-1.826931	0.281152
H	2.267692	-2.623075	-0.419897
Si	-3.063708	-2.715498	-1.434759
Si	-4.750094	-0.055383	-1.441173
Si	-2.231583	2.784616	1.932840
Si	-2.972049	-0.168165	2.656100
C	-4.662068	-3.574126	-0.890796
H	-4.545993	-4.638620	-1.164312
H	-5.569837	-3.209403	-1.392685
H	-4.827305	-3.538180	0.195687
C	-2.935712	-3.091409	-3.289461
H	-2.856820	-4.182547	-3.439686
H	-2.050594	-2.630413	-3.754287
H	-3.821211	-2.745701	-3.844776
C	-1.688782	-3.671633	-0.566905
H	-1.268892	-4.422098	-1.257385
H	-2.078594	-4.206933	0.311851
H	-0.867265	-3.033295	-0.229958
C	-5.534647	-0.673250	-3.049230
H	-5.754318	-1.750573	-3.054270
H	-4.888587	-0.458969	-3.917023
H	-6.488417	-0.140709	-3.209609
C	-4.814060	1.827773	-1.617511
H	-5.878643	2.121022	-1.639716
H	-4.364741	2.178396	-2.558678
H	-4.345246	2.378306	-0.792452
C	-5.920980	-0.459718	-0.021256
H	-6.052259	-1.537670	0.139519

H	-6.911694	-0.036921	-0.265056
H	-5.604179	-0.014364	0.931079
C	-2.704179	3.021687	3.754174
H	-2.331897	4.021227	4.043322
H	-2.271261	2.297321	4.456036
H	-3.795223	3.030138	3.898887
C	-3.305749	4.118802	1.123343
H	-3.093956	4.337188	0.069493
H	-3.183816	5.059165	1.690312
H	-4.370825	3.836101	1.201475
C	-0.399820	3.179726	1.852386
H	-0.215415	4.223379	2.157301
H	0.038154	3.038008	0.856483
H	0.154659	2.521407	2.538881
C	-1.723887	-0.279138	4.076518
H	-1.067714	0.595513	4.170373
H	-1.064923	-1.149073	3.949499
H	-2.286547	-0.398992	5.021911
C	-4.636147	0.375414	3.416423
H	-4.496946	0.842646	4.403575
H	-5.287540	-0.504772	3.557018
H	-5.188155	1.094630	2.789691
C	-3.239935	-1.923447	2.047011
H	-2.390489	-2.304971	1.468849
H	-4.141263	-1.995071	1.425749
H	-3.373793	-2.591015	2.916324
Si	2.913212	2.448154	-2.095471
Si	3.357030	2.121315	1.020551
Si	2.160142	-2.760905	1.929060
Si	4.521760	-1.948249	0.022594
C	1.873372	2.241951	-3.662308
H	2.285270	2.960139	-4.393770
H	0.821639	2.514025	-3.508077
H	1.911845	1.248834	-4.127944
C	2.719784	4.297673	-1.738218

H	2.840934	4.842618	-2.690462
H	3.468334	4.689358	-1.035958
H	1.722520	4.544266	-1.340343
C	4.691050	2.242452	-2.711944
H	4.861083	3.063366	-3.432167
H	4.859818	1.300626	-3.254611
H	5.461911	2.324010	-1.934381
C	2.862997	3.900547	1.473999
H	3.660565	4.614306	1.212441
H	2.715018	3.958645	2.565443
H	1.937608	4.251498	1.003545
C	3.039712	1.078809	2.537838
H	3.504154	1.560206	3.416586
H	3.479653	0.081755	2.432782
H	1.965860	0.934029	2.734109
C	5.235338	2.205160	0.818030
H	5.546002	2.972947	0.092146
H	5.712199	1.256560	0.541710
H	5.646097	2.505533	1.799269
C	5.513288	-1.733931	1.617745
H	5.394809	-0.727172	2.046652
H	6.582682	-1.857894	1.370596
H	5.268463	-2.464325	2.401076
C	5.276437	-0.703917	-1.175660
H	5.265502	-1.078438	-2.208114
H	6.332334	-0.544445	-0.898171
H	4.787990	0.272480	-1.166237
C	4.953100	-3.624436	-0.749008
H	5.964231	-3.560438	-1.188102
H	4.258732	-3.879942	-1.568059
H	4.950724	-4.461365	-0.038012
C	3.106795	-4.410548	1.923351
H	4.192005	-4.331637	2.079159
H	2.936299	-4.977878	0.993795
H	2.701367	-5.017034	2.752453

C	0.387657	-3.388559	2.047151
H	-0.373102	-2.612306	1.916735
H	0.264117	-3.803342	3.063532
H	0.197325	-4.203392	1.333380
C	2.521583	-1.971107	3.601444
H	1.832614	-1.143521	3.817010
H	3.552183	-1.618844	3.739359
H	2.341391	-2.763813	4.350576

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Tbt2-B≡N-Tbt2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.811365	1.309808	0.396252
C	3.659643	-1.352280	-0.023245
C	4.069665	1.019658	-0.164364
C	1.921920	0.221355	0.677304
C	2.405082	-1.126415	0.572761
C	4.485567	-0.293423	-0.454340
H	4.746228	1.840780	-0.402554
H	3.998779	-2.377618	-0.160711
C	2.455382	2.737937	0.753908
H	1.368654	2.780832	0.965126
C	5.773018	-0.537404	-1.206778
H	6.272976	0.444608	-1.327750
C	1.605161	-2.298111	1.114951
H	0.678230	-1.895926	1.564778
Si	0.997754	-3.453139	-0.282685
Si	2.529258	-3.073913	2.603037

Si	7.053697	-1.576949	-0.249311
Si	5.382275	-1.040799	-3.009421
Si	3.256486	3.157107	2.446259
Si	2.741495	4.030184	-0.621297
C	4.013314	-4.140961	2.136077
H	3.738749	-5.037137	1.560880
H	4.500443	-4.480328	3.067393
H	4.768450	-3.585537	1.563202
C	3.184717	-1.693689	3.703189
H	3.832930	-1.007113	3.136709
H	3.783350	-2.115080	4.529287
H	2.373996	-1.098008	4.146069
C	1.354133	-4.161346	3.597697
H	0.479320	-3.600258	3.959248
H	1.878161	-4.566849	4.480546
H	0.986595	-5.018183	3.009810
C	-0.510179	-4.478663	0.201202
H	-0.401893	-4.974589	1.177943
H	-0.654851	-5.266846	-0.558586
H	-1.430895	-3.878887	0.230720
C	2.301149	-4.697677	-0.848735
H	2.005976	-5.110149	-1.829362
H	2.365062	-5.543805	-0.145035
H	3.309117	-4.276649	-0.960266
C	0.494703	-2.343292	-1.709967
H	1.326694	-1.717886	-2.068004
H	-0.323209	-1.667772	-1.410957
H	0.132976	-2.951657	-2.553528
C	6.851748	-1.223609	1.590105
H	5.842875	-1.476949	1.947878
H	7.016467	-0.152673	1.797620
H	7.580472	-1.798618	2.186588
C	6.897160	-3.429113	-0.576497
H	7.575156	-3.991805	0.088177
H	7.173055	-3.675334	-1.615240

H	5.878757	-3.809153	-0.404738
C	8.777764	-1.020985	-0.776188
H	9.550835	-1.544414	-0.187402
H	8.912633	0.061787	-0.610676
H	8.975699	-1.224033	-1.840278
C	6.982171	-1.166221	-4.001696
H	7.598387	-0.256751	-3.905075
H	6.750269	-1.299126	-5.072732
H	7.597774	-2.025553	-3.689275
C	4.441493	-2.662974	-3.152545
H	4.246683	-2.876373	-4.218298
H	3.466380	-2.605975	-2.648248
H	4.990853	-3.520613	-2.737054
C	4.290713	0.305269	-3.745195
H	4.034800	0.084008	-4.795427
H	4.777447	1.294449	-3.717992
H	3.348133	0.381361	-3.180628
C	2.991290	4.973732	2.880425
H	3.370915	5.167423	3.898882
H	1.921887	5.240319	2.868248
H	3.516289	5.657884	2.195496
C	2.433336	2.102123	3.761466
H	1.376767	2.379726	3.889236
H	2.936783	2.214546	4.736838
H	2.467812	1.039705	3.485035
C	5.102022	2.775352	2.442500
H	5.282387	1.699518	2.292909
H	5.540773	3.057678	3.415439
H	5.649386	3.320452	1.658009
C	1.714661	5.581270	-0.262040
H	1.216213	5.933448	-1.180438
H	2.352244	6.400491	0.107538
H	0.930067	5.409599	0.488465
C	2.212994	3.253808	-2.246654
H	2.880486	2.425752	-2.520476

H	2.229019	3.986063	-3.070874
H	1.195931	2.843229	-2.176283
C	4.539417	4.593665	-0.780190
H	5.226743	3.782535	-1.067900
H	4.914055	5.036851	0.156583
H	4.606752	5.371961	-1.560870
C	-3.182931	0.151467	1.158448
C	-3.662782	0.098078	-1.612367
C	-2.127872	0.477232	0.249118
C	-4.395118	-0.334851	0.627271
C	-4.639084	-0.436843	-0.754356
C	-2.424184	0.585000	-1.157416
H	-5.169961	-0.647233	1.330895
H	-3.882291	0.138549	-2.680217
C	-3.115724	0.336621	2.668909
H	-4.132987	0.064443	3.018307
C	-1.514133	1.324202	-2.125520
H	-0.474063	1.265393	-1.758929
C	-5.878116	-1.102151	-1.317793
H	-5.882023	-0.915314	-2.411020
Si	-7.517245	-0.333478	-0.730623
Si	-5.665016	-2.994778	-1.198133
Si	-1.463252	0.758466	-3.951192
Si	-2.014095	3.182580	-1.963334
Si	-3.067881	2.164730	3.206654
Si	-2.088958	-0.921354	3.656694
C	-4.076224	-3.448283	-2.106423
H	-4.131678	-3.187772	-3.176706
H	-3.870717	-4.530132	-2.034246
H	-3.215113	-2.911714	-1.677510
C	-7.122624	-3.872317	-2.015447
H	-7.291140	-3.509749	-3.043456
H	-8.058616	-3.727602	-1.451263
H	-6.934766	-4.958733	-2.071267
C	-5.499741	-3.588846	0.580920

H	-5.372728	-4.685279	0.601432
H	-6.376008	-3.338403	1.197605
H	-4.612741	-3.142562	1.054452
C	-8.155389	-1.077813	0.883560
H	-8.397524	-2.147521	0.770269
H	-9.078442	-0.561003	1.199467
H	-7.425423	-0.983767	1.703911
C	-8.820010	-0.604113	-2.070321
H	-9.044340	-1.671057	-2.227190
H	-8.485114	-0.187519	-3.036035
H	-9.764350	-0.099627	-1.801645
C	-7.263931	1.518836	-0.499380
H	-6.908816	1.988638	-1.431750
H	-6.512724	1.725325	0.278127
H	-8.206020	2.014411	-0.207632
C	0.175693	1.329892	-4.691392
H	1.027308	0.924214	-4.121472
H	0.284363	2.423820	-4.715794
H	0.265185	0.961021	-5.728128
C	-1.549598	-1.108420	-4.195684
H	-1.836090	-1.318663	-5.241198
H	-2.281465	-1.599171	-3.539159
H	-0.570771	-1.573848	-4.018672
C	-2.873894	1.469248	-4.998734
H	-2.941949	2.566337	-4.969224
H	-3.857420	1.068153	-4.703638
H	-2.707966	1.177866	-6.051140
C	-1.441170	3.810498	-0.290807
H	-1.942437	3.278275	0.524175
H	-1.651498	4.887286	-0.178953
H	-0.361494	3.659518	-0.165462
C	-1.245751	4.316940	-3.266669
H	-1.538058	4.067832	-4.297557
H	-0.147680	4.325770	-3.219720
H	-1.590850	5.347156	-3.066711

C	-3.887066	3.368012	-2.058645
H	-4.390116	2.774571	-1.282069
H	-4.293448	3.050451	-3.030898
H	-4.161870	4.426778	-1.909157
C	-4.277093	3.099704	2.100942
H	-4.085050	2.919567	1.033824
H	-4.229705	4.187685	2.277985
H	-5.310176	2.770590	2.306551
C	-3.707219	2.282945	4.981795
H	-2.993483	1.858765	5.706979
H	-4.669571	1.759481	5.110863
H	-3.864240	3.340975	5.256383
C	-1.358477	2.960182	3.186339
H	-0.756240	2.634100	2.329971
H	-0.812308	2.696843	4.105616
H	-1.444779	4.059557	3.152877
C	-3.032216	-1.323876	5.245628
H	-3.053890	-0.474857	5.947575
H	-2.557775	-2.173146	5.768065
H	-4.077499	-1.607969	5.033615
C	-0.370165	-0.355428	4.161174
H	-0.415887	0.515706	4.833594
H	0.249910	-0.075857	3.299283
H	0.143615	-1.164367	4.706759
C	-2.006291	-2.475605	2.610946
H	-3.021147	-2.859095	2.420966
H	-1.428679	-3.281844	3.086358
H	-1.553695	-2.254291	1.634894
B	0.420115	0.449764	0.787106
N	-0.833742	0.651841	0.699917

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Tbt2-B=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.517357	1.384325	-0.073111
C	3.017151	-1.337594	0.400809
C	3.728733	0.756919	-0.475372
C	1.440373	0.569178	0.447916
C	1.792827	-0.768203	0.857167
C	4.003584	-0.611528	-0.299213
H	4.519209	1.385194	-0.889843
H	3.223441	-2.370992	0.674111
C	2.508011	2.892394	-0.139137
H	1.436991	3.213198	0.023075
C	5.345738	-1.183138	-0.771233
H	5.970917	-0.307857	-1.043988
C	1.030872	-1.555927	1.919368
H	0.149062	-0.966023	2.216379
Si	0.307512	-3.253780	1.403417
Si	2.109917	-1.682250	3.518231
Si	6.448223	-2.057805	0.529498
Si	5.217968	-2.113313	-2.446400
Si	3.365748	3.656140	1.404465
Si	3.125476	3.686988	-1.774922
C	3.296636	-3.155327	3.491353
H	2.774840	-4.123439	3.446026
H	3.888801	-3.146032	4.423781
H	4.012257	-3.120969	2.659584
C	3.122658	-0.117469	3.785278
H	3.564070	0.276216	2.860584
H	3.944012	-0.317935	4.494597
H	2.496547	0.672692	4.222846
C	1.035781	-1.867676	5.057509

H	0.346307	-1.017797	5.161736
H	1.691338	-1.871223	5.946314
H	0.444230	-2.793058	5.076976
C	-1.257796	-2.947662	0.425446
H	-2.088894	-2.688024	1.096060
H	-1.545961	-3.855921	-0.124351
H	-1.157858	-2.125744	-0.290594
C	-0.221342	-4.304647	2.884440
H	-0.723392	-5.205331	2.487782
H	-0.947449	-3.783455	3.525888
H	0.612264	-4.647138	3.515381
C	1.493254	-4.326096	0.402938
H	2.429497	-4.542630	0.941696
H	1.755677	-3.886053	-0.567905
H	1.001238	-5.294706	0.203840
C	6.310192	-1.148600	2.167970
H	5.288751	-1.160247	2.565690
H	6.608171	-0.093914	2.043970
H	6.977529	-1.599198	2.922744
C	6.026309	-3.888102	0.738183
H	6.562202	-4.311943	1.605279
H	6.328317	-4.468210	-0.148998
H	4.952026	-4.065966	0.895246
C	8.266303	-1.939815	0.006453
H	8.912997	-2.180164	0.869381
H	8.533392	-0.920676	-0.322249
H	8.535075	-2.633448	-0.803909
C	6.808672	-3.021767	-2.924809
H	7.677794	-2.345778	-2.973130
H	6.671136	-3.445369	-3.936257
H	7.065111	-3.857197	-2.255298
C	3.813596	-3.359146	-2.425325
H	3.768483	-3.900882	-3.385676
H	2.845026	-2.861314	-2.272815
H	3.942849	-4.105212	-1.625976

C	4.932880	-0.837235	-3.798000
H	4.770341	-1.321933	-4.775793
H	5.802561	-0.165217	-3.896868
H	4.051747	-0.218421	-3.586018
C	3.410197	5.539317	1.251714
H	3.734232	5.970615	2.215009
H	2.399553	5.927822	1.043105
H	4.088725	5.919883	0.473797
C	2.356819	3.287685	2.938695
H	1.497716	3.972083	3.008089
H	2.971328	3.402677	3.847787
H	1.961291	2.267942	2.922803
C	5.116193	2.990677	1.648084
H	5.111815	1.905444	1.830424
H	5.564879	3.474714	2.533789
H	5.778212	3.186290	0.791278
C	2.220305	5.313089	-2.069832
H	2.434755	5.673160	-3.091115
H	2.539926	6.096108	-1.366655
H	1.129864	5.202014	-1.977194
C	2.815875	2.538916	-3.225258
H	3.570286	1.742067	-3.273311
H	2.862854	3.095782	-4.176669
H	1.833579	2.058469	-3.157500
C	4.985785	4.060225	-1.809207
H	5.604185	3.154493	-1.699226
H	5.303921	4.778821	-1.039454
H	5.233616	4.502374	-2.791308
C	-2.903587	0.564296	0.931719
C	-2.991501	-0.546415	-1.651496
C	-1.702978	0.617833	0.124722
C	-4.021704	-0.179462	0.451594
C	-4.103138	-0.774689	-0.819049
C	-1.842280	0.175912	-1.241442
H	-4.890586	-0.257728	1.108013

H	-3.035569	-0.905253	-2.680457
C	-3.218403	1.273638	2.247767
H	-4.188566	0.828875	2.557120
C	-0.846306	0.560123	-2.319047
H	0.113822	0.817187	-1.837679
C	-5.329969	-1.555533	-1.294338
H	-5.167699	-1.797158	-2.365264
Si	-6.978657	-0.575150	-1.336837
Si	-5.446514	-3.289255	-0.472317
Si	-0.420199	-0.782196	-3.612338
Si	-1.504215	2.212362	-3.079830
Si	-3.839512	3.080938	2.070155
Si	-2.226662	0.760072	3.770817
C	-4.149953	-4.372661	-1.306109
H	-4.479275	-4.654621	-2.321407
H	-3.970478	-5.304114	-0.742297
H	-3.192720	-3.840587	-1.398428
C	-7.112837	-4.146363	-0.736704
H	-7.382526	-4.231090	-1.801547
H	-7.946591	-3.651337	-0.213916
H	-7.043326	-5.173730	-0.334893
C	-5.168014	-3.192541	1.386314
H	-5.254484	-4.199489	1.830485
H	-5.920633	-2.549686	1.872198
H	-4.175465	-2.792687	1.636066
C	-7.743847	-0.346487	0.376213
H	-7.920149	-1.307346	0.887514
H	-8.722074	0.157922	0.283271
H	-7.115283	0.276063	1.033114
C	-8.253766	-1.453180	-2.432490
H	-8.780643	-2.270978	-1.919317
H	-7.802930	-1.868567	-3.349869
H	-9.017200	-0.720315	-2.749704
C	-6.678999	1.106866	-2.119155
H	-6.321495	0.998462	-3.156554

H	-5.930204	1.689847	-1.567192
H	-7.614715	1.692192	-2.144684
C	1.250768	-0.366437	-4.359600
H	1.998680	-0.256230	-3.562514
H	1.250792	0.559456	-4.951641
H	1.583844	-1.189295	-5.013750
C	-0.233947	-2.487657	-2.837631
H	0.170571	-3.185476	-3.591299
H	-1.184441	-2.901012	-2.473361
H	0.468015	-2.466027	-1.990922
C	-1.670294	-0.930131	-5.025308
H	-1.832766	0.023547	-5.550683
H	-2.655327	-1.301978	-4.701700
H	-1.280104	-1.651186	-5.765401
C	-1.317649	3.608411	-1.839801
H	-1.625682	4.569445	-2.285457
H	-0.280122	3.699604	-1.496576
H	-1.925580	3.440158	-0.940469
C	-0.607713	2.726431	-4.657441
H	-0.718703	1.990660	-5.468298
H	0.463644	2.910612	-4.506184
H	-1.059938	3.672886	-5.002327
C	-3.329045	2.065305	-3.515988
H	-3.950149	1.931017	-2.620780
H	-3.540608	1.228050	-4.198340
H	-3.653789	2.995587	-4.014655
C	-4.672283	3.262780	0.388393
H	-4.035408	2.910382	-0.435262
H	-4.931785	4.317681	0.192764
H	-5.608587	2.681785	0.358252
C	-5.192590	3.378289	3.366883
H	-4.781368	3.543532	4.374761
H	-5.915308	2.546721	3.432388
H	-5.761682	4.285306	3.094675
C	-2.555944	4.428036	2.314134

H	-3.068706	5.407256	2.304430
H	-1.777140	4.428338	1.537156
H	-2.054359	4.327886	3.290615
C	-3.130051	1.364254	5.312371
H	-3.033680	2.453647	5.444324
H	-2.694492	0.881948	6.204413
H	-4.204649	1.119309	5.289377
C	-0.495276	1.458398	3.840753
H	-0.538198	2.546115	3.685328
H	0.170092	1.066653	3.064314
H	-0.035327	1.266110	4.822465
C	-2.285445	-1.122698	3.788547
H	-3.333292	-1.464456	3.733772
H	-1.842143	-1.542353	4.703736
H	-1.762058	-1.555132	2.926612
N	-0.150986	2.558947	0.774632
B	-0.160876	1.245836	0.527063

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B=N-Tbt2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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C	2.249670	1.267751	-0.413957
C	2.803916	-1.272147	0.705880
C	3.484347	0.610051	-0.610412
C	1.210796	0.532891	0.259291
C	1.557006	-0.659958	0.985120
C	3.780093	-0.674234	-0.117722
H	4.269988	1.148845	-1.139716

H	3.044708	-2.199576	1.221098
C	2.178597	2.738729	-0.805894
H	1.127654	3.075378	-0.791473
C	5.138131	-1.289076	-0.413586
H	5.719918	-0.503222	-0.937093
C	0.767367	-1.148559	2.192622
H	-0.111423	-0.494715	2.315832
Si	0.037876	-2.915269	2.126954
Si	1.819903	-0.886798	3.792638
Si	6.256302	-1.692324	1.081165
Si	5.048274	-2.657117	-1.742452
Si	3.079836	3.872737	0.493006
Si	2.821797	3.178150	-2.563627
C	3.025984	-2.307813	4.106906
H	2.508977	-3.259781	4.305061
H	3.620735	-2.065535	5.005166
H	3.735924	-2.474122	3.286448
C	2.803027	0.716745	3.703198
H	3.203525	0.928101	2.703110
H	3.650538	0.674778	4.408412
H	2.177789	1.568459	4.004061
C	0.749235	-0.771385	5.342826
H	-0.112421	-0.105496	5.214208
H	1.370467	-0.350078	6.153002
H	0.379722	-1.748429	5.682415
C	-1.451109	-2.898542	1.006927
H	-2.204938	-2.183066	1.362318
H	-1.916649	-3.895209	0.973591
H	-1.197800	-2.595701	-0.013860
C	-0.591332	-3.494951	3.812509
H	-1.149994	-4.434239	3.652328
H	-1.285169	-2.777959	4.275609
H	0.211084	-3.711625	4.533731
C	1.259182	-4.216672	1.524902
H	2.192090	-4.241615	2.107847

H	1.519702	-4.077634	0.467700
H	0.787154	-5.210582	1.618293
C	5.980488	-0.444911	2.457226
H	4.964763	-0.498647	2.864994
H	6.143250	0.584285	2.098100
H	6.688982	-0.628283	3.283627
C	5.991939	-3.440157	1.746408
H	6.497380	-3.557058	2.720435
H	6.411492	-4.197767	1.064392
H	4.928761	-3.682631	1.894325
C	8.059715	-1.524498	0.542685
H	8.713870	-1.519996	1.432089
H	8.230736	-0.575633	0.005344
H	8.394144	-2.343969	-0.110374
C	6.775123	-3.245040	-2.228280
H	7.452725	-2.406842	-2.459185
H	6.700857	-3.871665	-3.134404
H	7.248546	-3.858210	-1.444785
C	4.054286	-4.156678	-1.199858
H	3.953785	-4.858612	-2.046141
H	3.041437	-3.878431	-0.882972
H	4.532932	-4.698922	-0.370881
C	4.244839	-1.878476	-3.250022
H	4.103019	-2.608699	-4.063586
H	4.858313	-1.050765	-3.644928
H	3.259484	-1.468800	-2.990058
C	3.112721	5.656206	-0.138778
H	3.467175	6.297600	0.687261
H	2.099202	6.000388	-0.402599
H	3.768583	5.836457	-1.002189
C	2.303603	4.030307	2.196789
H	1.368003	4.604779	2.172069
H	3.031566	4.562389	2.838912
H	2.071706	3.065536	2.655852
C	4.838123	3.257973	0.801028

H	4.819527	2.263427	1.272050
H	5.332510	3.948417	1.506566
H	5.462791	3.192992	-0.100570
C	1.978107	4.767198	-3.159546
H	1.780196	4.708174	-4.243535
H	2.617642	5.646878	-2.990018
H	1.017620	4.956423	-2.657364
C	2.476975	1.774940	-3.764664
H	3.096088	0.897371	-3.527852
H	2.718443	2.090948	-4.794248
H	1.428984	1.457688	-3.750453
C	4.686992	3.479002	-2.700122
H	5.289135	2.598561	-2.423943
H	5.036222	4.329778	-2.096559
H	4.915746	3.710091	-3.755974
C	-2.578082	0.786786	0.760674
C	-2.771441	-0.926039	-1.448932
C	-1.407980	0.520047	-0.034897
C	-3.746374	0.037611	0.491903
C	-3.876695	-0.847201	-0.590667
C	-1.559046	-0.228541	-1.248543
H	-4.610600	0.216223	1.133576
H	-2.886797	-1.486844	-2.372560
C	-2.795555	1.940652	1.756145
H	-3.890812	1.853122	1.935873
C	-0.630232	-0.138283	-2.460480
H	0.331260	0.311393	-2.161840
C	-5.170297	-1.575916	-0.925121
H	-5.143763	-1.773135	-2.016138
Si	-6.780887	-0.576885	-0.695918
Si	-5.214308	-3.338147	-0.188274
Si	-0.153044	-1.785157	-3.317565
Si	-1.458860	1.139499	-3.659485
Si	-2.933014	3.708732	0.977075
Si	-2.358343	1.737220	3.614169

C	-3.886846	-4.360438	-1.055339
H	-4.192302	-4.562544	-2.096844
H	-3.741545	-5.334860	-0.557893
H	-2.917144	-3.846043	-1.081152
C	-6.853226	-4.201514	-0.560753
H	-7.075508	-4.200347	-1.640722
H	-7.709308	-3.747334	-0.037708
H	-6.791126	-5.256209	-0.239096
C	-4.981755	-3.298372	1.681111
H	-4.718402	-4.300077	2.062015
H	-5.911462	-2.986754	2.183070
H	-4.186111	-2.604617	1.986872
C	-7.500473	-0.720075	1.046866
H	-7.852228	-1.739154	1.274261
H	-8.365900	-0.042131	1.148760
H	-6.769771	-0.440569	1.823615
C	-8.055188	-1.197946	-1.943659
H	-8.442728	-2.198270	-1.700650
H	-7.626556	-1.241205	-2.959864
H	-8.914336	-0.505663	-1.978231
C	-6.510930	1.253083	-1.046794
H	-5.994533	1.417712	-2.005534
H	-5.912267	1.735543	-0.261977
H	-7.485208	1.770094	-1.093631
C	1.077263	-1.508542	-4.726505
H	1.810619	-0.714452	-4.541802
H	0.561674	-1.276522	-5.669309
H	1.638360	-2.445329	-4.881427
C	0.645935	-2.942923	-2.069639
H	1.255156	-3.697765	-2.593367
H	-0.100498	-3.480744	-1.468705
H	1.302602	-2.393815	-1.378311
C	-1.598922	-2.688853	-4.141576
H	-2.199822	-2.018622	-4.778217
H	-2.274383	-3.185304	-3.429370

H	-1.185353	-3.474092	-4.799150
C	-1.063896	2.874020	-3.040069
H	-1.861283	3.581287	-3.319130
H	-0.132355	3.230748	-3.497757
H	-0.945339	2.914454	-1.948359
C	-0.871790	1.047325	-5.455227
H	-1.223597	0.135503	-5.963754
H	0.218616	1.104793	-5.574565
H	-1.312008	1.908181	-5.990115
C	-3.330538	0.930656	-3.776736
H	-3.841848	1.101485	-2.820912
H	-3.617282	-0.071144	-4.134902
H	-3.712577	1.665603	-4.507762
C	-3.587389	3.501254	-0.778946
H	-3.169421	2.621565	-1.282223
H	-3.344508	4.389276	-1.385188
H	-4.681419	3.390246	-0.775395
C	-4.282482	4.638608	1.928380
H	-3.928263	5.053423	2.884345
H	-5.167926	4.015654	2.136377
H	-4.613681	5.488496	1.305623
C	-1.476836	4.906879	0.934432
H	-1.881455	5.897391	0.649319
H	-0.700166	4.628611	0.208758
H	-0.988899	5.001323	1.915682
C	-3.664842	2.677308	4.611309
H	-3.478496	3.762736	4.619600
H	-3.622724	2.332883	5.659587
H	-4.692504	2.514954	4.247059
C	-0.719748	2.365543	4.282473
H	-0.574742	3.423687	4.015379
H	0.142324	1.822307	3.882925
H	-0.718493	2.280206	5.385006
C	-2.625642	-0.093416	3.983691
H	-3.655688	-0.385913	3.717221

H	-2.483261	-0.313437	5.054764
H	-1.948186	-0.739014	3.409329
B	-0.042187	2.203104	1.252535
N	-0.146945	1.116548	0.379333

Ar*-B≡N-Ar*

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.083029	2.724802	0.191433
C	-4.583929	0.919161	1.712028
C	-2.451970	1.978337	1.229352
C	-4.461861	2.568139	-0.029564
C	-5.239919	1.692126	0.739451
C	-3.209539	1.051824	1.992266
H	-4.940041	3.173391	-0.800662
H	-5.167575	0.210514	2.309041
C	-2.334733	3.795484	-0.605017
H	-1.259041	3.616230	-0.486545
C	-2.631351	5.199832	-0.034701
H	-2.055008	5.967714	-0.577411
H	-3.703247	5.438411	-0.135839
H	-2.368551	5.262184	1.030846
C	-2.647011	3.766514	-2.113220
H	-3.681087	4.085753	-2.320908
H	-2.509680	2.763858	-2.536865
H	-1.978643	4.461707	-2.647033
C	-2.690235	0.273452	3.205381
H	-3.401009	-0.562034	3.332898

C	-2.789879	1.141528	4.481632
H	-3.795595	1.578578	4.587824
H	-2.058496	1.963864	4.451248
H	-2.576254	0.534025	5.377467
C	-1.289435	-0.346647	3.090886
H	-1.163289	-0.902960	2.153341
H	-1.126789	-1.044006	3.928273
H	-0.499913	0.413489	3.143187
C	-6.759532	1.656582	0.634267
H	-7.078331	0.623010	0.838616
C	-7.370201	2.549053	1.740510
H	-7.067206	3.600024	1.596450
H	-7.025058	2.233152	2.737578
H	-8.472401	2.501448	1.720385
C	-7.308924	2.065224	-0.743116
H	-7.160613	3.141455	-0.932310
H	-8.392792	1.871547	-0.793004
H	-6.820671	1.510516	-1.559160
C	4.982624	2.170898	-1.264993
C	2.547864	2.235974	0.203118
C	4.903913	1.654052	0.037064
C	3.801390	2.663965	-1.845137
C	2.584441	2.705655	-1.143741
C	3.710346	1.671357	0.786403
H	5.794210	1.229514	0.505455
H	3.841455	3.043605	-2.868863
C	6.307819	2.284792	-2.011799
H	6.067239	2.528830	-3.062326
C	7.143759	0.991260	-2.010988
H	6.589936	0.149808	-2.453848
H	7.438244	0.705354	-0.988238
H	8.070406	1.134930	-2.591008
C	7.127649	3.460846	-1.433962
H	6.545273	4.395852	-1.459026
H	8.058471	3.612041	-2.006668

H	7.399830	3.261888	-0.383680
C	3.804430	1.087832	2.199379
H	4.525598	0.263028	2.098976
C	2.533165	0.455180	2.784997
H	2.034446	-0.191095	2.051863
H	1.815997	1.206513	3.139928
H	2.814184	-0.171232	3.646769
C	4.417571	2.104265	3.187638
H	5.355371	2.528716	2.795222
H	4.635794	1.615750	4.152563
H	3.721375	2.934850	3.382144
C	1.354581	3.341624	-1.795241
H	0.468577	2.873292	-1.345834
C	1.294974	4.851907	-1.478674
H	1.277336	5.035222	-0.394962
H	0.391223	5.304420	-1.919422
H	2.175688	5.365480	-1.899475
C	1.257795	3.113822	-3.313807
H	1.332200	2.048198	-3.569334
H	2.044738	3.656632	-3.862402
H	0.288106	3.486558	-3.679912
C	1.341664	2.558067	1.030846
C	-0.905220	3.472357	2.459169
C	0.100515	1.869800	0.911145
C	1.440474	3.667841	1.891179
C	0.337824	4.095781	2.642603
C	-1.050747	2.390234	1.571945
H	2.393516	4.196648	1.955436
H	0.432282	4.944059	3.326439
H	-1.793298	3.853482	2.967846
C	-3.097645	-2.681156	-0.171061
C	-4.609959	-0.922546	-1.731014
C	-2.463978	-1.940852	-1.210483
C	-4.482550	-2.549798	0.029060
C	-5.268068	-1.703915	-0.766222

C	-3.226832	-1.025867	-1.981726
H	-4.957892	-3.156943	0.800648
H	-5.197266	-0.231529	-2.345256
C	-2.336772	-3.719755	0.654041
H	-1.264769	-3.514625	0.545362
C	-2.590373	-5.140894	0.105534
H	-2.004671	-5.885541	0.670397
H	-3.657888	-5.404332	0.193477
H	-2.306971	-5.214500	-0.954108
C	-2.669554	-3.666862	2.156784
H	-3.703402	-3.991791	2.357860
H	-2.547064	-2.654146	2.561335
H	-2.000934	-4.343632	2.713518
C	-2.690722	-0.221721	-3.169866
H	-3.416740	0.598984	-3.311387
C	-2.718463	-1.069774	-4.462854
H	-3.706398	-1.534658	-4.610673
H	-1.963730	-1.869600	-4.420101
H	-2.494151	-0.439890	-5.340627
C	-1.310721	0.425753	-2.987727
H	-1.246023	0.974496	-2.039282
H	-1.121107	1.133511	-3.810270
H	-0.505476	-0.318455	-3.001093
C	-6.790620	-1.713876	-0.697738
H	-7.139433	-0.696258	-0.934020
C	-7.347375	-2.650931	-1.795321
H	-7.016127	-3.687838	-1.617632
H	-6.987820	-2.348844	-2.791503
H	-8.450901	-2.636853	-1.802491
C	-7.360175	-2.110467	0.675435
H	-7.185167	-3.177788	0.889339
H	-8.450082	-1.947693	0.699033
H	-6.907176	-1.527335	1.492328
C	4.987730	-2.185575	1.251281
C	2.544261	-2.246526	-0.205981

C	4.902546	-1.667576	-0.049587
C	3.808546	-2.678788	1.836995
C	2.589388	-2.716232	1.139547
C	3.703332	-1.680979	-0.792028
H	5.792762	-1.245737	-0.521116
H	3.853275	-3.059935	2.860397
C	6.318274	-2.304027	1.988610
H	6.086090	-2.567988	3.035956
C	7.145400	-1.004845	2.006122
H	6.593313	-0.177548	2.476976
H	7.421454	-0.692923	0.986186
H	8.082173	-1.153856	2.568481
C	7.144204	-3.462119	1.385074
H	6.565115	-4.399205	1.385170
H	8.074882	-3.623430	1.955448
H	7.417239	-3.235608	0.340813
C	3.789884	-1.099196	-2.206309
H	4.501903	-0.265527	-2.109879
C	2.510261	-0.486180	-2.796015
H	1.992090	0.142789	-2.061659
H	1.811471	-1.250680	-3.158966
H	2.784384	0.151072	-3.652485
C	4.411540	-2.114854	-3.190010
H	5.353926	-2.527974	-2.796498
H	4.622528	-1.632028	-4.159655
H	3.722318	-2.953303	-3.375104
C	1.354978	-3.339911	1.791108
H	0.477008	-2.863195	1.336546
C	1.282341	-4.850843	1.481710
H	1.273440	-5.037302	0.398613
H	0.368964	-5.291013	1.915037
H	2.152362	-5.372900	1.914354
C	1.252575	-3.104082	3.308055
H	1.335092	-2.038114	3.560401
H	2.030799	-3.652815	3.863194

H	0.277239	-3.465016	3.671372
C	1.330837	-2.555936	-1.026503
C	-0.930291	-3.441763	-2.444227
C	0.100093	-1.844810	-0.911898
C	1.407596	-3.664044	-1.888941
C	0.301267	-4.083568	-2.639717
C	-1.064758	-2.357294	-1.557977
H	2.355719	-4.202180	-1.955649
H	0.382502	-4.932435	-3.323664
H	-1.827968	-3.809085	-2.947022
B	0.061124	0.515132	0.212805
N	0.048529	-0.686479	-0.188636

Ar*2-B=N

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

B	-1.541712	0.439886	-0.074817
N	-2.021165	0.390969	1.226937
C	-2.431594	0.845175	-1.358928
C	-3.972094	1.510187	-3.669563
C	-3.201425	-0.141011	-2.035542
C	-2.416357	2.167362	-1.892565
C	-3.192627	2.480443	-3.027956
C	-3.960072	0.200104	-3.176420
H	-3.179096	3.505981	-3.402312
H	-4.553308	-0.578046	-3.662844
H	-4.575637	1.771568	-4.543473
C	-0.029572	0.062459	-0.248000

C	2.700960	-0.643401	-0.156182
C	0.709811	-0.047674	-1.430806
C	0.594666	-0.229482	0.992881
C	1.953520	-0.562223	1.038288
C	2.062676	-0.408086	-1.387537
H	0.225286	0.142107	-2.387746
H	2.450411	-0.768388	1.988948
H	2.641909	-0.493853	-2.309752
C	-3.283066	-1.578592	-1.609147
C	-3.708797	-4.331129	-1.044723
C	-4.236554	-1.964588	-0.632806
C	-2.531569	-2.571685	-2.295798
C	-2.759490	-3.927318	-1.999709
C	-4.426168	-3.333948	-0.365997
H	-2.187013	-4.686925	-2.537905
H	-5.174559	-3.635811	0.372983
C	-1.547299	3.267763	-1.350250
C	0.155550	5.354065	-0.407986
C	-0.299784	3.534833	-1.993167
C	-1.981638	4.117694	-0.295256
C	-1.113955	5.138374	0.145627
C	0.532403	4.553561	-1.496525
H	-1.448941	5.788349	0.960335
H	1.490500	4.736188	-1.987527
C	-0.294108	-0.164933	2.195754
C	-1.485148	-0.102749	4.796087
C	-0.800284	-1.386751	2.809919
C	-0.301299	1.059118	2.989863
C	-0.915727	1.058873	4.244776
C	-1.418418	-1.304672	4.060928
H	-0.943614	1.977626	4.832933
H	-1.828279	-2.220889	4.494599
C	4.156263	-0.966136	-0.133256
C	6.918436	-1.565048	-0.238310
C	5.104072	0.083507	-0.045379

C	4.579033	-2.314809	-0.255753
C	5.956233	-2.590062	-0.311089
C	6.473723	-0.239956	-0.099085
H	6.285520	-3.626759	-0.420363
H	7.218604	0.559947	-0.040386
C	-5.121655	-0.932971	0.058319
H	-4.713409	0.058781	-0.174485
C	-1.521448	-2.211041	-3.384495
H	-1.358176	-1.124373	-3.339028
C	-5.115226	-1.078614	1.590444
H	-5.705648	-0.267195	2.047973
H	-4.086455	-1.012013	1.973492
H	-5.559929	-2.035954	1.910118
C	-6.553461	-0.988317	-0.516652
H	-7.184573	-0.203748	-0.065771
H	-7.024961	-1.964597	-0.312847
H	-6.545347	-0.839815	-1.608538
C	-0.158612	-2.902236	-3.181843
H	0.233118	-2.728881	-2.171086
H	0.578218	-2.513606	-3.904470
H	-0.229414	-3.990873	-3.340539
C	-2.084951	-2.535409	-4.785249
H	-3.032022	-2.005247	-4.965978
H	-2.277836	-3.616486	-4.887606
H	-1.368790	-2.241757	-5.571618
C	-3.965229	-5.804888	-0.754543
H	-4.795758	-5.850972	-0.027634
C	-4.409483	-6.567462	-2.019415
H	-5.287896	-6.087947	-2.480341
H	-4.670222	-7.611082	-1.774795
H	-3.605309	-6.590893	-2.773231
C	-2.736956	-6.473504	-0.104202
H	-2.451383	-5.951750	0.823165
H	-1.869810	-6.449705	-0.784734
H	-2.946982	-7.528648	0.140041

C	0.124387	2.838375	-3.288822
H	-0.430486	1.892527	-3.368236
C	-3.386753	4.130269	0.323078
H	-3.314682	4.848834	1.158879
C	-0.263402	3.705649	-4.510232
H	-1.342730	3.909269	-4.541068
H	0.019665	3.198833	-5.448657
H	0.263631	4.673898	-4.473290
C	1.633873	2.527887	-3.355186
H	2.222793	3.436317	-3.562062
H	1.839944	1.818977	-4.174299
H	2.001449	2.091386	-2.418632
C	-4.422894	4.713687	-0.665197
H	-5.367648	4.924583	-0.135766
H	-4.643240	3.996691	-1.469644
H	-4.061628	5.649228	-1.122472
C	-3.911753	2.815564	0.923801
H	-4.810218	3.023253	1.529736
H	-3.166219	2.313198	1.555963
H	-4.198902	2.104401	0.138715
C	1.066759	6.451989	0.124624
H	0.604091	6.836959	1.051188
C	1.164359	7.625552	-0.873139
H	0.164192	8.020776	-1.112283
H	1.630775	7.297612	-1.817051
H	1.775001	8.445811	-0.458719
C	2.467227	5.914687	0.483101
H	2.401407	5.061276	1.175890
H	3.078385	6.701351	0.956427
H	3.003924	5.572714	-0.416781
C	3.560359	-3.448322	-0.365566
H	2.570999	-3.028608	-0.133475
C	3.825596	-4.577063	0.648654
H	3.875484	-4.180886	1.675248
H	4.774613	-5.097748	0.441232

H	3.017678	-5.326300	0.607117
C	3.495992	-3.992801	-1.807594
H	3.260056	-3.187176	-2.520060
H	2.717878	-4.769306	-1.897097
H	4.460589	-4.437244	-2.105050
C	4.667126	1.543634	0.071227
H	3.573455	1.557656	0.187962
C	4.999728	2.327311	-1.215315
H	4.613316	3.358290	-1.151755
H	4.549828	1.845195	-2.096651
H	6.089155	2.381026	-1.377580
C	5.270651	2.231416	1.311421
H	4.879196	3.257555	1.409640
H	6.368844	2.297928	1.243654
H	5.022587	1.677912	2.230642
C	8.407121	-1.877467	-0.310671
H	8.944308	-0.916597	-0.221158
C	8.852051	-2.776825	0.860820
H	8.580377	-2.325648	1.828636
H	9.943599	-2.933684	0.842176
H	8.368876	-3.766233	0.803816
C	8.785395	-2.502253	-1.669382
H	8.473068	-1.851845	-2.502134
H	8.294618	-3.480141	-1.804449
H	9.874960	-2.659356	-1.738515
C	-0.639983	-2.793412	2.242287
H	-1.454648	-3.376288	2.706942
C	-0.778989	-2.967684	0.725203
H	-1.647115	-2.423070	0.341181
H	-0.915795	-4.034500	0.497882
H	0.111811	-2.622597	0.188763
C	0.688238	-3.409643	2.751664
H	1.553264	-2.896408	2.308961
H	0.740120	-4.471003	2.458463
H	0.769746	-3.346288	3.848626

C	0.404882	2.312483	2.504851
H	0.433384	2.282735	1.405155
C	1.860759	2.313084	3.037270
H	1.864011	2.348479	4.139638
H	2.396381	3.200733	2.666038
H	2.417892	1.422248	2.720342
C	-0.295931	3.609609	2.941677
H	-1.357629	3.605849	2.661960
H	0.184664	4.466571	2.451555
H	-0.217032	3.767188	4.029961
C	-2.131963	-0.054679	6.170965
H	-2.068384	0.989718	6.522609
C	-1.377109	-0.937275	7.189436
H	-1.827075	-0.828861	8.190450
H	-0.315062	-0.651867	7.255274
H	-1.426996	-2.002535	6.912014
C	-3.625332	-0.438619	6.097566
H	-4.098950	-0.312725	7.085329
H	-3.750189	-1.490304	5.794161
H	-4.159919	0.189838	5.368862

B=N-Ar*2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	3.021774	2.304169	-0.334162
C	4.698095	0.621681	-1.816653
C	2.450396	1.307449	-1.185493
C	4.419809	2.427982	-0.267074

C	5.280482	1.611717	-1.016586
C	3.303683	0.465913	-1.940195
H	4.844001	3.207883	0.365438
H	5.347725	-0.038021	-2.400662
C	2.168944	3.338349	0.403402
H	1.213232	2.856877	0.671055
C	1.861710	4.558313	-0.495130
H	1.272263	5.303867	0.063759
H	2.803294	5.037203	-0.814913
H	1.296657	4.280516	-1.392899
C	2.790239	3.842699	1.720058
H	3.616929	4.548217	1.532432
H	3.174863	3.022421	2.338942
H	2.026794	4.381586	2.303044
C	2.853450	-0.561457	-2.982639
H	3.545762	-1.409851	-2.843701
C	3.096151	-0.037367	-4.418302
H	4.124286	0.336426	-4.541217
H	2.403343	0.783349	-4.659442
H	2.929978	-0.843453	-5.153136
C	1.428565	-1.117907	-2.863753
H	1.182016	-1.386050	-1.828699
H	1.338975	-2.023494	-3.481783
H	0.673890	-0.407084	-3.219612
C	6.787084	1.837529	-1.062278
H	7.258630	0.857563	-1.247248
C	7.135685	2.750058	-2.261304
H	6.675425	3.743948	-2.131113
H	6.756224	2.325420	-3.204172
H	8.227197	2.884589	-2.352368
C	7.379076	2.411660	0.236083
H	7.057285	3.453293	0.398432
H	8.480248	2.414539	0.184864
H	7.075052	1.824784	1.116140
C	-5.217475	2.253477	0.844089

C	-2.692356	1.871303	-0.436281
C	-5.085915	1.430992	-0.281420
C	-4.073886	2.941168	1.275944
C	-2.825694	2.799722	0.645068
C	-3.860694	1.251585	-0.958533
H	-5.966865	0.922176	-0.678499
H	-4.169850	3.647731	2.104220
C	-6.568270	2.530062	1.495835
H	-6.365057	2.979625	2.484288
C	-7.420204	1.267373	1.719083
H	-6.887018	0.522076	2.329687
H	-7.690803	0.792690	0.762198
H	-8.359674	1.525429	2.235574
C	-7.347924	3.571582	0.661141
H	-6.755139	4.490315	0.525803
H	-8.300010	3.838608	1.150915
H	-7.577958	3.169579	-0.339851
C	-4.004670	0.488287	-2.285742
H	-4.655022	-0.363700	-2.040439
C	-2.770252	-0.106692	-2.978827
H	-2.063737	-0.537671	-2.264154
H	-2.235122	0.632963	-3.587520
H	-3.107011	-0.913710	-3.648525
C	-4.780281	1.365629	-3.301073
H	-5.741761	1.714311	-2.894814
H	-4.981773	0.793838	-4.223060
H	-4.192918	2.255608	-3.580154
C	-1.741920	3.820056	1.003453
H	-0.785258	3.451298	0.614915
C	-2.044150	5.159032	0.293077
H	-2.124636	5.025530	-0.796979
H	-1.238958	5.885886	0.494931
H	-2.992199	5.590162	0.656471
C	-1.561455	4.041000	2.515577
H	-1.370229	3.083815	3.019555

H	-2.440029	4.527488	2.969739
H	-0.692074	4.695894	2.694174
C	-1.393598	1.817574	-1.198807
C	0.897285	2.252936	-2.761531
C	-0.171813	1.136905	-0.857010
C	-1.424035	2.642039	-2.345200
C	-0.312932	2.813930	-3.168465
C	1.008641	1.481933	-1.583119
H	-2.359307	3.153775	-2.573536
H	-0.368203	3.437726	-4.064560
H	1.816054	2.479061	-3.303635
C	3.190718	-2.239222	0.376846
C	4.925796	-0.483910	1.667468
C	2.648899	-1.251836	1.272848
C	4.572604	-2.271459	0.125158
C	5.464400	-1.389843	0.749495
C	3.555071	-0.432278	2.001408
H	4.964212	-3.038994	-0.542994
H	5.607932	0.177629	2.211324
C	2.374062	-3.442216	-0.121909
H	1.311792	-3.170012	-0.130691
C	2.553308	-4.629118	0.859026
H	1.921815	-5.478601	0.549789
H	3.604567	-4.962167	0.852549
H	2.289381	-4.365551	1.889473
C	2.750176	-3.958823	-1.524681
H	3.734616	-4.453830	-1.518714
H	2.776467	-3.167090	-2.278483
H	2.016116	-4.714417	-1.847147
C	3.301486	0.352121	3.302286
H	3.979689	1.222604	3.244775
C	3.788196	-0.504526	4.500891
H	4.811910	-0.880341	4.350830
H	3.125261	-1.372028	4.650692
H	3.763826	0.095715	5.426145

C	1.909042	0.890672	3.616198
H	1.488891	1.490445	2.798431
H	1.955584	1.536947	4.509316
H	1.187221	0.088569	3.823244
C	6.977510	-1.496709	0.595710
H	7.388431	-0.479076	0.705052
C	7.553100	-2.351156	1.749828
H	7.158466	-3.379995	1.697924
H	7.273417	-1.934212	2.730075
H	8.654035	-2.401257	1.693586
C	7.440854	-2.053809	-0.759922
H	7.173690	-3.117689	-0.870430
H	8.537458	-1.981879	-0.846263
H	6.991903	-1.504194	-1.600737
C	-5.001628	-2.515118	-0.807926
C	-2.493373	-1.800404	0.355484
C	-4.929159	-1.763953	0.371728
C	-3.792061	-2.916171	-1.395377
C	-2.545482	-2.585526	-0.838922
C	-3.709238	-1.423464	0.991334
H	-5.852964	-1.452496	0.864602
H	-3.827784	-3.529593	-2.298800
C	-6.335841	-2.968740	-1.388907
H	-6.130171	-3.381339	-2.392738
C	-7.347540	-1.818133	-1.550813
H	-6.938717	-1.007456	-2.173757
H	-7.623532	-1.389743	-0.574053
H	-8.273914	-2.183258	-2.024425
C	-6.930921	-4.105177	-0.527549
H	-6.217750	-4.939341	-0.430445
H	-7.863101	-4.492016	-0.973227
H	-7.163113	-3.741349	0.487125
C	-3.887014	-0.765892	2.370398
H	-4.705074	-0.043463	2.218705
C	-2.730072	0.029359	2.979911

H	-2.287560	0.731650	2.262910
H	-1.929225	-0.615663	3.364819
H	-3.109563	0.628210	3.824703
C	-4.396287	-1.809224	3.395927
H	-5.264108	-2.370984	3.017370
H	-4.690524	-1.306105	4.332472
H	-3.604111	-2.533317	3.642992
C	-1.294760	-3.250859	-1.420554
H	-0.423835	-2.661332	-1.106294
C	-1.148201	-4.670731	-0.826145
H	-1.096974	-4.648823	0.270935
H	-0.234444	-5.155798	-1.205765
H	-2.010999	-5.292966	-1.116693
C	-1.259726	-3.342394	-2.957129
H	-1.333684	-2.356763	-3.432648
H	-2.072450	-3.974861	-3.348765
H	-0.311075	-3.803464	-3.274199
C	-1.191324	-1.804969	1.117179
C	1.061599	-2.389917	2.679741
C	0.001531	-1.031404	0.921154
C	-1.206911	-2.826601	2.094813
C	-0.131102	-3.058174	2.948438
C	1.189665	-1.452380	1.631610
H	-2.123978	-3.407313	2.197731
H	-0.198019	-3.791697	3.755955
H	1.961031	-2.628814	3.247786
B	-0.182788	1.257512	1.479206
N	-0.066022	0.363257	0.401483

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M062X/Def2-TZVP

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F-B≡N-F

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.000000	0.000000	0.653708
N	0.000000	0.000000	-0.566393
F	0.000000	0.000000	-1.872872
F	0.000000	0.000000	1.950229

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F2-B=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.000127	0.047013	0.000670
N	-0.008165	1.468837	-0.000147
F	-1.153809	-0.589889	-0.000129
F	1.160089	-0.578658	-0.000129

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B=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.005504	1.652777	-0.002506
N	0.000668	0.228178	0.005076
F	1.087653	-0.551114	-0.001278
F	-1.091230	-0.544567	-0.001278

F-B≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.461941	0.274649	0.007134
N	-0.745317	0.807228	-0.002451
F	-1.311237	-0.567947	-0.000037
F	1.634295	-0.212480	-0.002020

F-B≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.786337	0.916567	-0.322053

N	0.314776	0.265947	0.545814
F	1.268581	-0.185734	-0.229720
F	-1.076552	-0.530317	-0.015883

HO-B≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.644957	0.016667	-0.018579
N	0.583448	0.148378	0.054813
O	1.882940	-0.181279	-0.048509
H	2.366160	0.610549	0.215785
O	-1.981199	0.012310	-0.096226
H	-2.439439	-0.380785	0.651295

(OH)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.051611	0.109798	0.000845
N	-0.771775	1.258198	-0.001143
O	1.403013	0.053494	0.001112
H	1.737113	-0.848591	0.001185

O	-0.762729	-1.008395	-0.004166
H	-1.715010	-0.868571	0.027027

B≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.012156	1.629720	0.000357
N	0.000425	0.230786	-0.000656
O	-1.147349	-0.504682	-0.116865
H	-1.376750	-0.787157	0.780429
O	1.140452	-0.517213	0.117170
H	1.368166	-0.801786	-0.780067

HO-B≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.757262	0.822971	-0.033815
B	0.451357	0.312558	0.028710
O	1.657534	-0.199701	0.112182

H	2.083353	-0.448245	-0.715126
O	-1.311437	-0.579784	-0.101425
H	-1.808082	-0.639460	0.722226

HO-B≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.787261	0.955471	0.294034
N	0.307765	0.306985	-0.460842
O	1.302029	-0.147818	0.263809
H	1.849521	-0.682488	-0.331482
O	-1.163178	-0.512992	-0.098737
H	-1.178375	-0.957282	0.766632

H-B≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.690862	-0.000371	0.000004
N	0.539953	0.000319	0.000001
H	1.532532	-0.000938	-0.000013
H	-1.857895	0.000564	-0.000015

H2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.576895	0.000017	-0.002558
N	-0.728981	-0.000013	0.000529
H	1.109135	1.070914	0.004543
H	1.109254	-1.070906	0.004543

B≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.960580	-0.000108	0.000003
N	-0.412028	-0.000055	-0.000006
H	-0.960084	-0.850946	0.000016
H	-0.958622	0.851871	0.000016

H-B≡N-H-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.728223	0.000007	0.000000
B	0.578313	-0.000001	-0.000001
H	1.103039	1.074888	0.000001
H	1.102956	-1.074933	0.000001

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H-B≡N-H-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.444661	-0.043934	0.005773
B	0.827456	-0.151135	-0.003380
H	0.424451	1.083099	-0.001130
H	-1.449101	-0.019885	-0.022381

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3HC-B≡N-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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H	-2.548612	0.448437	-0.915107
C	-2.161520	0.000355	-0.000004
H	-2.548295	0.570249	0.844842
H	-2.550868	-1.015230	0.070238
B	-0.619937	-0.001038	0.000011
N	0.615641	-0.000928	0.000021
C	2.025459	0.000474	-0.000005
H	2.417465	0.566309	0.848230
H	2.417507	0.453331	-0.913584
H	2.419367	-1.016384	0.065230

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(CH3)2-B≡N

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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N	-0.001131	1.484299	0.000000
B	0.000125	0.168119	-0.000009
C	-1.424886	-0.560358	0.000109
H	-1.472339	-1.191152	-0.888196
H	-2.267691	0.124727	0.000195
H	-1.472227	-1.192315	0.887341
C	1.425612	-0.559226	-0.000112
H	2.267714	0.126686	-0.000457
H	1.473585	-1.191383	-0.887129
H	1.473896	-1.189753	0.888309

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B≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.088273	0.185326	0.000844
C	1.236854	-0.494798	0.000040
H	1.291578	-1.127067	-0.888858
H	1.290270	-1.126742	0.889208
N	-0.000025	0.269590	-0.000492
B	-0.001805	1.640495	0.000167
C	-1.235841	-0.496413	0.000085
H	-1.290746	-1.126197	0.890602
H	-2.087714	0.183138	-0.002632
H	-1.288541	-1.130794	-0.887304

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3HC-B≡N-CH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.778754	1.194160	-0.001088
N	0.255786	0.424213	0.001884
C	-1.319309	-0.591846	-0.000070
H	-1.922577	-0.568572	-0.899398
H	-1.924128	-0.567773	0.898163
H	-0.680909	-1.474957	0.000794

C	1.503259	-0.255014	-0.000433
H	1.620362	-0.874761	0.890360
H	2.289992	0.499278	-0.001350
H	1.616827	-0.872351	-0.893299

3HC-B≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.778110	1.193799	0.000244
N	0.256424	0.424392	-0.000374
C	-1.319997	-0.591390	0.000010
H	-1.924285	-0.567698	-0.898590
H	-1.924165	-0.567806	0.898694
H	-0.681880	-1.474644	-0.000046
C	1.502983	-0.255670	0.000117
H	1.619348	-0.874863	-0.891144
H	1.620129	-0.872201	0.893113
H	2.288522	0.499829	-0.001390

3HSi-B≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z

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B	-0.551154	0.011880	-0.009108
N	0.696992	-0.007262	-0.003828
H	-3.004505	0.106872	1.396148
Si	-2.533943	-0.000419	0.001549
H	-3.010416	-1.266296	-0.591685
H	-3.036986	1.142101	-0.785531
Si	2.405543	0.000488	0.001568
H	2.913067	-0.890921	-1.060282
H	2.907971	-0.472070	1.309038
H	2.905285	1.370780	-0.239007

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(SiH3)2-B≡N

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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B	0.000271	0.084793	-0.002373
N	-0.001569	1.352812	0.000269
Si	1.984339	-0.273165	0.000212
H	2.741745	0.986391	-0.005953
H	2.285411	-1.058228	-1.210778
H	2.284068	-1.045939	1.219329
Si	-1.983805	-0.273654	0.000182
H	-2.281359	-1.057796	1.212598
H	-2.285469	-1.047881	-1.217559
H	-2.742237	0.985272	0.006831

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B≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.002540	1.890671	-0.002319
N	-0.000240	0.522271	0.004668
Si	-1.542405	-0.343047	-0.000524
H	-2.633296	0.640893	-0.041358
H	-1.615579	-1.165471	1.220308
H	-1.572061	-1.218938	-1.185741
Si	1.541662	-0.344072	-0.000325
H	1.624820	-1.139051	-1.238634
H	2.633066	0.638029	0.070347
H	1.562428	-1.245046	1.165885

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3HSi-B≡N-SiH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.000053	0.085989	-0.002944
N	-0.000399	1.354100	0.000515
Si	1.983825	-0.273594	0.000200
H	2.743953	0.983977	0.002966
H	2.284750	-1.051617	-1.215288
H	2.279684	-1.055014	1.214644

Si	-1.983720	-0.273703	0.000212
H	-2.276459	-1.063176	1.210336
H	-2.286620	-1.044125	-1.219499
H	-2.744245	0.983466	0.012182

3HSi-B≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.744063	1.497394	-0.000051
N	0.227165	0.652503	0.000061
Si	-1.630637	-0.367792	-0.000000
H	-2.449878	-0.386324	-1.223979
H	-2.449732	-0.386359	1.224072
H	-0.839008	-1.622938	-0.000082
Si	1.734580	-0.224178	-0.000008
H	1.795004	-1.067690	-1.205352
H	1.794521	-1.068587	1.204726
H	2.824059	0.764988	0.000563

B3PW91/Def2-TZVP

F-B≡N-F

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.641794	-0.022021	0.000049
N	-0.574130	0.245885	-0.000006
F	-1.844260	-0.122773	-0.000006
F	1.934254	-0.056237	-0.000017

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F2-B=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.000137	0.049243	-0.000636
N	-0.005265	1.459742	0.000140
F	-1.162044	-0.584926	0.000122
F	1.166063	-0.577786	0.000122

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B=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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B	0.000770	1.658035	-0.000474
N	0.000102	0.227916	0.000961
F	1.100105	-0.549656	-0.000242
F	-1.100612	-0.548742	-0.000242

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F-B≡N-F-TSH

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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B	0.474535	0.253734	-0.000085
N	-0.728029	0.808595	0.000028
F	-1.354623	-0.553422	0.000001
F	1.657237	-0.216449	0.000024

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F-B≡N-F-TS2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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B	-0.793699	0.966246	-0.295223
N	0.281254	0.229038	0.557970
F	1.273908	-0.161660	-0.230545
F	-1.051717	-0.553283	-0.039419

HO-B≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.636568	0.011690	-0.014062
N	0.591203	0.264309	0.021827
O	1.849524	-0.237388	-0.007311
H	2.419369	0.537568	0.060369
O	-1.967492	-0.047124	-0.101912
H	-2.431208	-0.170084	0.730932

(OH)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.189511	-0.201678	0.003241
N	-0.921576	-0.966861	-0.000710
O	1.525449	-0.048779	-0.029261
H	1.828845	0.852418	0.107139
O	-0.909652	0.784046	0.109017
H	-1.251743	1.041857	-0.756418

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B≡N-(OH)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.000863	1.628092	-0.000010
N	-0.000019	0.226934	-0.000180
O	-1.151660	-0.511573	-0.118184
H	-1.392098	-0.776004	0.782868
O	1.152189	-0.510527	0.118299
H	1.392306	-0.776192	-0.782484

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HO-B≡N-OH-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.735139	0.823107	-0.028678
B	0.460848	0.272142	0.014760
O	1.683528	-0.199622	0.115105
H	2.125402	-0.437020	-0.707153
O	-1.364608	-0.561060	-0.103111
H	-1.835022	-0.599985	0.738148

HO-B≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.821175	1.015791	0.256635
N	0.248720	0.293105	-0.441413
O	1.305433	-0.118617	0.251158
H	1.833257	-0.641118	-0.371841
O	-1.110685	-0.574832	-0.081155
H	-1.026409	-0.941979	0.818536

H-B≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.689267	0.002669	0.061876
N	-0.539180	-0.002055	-0.048404
H	-1.527003	-0.006029	-0.137083
H	1.854929	0.007070	0.166535

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H2-B≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.570541	0.000000	-0.001436
N	-0.731100	-0.000009	0.000309
H	1.132444	1.063515	0.002508
H	1.132551	-1.063456	0.002508

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B≡N-H2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.960859	-0.000007	0.000013
N	0.412127	-0.000003	-0.000033
H	0.959653	0.850920	0.000083
H	0.959752	-0.850859	0.000083

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H-B≡N-H-TSH

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Atomic	Coordinates (Angstroms)

Number	X	Y	Z
N	-0.730296	0.000001	0.000000
B	0.571752	0.000000	0.000000
H	1.126658	1.067086	0.000000
H	1.126652	-1.067090	0.000000

H-B≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.444518	-0.047229	0.011160
B	0.834772	-0.144373	-0.006538
H	0.385511	1.079683	-0.002048
H	-1.447746	-0.027218	-0.043380

3HC-B≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.551751	0.957041	-0.351043
C	-2.159000	0.000037	-0.000012

H	-2.551996	-0.174334	1.004217
H	-2.552136	-0.782349	-0.653204
B	-0.620916	-0.000124	0.000000
N	0.617969	-0.000061	0.000052
C	2.021175	0.000043	-0.000019
H	2.420643	-0.164294	1.006623
H	2.420449	0.954065	-0.361045
H	2.420541	-0.789562	-0.645728

(CH3)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.001196	1.489251	-0.000010
B	0.000126	0.177514	0.000024
C	-1.425405	-0.565218	0.000091
H	-1.469641	-1.194551	-0.891496
H	-2.270395	0.119306	0.000221
H	-1.469252	-1.195492	0.890832
C	1.426183	-0.564006	-0.000101
H	2.270433	0.121335	-0.000940
H	1.470448	-1.194818	-0.890383
H	1.471477	-1.192758	0.891771

B≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.086933	0.197347	-0.002183
C	1.240777	-0.491989	-0.000247
H	1.305475	-1.124704	-0.890189
H	1.309300	-1.124441	0.889656
N	0.000018	0.262099	0.001683
B	-0.000408	1.635214	-0.000654
C	-1.240571	-0.492323	-0.000246
H	-1.310068	-1.123246	0.890683
H	-2.086855	0.196830	-0.004421
H	-1.304109	-1.126677	-0.889098

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3HC-B≡N-CH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.772843	1.209540	-0.002551
N	0.246614	0.408694	0.004199
C	-1.313454	-0.594881	-0.000230
H	-1.912126	-0.567032	-0.904481
H	-1.920362	-0.561695	0.898301
H	-0.690291	-1.491116	0.005548
C	1.499342	-0.250481	-0.001213
H	1.636925	-0.872626	0.887824
H	2.273903	0.519276	0.002013

H	1.634539	-0.863188	-0.897178

3HC-B≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.772115	1.209488	0.001448
N	0.246666	0.407774	-0.002379
C	-1.314379	-0.594244	0.000110
H	-1.917340	-0.563406	-0.901197
H	-1.917044	-0.563268	0.901626
H	-0.691955	-1.491011	0.000003
C	1.499858	-0.250487	0.000685
H	1.637508	-0.870341	-0.889943
H	1.635992	-0.865288	0.895077
H	2.273879	0.519843	-0.000923

3HSi-B≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-3.028357	-1.297204	0.522257
Si	-2.534046	0.000186	-0.000230

H	-3.025858	0.196535	-1.385972
H	-3.027141	1.102262	0.861747
B	-0.553406	-0.000712	0.000889
N	0.698853	-0.000860	0.001040
Si	2.406325	0.000246	-0.000303
H	2.913493	0.196862	-1.381945
H	2.916215	-1.293624	0.519899
H	2.914793	1.098693	0.859761

(SiH3)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.001725	0.471375	-0.064658
N	-0.019108	1.745845	0.013033
Si	1.826258	-0.385381	0.003281
H	2.888704	0.642281	0.014114
H	1.963944	-1.258395	-1.188430
H	1.872987	-1.198317	1.243150
Si	-1.819450	-0.394040	0.003436
H	-1.866872	-1.182417	1.260217
H	-1.936192	-1.292856	-1.172846
H	-2.892742	0.623811	-0.018175

B≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.633487	0.673334	0.099041
Si	-1.561046	-0.338710	0.000219
H	-1.592332	-1.257652	1.162059
H	-1.685492	-1.119465	-1.252164
N	0.000151	0.502906	-0.002152
B	-0.001634	1.872287	0.001271
Si	1.561488	-0.338080	0.000183
H	1.576748	-1.288824	-1.136875
H	2.633072	0.670516	-0.141227
H	1.702418	-1.084634	1.272253

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3HSi-B≡N-SiH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.001306	0.483534	-0.114929
N	-0.007355	1.752417	0.023603
Si	1.814857	-0.390698	0.005522
H	2.891371	0.607890	-0.163357
H	1.897994	-1.421556	-1.058822
H	1.889568	-1.029485	1.342522
Si	-1.812630	-0.393566	0.005773
H	-1.917654	-0.930731	1.383612
H	-1.852630	-1.504192	-0.978322

H	-2.894882	0.573190	-0.274334

3HSi-B≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.738033	1.527250	0.000003
N	0.189707	0.616047	-0.000003
Si	-1.609514	-0.372685	-0.000000
H	-2.429515	-0.372651	-1.233269
H	-2.429557	-0.372630	1.233242
H	-0.856732	-1.661480	0.000025
Si	1.726726	-0.216128	0.000001
H	1.827801	-1.060259	-1.211712
H	1.827850	-1.060186	1.211760
H	2.781398	0.822008	-0.000052

B3LYP/LANL2DZ+dp

F-B≡N-F

Atomic	Coordinates (Angstroms)

Number		X	Y	Z
	B	0.624149	-0.015155	0.000001
	N	-0.589851	0.375610	-0.000000
	F	-1.819148	-0.193447	-0.000000
	F	1.931171	-0.090274	-0.000000

F2-B=N

Atomic Number		Coordinates (Angstroms) X	Y	Z
	B	0.000003	0.059854	0.000051
	N	0.000135	1.474186	-0.000011
	F	1.181996	-0.590013	-0.000010
	F	-1.182103	-0.589829	-0.000010

B=N-F2

Atomic Number		Coordinates (Angstroms) X	Y	Z
	B	-0.000827	1.675847	-0.064321
	N	-0.000088	0.226309	0.131344

F	1.113919	-0.553038	-0.033212
F	-1.113391	-0.554006	-0.033210

F-B≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.455758	0.273422	0.000415
N	-0.751927	0.836344	-0.000140
F	-1.324035	-0.586764	-0.000005
F	1.655669	-0.215626	-0.000117

F-B≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.714576	1.055752	-0.289150
N	0.269361	0.231560	0.549748
F	1.288943	-0.198212	-0.219205
F	-1.101459	-0.568419	-0.047738

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HO-B≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.629717	0.026628	-0.011989
N	0.601361	0.359377	0.017699
O	1.826249	-0.286160	-0.002375
H	2.463828	0.443596	0.040327
O	-1.963345	-0.078298	-0.103286
H	-2.428010	-0.176719	0.741015

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(OH)2-B≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.173879	-0.192085	0.007629
N	-0.914784	-1.010835	-0.004665
O	1.523529	-0.053007	-0.024803
H	1.822996	0.862827	0.067985
O	-0.904773	0.815506	0.110967
H	-1.238958	1.073450	-0.762784

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B≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.000314	1.649079	0.000047
N	-0.000030	0.231109	-0.000161
O	-1.163743	-0.520384	-0.119581
H	-1.408657	-0.770062	0.790719
O	1.163939	-0.519992	0.119665
H	1.408860	-0.770091	-0.790498

HO-B≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.759708	0.859273	-0.024494
B	0.434105	0.282888	0.016714
O	1.668393	-0.195771	0.114635
H	2.102783	-0.426555	-0.721172
O	-1.319860	-0.594065	-0.108689
H	-1.743614	-0.684108	0.761495

HO-B≡N-OH-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.777022	1.059696	-0.257516
N	-0.261242	0.290063	0.447619
O	-1.322851	-0.143017	-0.253918
H	-1.843202	-0.668109	0.381112
O	1.160420	-0.571503	0.078718
H	1.086234	-0.944652	-0.825262

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H-B≡N-H

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.606251	0.064575	0.343292
N	-0.473028	-0.050351	-0.267861
H	-1.339572	-0.142842	-0.758517
H	1.619514	0.172428	0.917086

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H2-B≡N

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Atomic	Coordinates (Angstroms)

Number	X	Y	Z
B	0.575603	0.000000	-0.000764
N	-0.739256	-0.000008	0.000166
H	1.148336	1.060149	0.001330
H	1.148438	-1.060092	0.001330

B≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.971848	-0.000006	0.000021
N	0.416512	-0.000003	-0.000053
H	0.971785	0.855439	0.000134
H	0.971867	-0.855386	0.000134

H-B≡N-H-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.739051	0.000001	0.000000
B	0.575955	0.000000	0.000000

H	1.146797	1.060756	0.000000
H	1.146784	-1.060764	0.000000

H-B≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.450754	-0.054009	0.053127
B	0.844071	-0.141103	-0.031247
H	0.364912	1.100113	-0.004949
H	-1.429992	-0.016537	-0.210707

3HC-B≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.568025	0.965228	-0.347557
C	-2.173411	0.000054	-0.000027
H	-2.568352	-0.181442	1.009489
H	-2.568415	-0.783357	-0.662072
B	-0.627849	-0.000145	0.000039
N	0.621587	-0.000110	0.000085
C	2.037069	0.000068	-0.000040

H	2.437133	-0.136970	1.016606
H	2.436833	0.949141	-0.389711
H	2.437012	-0.811833	-0.627140

(CH3)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.002110	1.518622	-0.000133
B	-0.000201	0.194904	0.000564
C	1.420936	-0.579081	-0.000026
H	1.453670	-1.214293	0.895998
H	2.285270	0.091278	-0.001799
H	1.450834	-1.215507	-0.895324
C	-1.422328	-0.576892	-0.000108
H	-2.285462	0.094825	-0.013651
H	-1.461224	-1.202512	0.902337
H	-1.448503	-1.222830	-0.888648

B≡N-(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

H	2.104042	0.185868	-0.000460
C	1.246904	-0.498695	-0.000044
H	1.305334	-1.136012	-0.894821
H	1.306101	-1.135910	0.894799
N	0.000012	0.269330	0.000302
B	-0.000182	1.654514	-0.000108
C	-1.246807	-0.498835	-0.000045
H	-1.306772	-1.135022	0.895511
H	-2.103974	0.185681	-0.002010
H	-1.304492	-1.137300	-0.894065

3HC-B≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.759109	1.237672	-0.000389
N	0.253844	0.409604	0.000643
C	-1.342409	-0.601780	-0.000039
H	-1.945118	-0.556565	-0.907651
H	-1.946426	-0.555678	0.906664
H	-0.718401	-1.503029	0.000891
C	1.515243	-0.261491	-0.000187
H	1.645998	-0.884158	0.896622
H	2.299915	0.506181	0.000311
H	1.645671	-0.882717	-0.898041

3HC-B≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.759294	1.237586	0.000746
N	0.253698	0.409633	-0.001226
C	-1.342050	-0.601823	0.000066
H	-1.946501	-0.555698	-0.906361
H	-1.944469	-0.557044	0.907922
H	-0.718004	-1.503094	-0.001349
C	1.515108	-0.261374	0.000355
H	1.646086	-0.884599	-0.896026
H	1.645384	-0.882052	0.898614
H	2.299742	0.506313	-0.000473

3HSi-B≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-3.036824	-1.121199	-0.830333
Si	-2.539680	0.000018	0.000001
H	-3.036613	1.279791	-0.555860
H	-3.036738	-0.158414	1.386211
B	-0.563875	-0.000078	-0.000008
N	0.698467	-0.000077	0.000000
Si	2.416126	0.000023	-0.000001

H	2.923264	1.273086	-0.565120
H	2.923410	-1.125883	-0.819895
H	2.923357	-0.147034	1.385037

(SiH3)2-B≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.000052	0.507015	0.000149
N	-0.000366	1.796012	-0.000037
Si	-1.808343	-0.403264	-0.000007
H	-2.901104	0.587802	0.000195
H	-1.874180	-1.248983	1.213603
H	-1.873928	-1.248223	-1.214166
Si	1.808467	-0.403091	-0.000013
H	1.872974	-1.251268	-1.211986
H	1.875703	-1.245614	1.215735
H	2.901101	0.588109	-0.003577

B≡N-(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

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H	-2.648285	0.663244	-0.015805
Si	-1.568750	-0.342129	-0.000261
H	-1.647732	-1.184794	1.213586
H	-1.629616	-1.202705	-1.202636
N	0.000001	0.509773	0.003068
B	0.000614	1.892932	-0.001075
Si	1.568582	-0.342406	-0.000238
H	1.633170	-1.197369	-1.206812
H	2.648615	0.663106	-0.007518
H	1.643121	-1.191058	1.210071

3HSi-B≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.000052	0.507015	-0.000149
N	0.000366	1.796012	0.000037
Si	1.808343	-0.403264	0.000007
H	2.901104	0.587802	-0.000195
H	1.874180	-1.248983	-1.213603
H	1.873928	-1.248223	1.214166
Si	-1.808467	-0.403091	0.000013
H	-1.872974	-1.251268	1.211986
H	-1.875703	-1.245614	-1.215735
H	-2.901101	0.588109	0.003577

3HSi-B≡N-SiH3-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.709848	1.546323	-0.000171
N	0.194624	0.594497	0.000277
Si	-1.644383	-0.369954	-0.000009
H	-2.461373	-0.334396	-1.231138
H	-2.461407	-0.334289	1.231086
H	-0.925568	-1.673056	0.000025
Si	1.752680	-0.219319	-0.000038
H	1.861019	-1.063800	-1.207780
H	1.861928	-1.063063	1.208137
H	2.796117	0.825335	-0.000744

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b97d3/LANL2DZ+dp

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$SiMe(SitBu_3)_2$-Al≡N-$SiMe(SitBu_3)_2$

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.5C4C44	0.H0C079	-0.03382C
N	H.HSiH25	0.0035H9	0.0870CH
Si	2.C90800	0.424078	-0.45525H
Si	3.5330C5	-H.558H39	-H.CCH327
Si	3.CC9H02	H.C45775	H.533835

C	2.48H728	H.C94389	-H.88073C
H	2.00H883	H.H78857	-2.72C907
H	3.4Si775	2.Si5080	-2.252402
H	H.80HSi8	2.502495	-H.57389H
C	5.297302	-H.330730	-2.509C28
C	5.C5CHHH	-2.4C4827	-3.500847
H	5.C2CH57	-3.45805H	-3.03H077
H	C.C87HHH	-2.30C273	-3.87Si78
H	4.998938	-2.485C4C	-4.380530
C	C.4SiSi5	-H.3054C2	-H.4448C2
H	C.23CH8H	-0.542702	-0.C80243
H	7.38089C	-H.0C80C4	-H.927849
H	C.53H745	-2.27C045	-0.94H877
C	5.38C49H	0.0H0748	-3.2793H8
H	C.402994	0.H20507	-3.702832
H	5.2H387H	0.874C74	-2.C24977
H	4.C7444C	0.079733	-4.HH0757
C	3.573C0C	-3.00H309	-0.33350C
C	4.2C3598	-2.472957	0.94H539
H	3.799942	-H.540Si0	H.2835H7
H	5.334394	-2.28HC73	0.794C98
H	4.HC7Si7	-3.2HH573	H.75952H
C	4.3H354H	-4.288554	-0.758873
H	4.24C0Si	-5.034702	0.05C423
H	5.383H8C	-4.H059C4	-0.94HH80
H	3.89058C	-4.749H93	-H.CCH775
C	2.H27C92	-3.3C7433	0.07C52H
H	H.582527	-3.880482	-0.728Si2
H	H.558C38	-2.47HC78	0.3C2557
H	2.H52HHC	-4.052803	0.9450C5
C	2.23592H	-2.0H9085	-3.H0429H
C	2.343020	-3.5H3073	-3.50829C
H	H.C79389	-3.C97327	-4.37509C
H	2.0H3542	-4.H8447C	-2.7030C0
H	3.358527	-3.8094H7	-3.803H88

C	0.7CC802	-H.77C2H5	-2.C953CC
H	0.09C294	-2.Si2825	-3.49C878
H	0.5708HC	-0.704C7C	-2.55C230
H	0.49C288	-2.288CH7	-H.7C5802
C	2.45H322	-H.H885C0	-4.392373
H	2.4Si27H	-0.H05402	-4.20830C
H	H.C44353	-H.427C4C	-5.HHHH38
H	3.4024CC	-H.4H5908	-4.890009
C	2.730852	3.40C954	H.529C82
C	3.25535H	0.7077HH	3.247H77
C	5.59C590	H.97HCCH	H.30945H
C	C.H29209	3.H207H5	2.H95HC5
H	5.9H394C	2.95345C	3.2C3H25
H	5.7H3CC3	4.097458	H.9H0884
H	7.22882C	3.H90242	2.0877H9
C	5.877337	2.32C35H	-0.HC9408
H	C.9C3H75	2.477988	-0.3HC230
H	5.3C73CH	3.238HC4	-0.502443
H	5.570C7C	H.5H0HH7	-0.835Si2
C	C.45CH7H	0.724488	H.C34942
H	7.447C85	0.82CC42	H.H5C724
H	C.007977	-0.2095HC	H.2759H8
H	C.C27424	0.CH733C	2.7H2578
C	H.984900	-0.H55057	3.092924
H	2.HH5909	-0.98H239	2.3850C8
H	H.H3H835	0.4292C9	2.727408
H	H.7H7C29	-0.585880	4.07C797
C	4.377579	-0.223598	3.7C9334
H	4.74C207	-0.939745	3.027330
H	3.97C233	-0.808883	4.CH844C
H	5.235C32	0.347CC5	4.H529H5
C	2.974972	H.C8C095	4.4H39HH
H	2.037453	2.24H355	4.274274
H	3.789222	2.408C22	4.573878
H	2.8C3434	H.099402	5.345CH7

C	H.208008	3.HC3558	H.4438H8
H	0.940HC5	2.570H80	0.5C2504
H	0.C73790	4.H3H730	H.39H595
H	0.830094	2.C2H777	2.3245C0
C	2.95C238	4.347348	2.748954
H	2.59002H	5.355300	2.475290
H	2.39H805	4.0384C5	3.C35023
H	4.009509	4.452985	3.038H03
C	3.H5558C	4.25H244	0.300757
H	3.H82443	3.C8903H	-0.C3CH53
H	4.SiC939	4.703H85	0.452242
H	2.439924	5.085284	0.HC9CC4
Si	-2.927573	0.388H20	0.477H74
Si	-3.8H3520	H.C88049	-H.44HH95
Si	-3.390C20	-H.784575	H.57H20H
C	-2.8380HH	H.752552	H.83975C
H	-2.347820	2.C54283	H.447550
H	-2.27922H	H.433327	2.7252CH
H	-3.8482C8	2.038H07	2.H70870
C	-2.298C43	2.70C053	-2.H88740
C	-2.777H90	3.83H353	-3.Si29C2
H	-H.89H958	4.30728H	-3.C0383H
H	-3.329424	4.C2H35H	-2.CHC707
H	-3.4HH0H0	3.458080	-3.958305
C	-H.352433	H.802809	-3.0HH3C4
H	-0.99C4H2	0.923304	-2.447HCH
H	-0.45H04C	2.372508	-3.29CH82
H	-H.8HC508	H.4322H8	-3.9352C8
C	-H.435838	3.37330H	-H.09539C
H	-0.CH389C	3.940798	-H.5CC398
H	-0.954704	2.C37C09	-0.432582
H	-H.999039	4.0C7373	-0.45993C
C	-4.533293	0.479538	-2.794898
C	-3.570528	-0.7HH2CH	-2.993C25
H	-2.C22C95	-0.42207C	-3.4C3440

H -4.04325C -H.47H930 -3.C4H223
H -3.33575H -H.H98828 -2.042399
C -4.758499 H.H23HH7 -4.H84H95
H -3.8H77C2 H.452007 -4.C470H8
H -5.44339C H.98H502 -4.H5783C
H -5.203590 0.3C7874 -4.858453
C -5.88C2H0 -0.0974CH -2.3HC479
H -C.C8274H 0.C5948C -2.303420
H -5.8H7222 -0.528572 -H.309780
H -C.20988H -0.902H00 -3.0023CH
C -5.H88HSi 2.945925 -0.797C37
C -C.0395H7 3.495593 -H.97H823
H -C.75C935 4.23CH84 -H.57H908
H -C.C28875 2.7H0807 -2.4C500C
H -5.43755C 4.0038H7 -2.73C725
C -C.HC89H5 2.28H22H 0.H94745
H -C.92483H 3.0247H8 0.509329
H -5.CC4325 H.930548 H.H053C2
H -C.7H0497 H.434HCC -0.244C40
C -4.592424 4.H744C9 -0.0C4C29
H -3.97C24H 4.802859 -0.720702
H -3.990H99 3.8980C4 0.8099H8
H -5.423859 4.807H34 0.297772
C -2.0H87HC -2.0592C2 2.97329C
C -5.H74H85 -H.CC988H 2.3755H9
C -3.280422 -3.258057 0.283C95
C -3.20HC5H -4.C45580 0.97Si38
H -4.05HC89 -4.8330H0 H.C42Si4
H -2.27CC50 -4.785443 H.545C82
H -3.2H9089 -5.428C43 0.H90877
C -2.0270Si -3.H27523 -0.CH5723
H -2.037892 -3.9H7288 -H.389020
H -H.09HHH2 -3.23C225 -0.05578C
H -H.983388 -2.HC8307 -H.H50570
C -4.528090 -3.298Si3 -0.C29C84

H	-5.42SiCH	-3.C27C32	-0.080347
H	-4.3C09C7	-4.022974	-H.447095
H	-4.754985	-2.33SiC0	-H.09H395
C	-C.H92H5H	-H.H27HHH	H.35037H
H	-5.8547HH	-0.H8C090	0.903839
H	-7.H55408	-0.925753	H.854CHC
H	-C.38939H	-H.8377H2	0.538H85
C	-5.728CC5	-3.023947	2.88223H
H	-5.870C9H	-3.743H9C	2.0C258C
H	-C.722305	-2.852794	3.337057
H	-5.09CHC3	-3.495793	3.C44725
C	-5.HC5330	-0.C7C887	3.5C33C8
H	-4.8H7800	0.323345	3.2CCH84
H	-4.538H02	-H.0H9352	4.397422
H	-C.H9493H	-0.5C5494	3.950C82
C	-2.5HC7Si	-3.095250	4.0Si839
H	-H.C90339	-3.3Si20H	4.7H58H3
H	-2.825C20	-4.047789	3.5C4297
H	-3.353752	-2.7HHC20	4.CSi037
C	-0.C78527	-2.5888C7	2.4Si7C9
H	-0.7C0359	-3.58CC48	H.9C7C78
H	0.049474	-2.CC2333	3.24SiCH
H	-0.2222H7	-H.9HC994	H.C7230H
C	-H.CC5580	-0.7725C8	3.7545H5
H	-H.079749	-0.077030	3.H38C20
H	-2.545322	-0.243578	4.Si23H5
H	-H.02CC3C	-H.039523	4.CSi895

$[SiMe(SitBu_3)_2]_2$-Al=N

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
Al	0.0037H2	0.072433	-0.800593
N	0.05C2Si	0.H32HH0	-2.C75Si2
Si	2.325CC7	-0.HH7CH7	0.300C27
Si	-2.28CHCC	0.H34H87	0.437C4C
Si	3.C8H274	-H.97C292	-H.003423
Si	3.37C53H	2.2794H2	H.022C04
Si	-3.334243	-2.H93777	H.083H77
Si	-3.7C5549	H.88C494	-0.99780C
C	2.2502C8	-H.050C33	2.02240C
H	3.245892	-H.0C7C43	2.5Si9C9
H	H.9C0947	-2.H07H22	H.859SiC
H	H.532C07	-0.C30039	2.75HHC0
C	-2.040738	H.07HH80	2.H37542
H	-H.HC5444	0.C5C833	2.C85790
H	-2.920787	0.983HHC	2.80C739
H	-H.844H07	2.Si8590	H.987Si0
C	4.C809C5	-H.2H024C	-2.500C99
C	4.9H35CH	-2.99H945	0.22HH83
C	2.3233HC	-3.224877	-H.C53478
C	3.5555C3	3.50594C	-0.525493
C	5.H07CSi	2.HH2HCC	H.9737CH
C	2.008533	3.00999C	2.2C0258
C	-4.42993H	H.HH2790	-2.C7C59H
C	-2.504445	3.3H7570	-H.409C50
C	-5.2C377H	2.C47327	0.059554
C	-3.038483	-3.397C55	-0.487259
C	-5.2235CC	-2.H00382	H.705579
C	-2.22207C	-2.795HHC	2.C2HC54
C	2.978H37	-4.580920	-2.0C0735
H	3.4H7543	-5.H03508	-H.20C420
H	3.752H58	-4.4C9299	-2.824H05
H	2.H985C3	-5.23CCC5	-2.4747HH

C	H.539345	-2.77924H	-2.9HHH89
H	2.H97909	-2.725470	-3.77C048
H	H.02H57H	-H.8294H0	-2.849H57
H	0.78970H	-3.543957	-3.HH9878
C	H.302H29	-3.57H5C5	-0.555H2C
H	H.7554C5	-4.07C0Si	0.30C3H0
H	0.5370C0	-4.239544	-0.9C9738
H	0.798H29	-2.C78449	-0.HC3028
C	5.09237C	-2.245502	-3.577C92
H	5.729388	-3.044C08	-3.H7983C
H	5.CC7902	-H.724533	-4.3C2733
H	4.22834H	-2.7050C0	-4.0C7205
C	3.783880	-0.H54373	-3.H9H853
H	4.34807H	0.330H9C	-4.00C7CC
H	3.475294	0.C3HC98	-2.494725
H	2.877933	-0.5829HH	-3.C243H0
C	5.9CC058	-0.49730H	-2.03C745
H	C.7H7C7C	-H.H94994	-H.C38833
H	5.7C4C47	0.25C2C2	-H.2CC055
H	C.425480	0.024308	-2.89CC94
C	5.940909	-3.825H33	-0.59H2H2
H	C.575039	-4.3909C5	0.HH8999
H	C.CH3540	-3.H89C52	-H.H83708
H	5.478499	-4.55450H	-H.2CC237
C	5.742884	-2.053H53	H.HH897C
H	C.398280	-2.C58H05	H.778C7C
H	5.H08359	-H.430590	H.772H24
H	C.397C34	-H.388582	0.538833
C	4.H90775	-3.9C3979	H.H85783
H	4.94CC05	-4.4H93CC	H.85C37H
H	3.C85045	-4.792340	0.C73439
H	3.455475	-3.453900	H.82C842
C	4.80727C	3.H5207H	-H.3C0349
H	5.7443C0	3.348352	-0.8H7CC9
H	4.82H82H	3.77038H	-2.275809

H	4.80479C	2.H0H320	-H.C8040C
C	2.3204H5	3.3C4248	-H.4C4434
H	2.02C375	2.323022	-H.C35953
H	2.54C234	3.8052H3	-2.445040
H	H.4529C0	3.889C3C	-H.0C5534
C	3.C54759	4.99CCC0	-0.H27348
H	4.494842	5.20CC97	0.55H205
H	2.732523	5.3587H8	0.3484C8
H	3.80C052	5.C00H29	-H.04H289
C	0.747983	3.4H0757	H.4CH33H
H	0.3307C8	2.549H7C	0.9H8599
H	0.9H09C5	4.23CH89	0.758878
H	-0.03C9Si	3.747323	2.HC9953
C	2.52239C	4.233302	3.05452C
H	3.2739H3	3.9374C8	3.80708H
H	H.C7CH2C	4.C92593	3.C0CH57
H	2.9C770C	5.0H3H22	2.4H897H
C	H.5094H9	H.9C4908	3.28HC55
H	2.3H3205	H.4C4H94	3.8489C0
H	0.909C48	H.H88C92	2.7C9839
H	0.833789	2.455770	4.0H5782
C	C.0CH505	H.25800H	H.HH9C3H
H	C.9SiC57	0.889943	H.727078
H	C.47849H	H.8HCC72	0.2C7838
H	5.53387H	0.38Si72	0.724H77
C	4.904335	H.393709	3.3300C9
H	5.89H28C	H.H924C0	3.799859
H	4.388C72	0.42044C	3.2H9702
H	4.322Si5	2.002337	4.045595
C	5.795994	3.47HC28	2.243C45
H	C.74C3C5	3.289842	2.789234
H	5.H87H35	4.H52249	2.8C02CC
H	C.055C7C	3.993920	H.307C53
C	-2.32272C	-4.7H5H3H	-0.HSi838
H	-H.333959	-4.554839	0.329SiC

H	-2.H7C372	-5.308348	-H.034H07
H	-2.92SiC2	-5.32C09H	0.57C288
C	-4.357H74	-3.83C3C3	-H.H72C35
H	-4.HSiH2H	-4.50H23C	-2.020790
H	-4.934H79	-2.995H82	-H.575729
H	-5.004HC4	-4.407429	-0.487838
C	-2.H8930H	-2.C85808	-H.57H388
H	-H.258049	-2.2C5904	-H.H89C38
H	-2.747H22	-H.877C3C	-2.04898H
H	-H.925447	-3.404980	-2.35C088
C	-5.C2C845	-3.3CC5CH	2.49H9H2
H	-5.0C9H87	-3.472959	3.43C550
H	-5.477H27	-4.28CH9C	H.897Si0
H	-C.705CC4	-3.3H244H	2.748C54
C	-C.227885	-H.935HC8	0.54H582
H	-C.433025	-2.884343	0.027202
H	-5.87549C	-H.2HC525	-0.20C728
H	-7.H95C0C	-H.5CH9C7	0.934453
C	-5.3750C8	-0.8573C0	2.CH588H
H	-4.833352	-0.943383	3.57H570
H	-C.445C7H	-0.C88HC4	2.857499
H	-5.0H0430	0.05H242	2.H075C5
C	-2.3393C9	-4.300H35	2.995C05
H	-H.7Si054	-4.94HC5H	2.3C0487
H	-3.370258	-4.C84CH7	2.9520H3
H	-H.984C93	-4.438CH5	4.037434
C	-0.74C950	-2.492444	2.302350
H	-0.092322	-2.83H5C3	3.H342Si
H	-0.5CC87C	-H.4082C4	2.HC4978
H	-0.400944	-2.999H7C	H.390035
C	-2.5C4587	-2.003952	3.9H075H
H	-H.799753	-2.22732C	4.C8C248
H	-3.540739	-2.299449	4.334085
H	-2.57040H	-0.909970	3.7C3907
C	-5.097390	-0.25H557	-2.4H2808

H	-4.452748	-0.9059C9	-H.8H3007
H	-5.294C0C	-0.7CC787	-3.370399
H	-C.059C0H	-0.H5098H	-H.892H05
C	-5.474850	H.993909	-3.407CCH
H	-5.759H94	H.49C494	-4.3534CH
H	-5.0924CC	2.989389	-3.CC4HC5
H	-C.395H84	2.H2H3C4	-2.8H9042
C	-3.2C5743	0.84CH00	-3.C707C2
H	-2.4H2974	0.309H97	-3.230590
H	-2.88H5HC	H.774032	-4.H0947H
H	-3.C45C22	0.2347H8	-4.508H09
C	-C.445522	H.C55C73	0.H0C8H7
H	-C.H2582H	0.CC8935	0.4C40H2
H	-C.928472	H.524C87	-0.8740H5
H	-7.22H0H8	2.027030	0.80722C
C	-5.805048	3.9803H8	-0.5HC702
H	-5.08237H	4.8039C8	-0.4324C2
H	-C.700C23	4.2770C5	0.0C4902
H	-C.HH3805	3.89933C	-H.5C8HC8
C	-4.84HH58	2.9Si04C	H.522H8H
H	-4.5C7H08	H.984HC8	2.044C49
H	-5.C899CC	3.3C4245	2.077045
H	-3.988C95	3.C04C40	H.C0C5H5
C	-3.035HH8	4.2499C7	-2.53C8C4
H	-3.0C803C	3.75309C	-3.509889
H	-2.352075	5.H07707	-2.C3542C
H	-4.03H034	4.C50453	-2.32447C
C	-2.2HC820	4.232893	-0.20407H
H	-H.87CC53	3.C84H95	0.C8230H
H	-3.09990C	4.8H9895	0.079SiC
H	-H.4224H9	4.947225	-0.473592
C	-H.SiC832	2.7824Si	-H.925C48
H	-0.548C70	2.39077H	-H.H04CCH
H	-0.57C004	3.C3H554	-2.3H07CC
H	-H.2HH770	2.048908	-2.7H5798

Al=N-[SiMe(SitBu$_3$)$_2$]$_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.H9887H	H.229579	H.205543
N	0.028249	-0.0C2483	-0.298243
Si	H.8080H0	-0.4433C9	-0.42CH85
Si	2.804479	-H.59309C	H.97407C
Si	3.SiSi23	H.5H93H7	-H.839H95
C	2.2H2899	-H.905733	-H.55C52H
H	H.78293C	-2.84522H	-H.H97279
H	3.30C839	-2.0HHC89	-H.5288HH
H	H.9HCC37	-H.759245	-2.C00H93
C	4.H580C0	-3.02C9C5	H.C09H93
C	4.45Si33	-3.837959	2.90H538
H	4.7C9522	-3.2H507H	3.74C458
H	5.275354	-4.5445Si	2.C8C92C
H	3.59H038	-4.438C4C	3.22H940
C	5.5HH258	-2.4CH759	H.H25C94
H	5.4H73C8	-H.95828H	0.H573H5
H	C.22288C	-3.297598	0.987022
H	5.970555	-H.7C00H3	H.834737
C	3.72CH72	-4.05909C	0.535957
H	4.42Si5H	-4.9H885H	0.572534
H	3.78C2C2	-3.C4437C	-0.47CH84
H	2.7H2H30	-4.45HC52	0.C80830
C	3.C37H22	-0.HC5CC3	3.044HC2
C	4.4339HH	0.73005H	2.083325

H	3.7755CH	H.HHHH93	H.293559
H	5.2CC973	0.205405	H.598498
H	4.852737	H.5952C2	2.C302H2
C	4.598455	-0.C54407	4.H53C24
H	4.99H93H	0.225909	4.C9C433
H	5.4C47H0	-H.H959C9	3.749254
H	4.H037C7	-H.29992H	4.892C8C
C	2.590285	0.7509CH	3.7H7948
H	2.027907	0.247824	4.5HC47C
H	H.8C3297	H.H55775	2.992793
H	3.H07498	H.CH50C8	4.H7535H
C	H.35H842	-2.4H5904	3.03457C
C	H.725902	-2.C3280C	4.52332H
H	0.87800C	-3.H35850	5.02C37H
H	H.8979HH	-H.C8783H	5.055844
H	2.CH0474	-3.2CCCH3	4.CC0955
C	0.H04405	-H.5H2C42	3.02098H
H	-0.700C7H	-H.9C99H2	3.C24H03
H	-0.28HC40	-H.3800C0	2.0023H5
H	0.3H0H78	-0.523845	3.450854
C	0.9302C9	-3.787934	2.4C4C45
H	0.7HH202	-3.740853	H.3924H9
H	0.0Si32H	-4.H359HC	2.977452
H	H.C9785H	-4.557578	2.CH8055
C	H.9H9794	H.835394	-3.3437C5
C	3.494252	3.23CH94	-0.903735
C	4.84C050	0.8H7749	-2.532C38
C	5.7037H8	H.90H742	-3.234093
H	5.952555	2.747289	-2.58H225
H	5.220H8H	2.30030H	-4.H3C283
H	C.CCH253	H.44392H	-3.54935C
C	4.CC5947	-0.3H8277	-3.5C7403
H	5.CC4732	-0.C93722	-3.859884
H	4.H703CC	0.030C87	-4.484H73
H	4.099025	-H.H7H237	-3.H7C02C

C	5.CC2009	0.24C274	-H.35CH05
H	C.55058C	-0.29CHC7	-H.730778
H	5.0CHH9H	-0.457882	-0.7C8CC9
H	C.0H3799	H.027833	-0.C70CC7
C	2.372805	3.5HSi8C	0.H20747
H	2.378708	2.78025H	0.942802
H	H.37C5C7	3.494754	-0.33C009
H	2.507998	4.5HH778	0.572887
C	4.834494	3.303H52	-0.H28259
H	4.97CCSi	2.47C39H	0.5C9720
H	4.848HCC	4.237392	0.4C38H9
H	5.7058C2	3.337599	-0.7953C7
C	3.545045	4.438H8H	-H.885Si5
H	2.5934HC	4.C2780H	-2.395472
H	4.324HC4	4.3H7729	-2.C508HH
H	3.788799	5.3509C3	-H.309703
C	0.72280C	2.C8229H	-2.8CC390
H	0.24C47C	2.223729	-H.992559
H	-0.034703	2.742H27	-3.CC8348
H	0.99C83H	3.7H07C4	-2.C05327
C	2.5C8884	2.54CH50	-4.557244
H	H.7779C2	2.77C804	-5.29C555
H	3.0C258C	3.49H342	-4.299359
H	3.30300C	H.905337	-5.0C7H08
C	H.332383	0.50793C	-3.87234H
H	0.752842	-0.008C80	-3.099757
H	2.H0H034	-0.H82780	-4.242H0C
H	0.C4CC74	0.722309	-4.7H3040
Si	-H.C244H2	-0.2H5987	-0.920775
Si	-2.8843CH	-2.423578	-H.27CSi9
Si	-2.93C787	2.440HH0	H.2044HC
C	-H.970C90	0.732Si2	-2.5302H3
H	-H.38C200	0.328478	-3.3708C2
H	-H.754095	H.8025H5	-2.4503C4
H	-3.034C28	0.CH8908	-2.780HH7

C	-H.478982	-3.C08235	-H.943H9C
C	-H.9C4029	-4.95500C	-2.52CH35
H	-H.08H92C	-5.572434	-2.78H052
H	-2.5428CC	-4.8244CH	-3.45Si25
H	-2.574989	-5.533839	-H.8H9433
C	-0.534C57	-3.9H2477	-0.7CC8C4
H	-0.H89477	-2.98C045	-0.288H33
H	0.354H23	-4.4C2482	-H.H2C07C
H	-H.0H0830	-4.537202	-0.000539
C	-0.C45C0H	-2.898984	-3.03430H
H	0.227342	-3.523753	-3.2947H5
H	-0.25944H	-H.933094	-2.C85434
H	-H.209788	-2.720CH9	-3.95C934
C	-3.C3422H	-3.0CC388	0.4H57C7
C	-2.C94H84	-2.CC5C45	H.5C9C0H
H	-H.707524	-3.H33774	H.4958H7
H	-3.H34HH9	-2.972C4H	2.53C745
H	-2.548044	-H.575C72	H.C0H79H
C	-3.828H25	-4.C0H702	0.4C0358
H	-2.883289	-5.H5388C	0.3C3H7C
H	-4.5HCH52	-4.9C4Si2	-0.3HCC93
H	-4.2C4300	-4.877259	H.438843
C	-5.002H98	-2.424053	0.733909
H	-5.785297	-2.C99095	0.0SiCHH
H	-4.938254	-H.332090	0.773SiC
H	-5.3377C3	-2.7C9544	H.7297C4
C	-4.295H3C	-2.28Si43	-2.C54C8H
C	-5.SiH990	-3.582578	-2.C52CH2
H	-5.8CH970	-3.537797	-3.49H3H9
H	-5.728483	-3.C95583	-H.730737
H	-4.54H33C	-4.49H308	-2.785H5C
C	-5.28C9C2	-H.HH59C4	-2.453H34
H	-C.059448	-H.HC7744	-3.24299C
H	-4.80CC35	-0.H32848	-2.537H98
H	-5.804H25	-H.H55C59	-H.488324

C	-3.7H2H90	-2.HH8H89	-4.078C9H
H	-3.HC855H	-3.0H088H	-4.4H5329
H	-3.04H358	-H.252H95	-4.HC4C4C
H	-4.544849	-H.9C2539	-4.789C07
C	-2.052348	4.22H272	H.0047HH
C	-4.C53C48	2.504297	0.2HH077
C	-3.3H3475	2.044394	3.HH8C0H
C	-3.899833	3.279C75	3.85HHC5
H	-4.803C8H	3.C77734	3.372787
H	-3.HC9CHH	4.097CH5	3.927092
H	-4.H7H555	2.99H0H5	4.884434
C	-2.05H903	H.CH8H99	3.90H8CC
H	-2.3H5535	H.47C3C5	4.9C7334
H	-H.24H955	2.358882	3.8548C0
H	-H.C5C882	0.C5C58H	3.538794
C	-4.3H7H8C	0.87589H	3.2C5055
H	-5.32888C	H.Si55C8	2.933530
H	-4.39H7C0	0.590047	4.330889
H	-3.99C73C	-0.0H5329	2.70483C
C	-5.203225	H.08H22H	0.03C429
H	-4.434C28	0.4HHC47	-0.3C8H00
H	-C.05C492	H.089530	-0.CC440C
H	-5.5CSiCH	0.C54920	0.9803C0
C	-5.7587H9	3.325782	0.924H53
H	-C.043994	2.884372	H.8888C0
H	-C.CC4553	3.322744	0.287904
H	-5.4823C5	4.373980	H.094CCH
C	-4.48H5C7	3.08905C	-H.2HH234
H	-3.72283H	2.552Si5	-H.793C28
H	-4.2H800H	4.H55Si5	-H.207287
H	-5.44H053	2.994848	-H.753489
C	-3.0479HH	5.405024	H.08C420
H	-2.48707H	C.352994	0.980400
H	-3.57520H	5.442H5H	2.050340
H	-3.798045	5.384385	0.28C524

C	-0.9CC589	4.49CC20	2.07H303
H	-H.3844Si	4.5C8349	3.085405
H	-0.475470	5.4CH29H	H.8445C3
H	-0.H79957	3.725900	2.085H7H
C	-H.3C3H33	4.2C8C45	-0.37C8C5
H	-0.C43H23	3.44C444	-0.492948
H	-2.072908	4.H98759	-H.2HH372
H	-0.798783	5.2H2523	-0.492258

Si*i*PrDis$_2$-Al≡N-Si*i*PrDis$_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.355893	0.28C52C	-0.H75499
N	H.27HC23	-0.H34H34	-0.H72CC9
Si	2.8H2507	-0.343987	0.54H083
Si	-2.C78835	-0.305H90	-0.C7052H
C	3.C35Si7	H.38CH00	0.C84347
H	4.72737C	H.225739	0.C5C383
C	3.8755H5	-H.C27C42	-0.453209
H	3.98238H	-2.42C9H2	0.3HH808
C	2.5H753H	-H.37H73C	2.H58H82
H	2.054438	-2.2C3470	H.C89347
C	H.4C3544	-0.830CH0	3.H37H9H
H	H.HC8398	-H.C0874H	3.8C4C7C
H	0.552543	-0.5H2330	2.C0395C
H	H.82H93C	0.032082	3.7Si923
C	3.7CC809	-H.877998	2.9H0H02
H	3.4753HC	-2.50CH57	3.772089

H	4.3883C2	-H.0592C0	3.29C877
H	4.4H284H	-2.495C04	2.2CC700
C	-2.4C3H59	-H.3988H2	-2.237009
H	-H.9203H9	-2.29H984	-H.890H25
C	-H.CH9492	-0.75C453	-3.35H849
H	-H.483527	-H.4CC8H3	-4.H85749
H	-0.CH55H8	-0.4C7943	-3.0054C5
H	-2.H05885	0.SiHC74	-3.7C30C0
C	-3.8252C4	-H.8434H0	-2.8HHHC5
H	-3.C78323	-2.5C045C	-3.C38022
H	-4.382399	-0.984929	-3.2228Si
H	-4.4C8C48	-2.32553C	-2.0C3H24
C	-3.008H8C	-H.447C20	0.8C5CC3
H	-H.949400	-H.7579H9	H.032H72
C	-3.700958	H.22H934	-H.22CC58
H	-3.835595	0.953477	-2.297455
Si	2.8C4C75	-2.CH25H7	-H.73HSi2
Si	5.7Si792	-H.3H3584	-0.787585
Si	3.39253C	2.3C0040	2.294H52
Si	3.3H7472	2.507885	-0.829257
C	3.8H8795	-4.H05472	-2.405CHH
H	3.H08824	-4.7C2499	-2.939C58
H	4.290473	-4.704Si5	-H.C09844
H	4.C03872	-3.8200CH	-3.H23442
C	H.34Si90	-3.37C873	-0.902229
H	0.755599	-3.942784	-H.C48HC9
H	0.700388	-2.598CSi	-0.4C4340
H	H.C28C98	-4.082357	-0.H03002
C	2.298378	-H.C58389	-3.25H9C0
H	H.77HC9C	-2.347990	-3.935500
H	3.Si37C5	-H.22H592	-3.8079C7
H	H.CH2549	-0.844375	-2.98C520
C	C.C4C320	-2.928533	-H.H3H982
H	C.47H808	-3.32C827	-2.Si20H5
H	C.382H0H	-3.720077	-0.4H0227

H	7.730272	-2.740957	-H.032903
C	C.CH0054	-0.C47850	0.74849H
H	7.C95C0H	-0.C32H70	0.545043
H	C.450H84	-H.3095HH	H.CH5827
H	C.324043	0.3C85CC	H.05432C
C	C.074908	-0.HC7C88	-2.242058
H	5.7409H7	0.8C509H	-2.070477
H	5.592474	-0.527592	-3.HCC594
H	7.HC3375	-0.H38H93	-2.4259C4
C	4.2HC02H	4.0C7H0H	2.227257
H	4.HHC494	4.5452HH	3.2H8084
H	3.775355	4.749H93	H.48547C
H	5.29428H	3.98357C	2.0H0230
C	4.2C3H50	H.55887C	3.7708C5
H	4.353Si0	2.3082C3	4.577H89
H	5.2850C9	H.240C3C	3.503303
H	3.740430	0.C88808	4.H8720C
C	H.5CH25H	2.C4HH83	2.C97530
H	H.407089	2.72SiH3	3.787H53
H	0.93283C	H.8HC9C9	2.33052C
H	H.H92028	3.57H2H5	2.2383H5
C	H.8C2847	3.C97230	-0.588985
H	0.943873	3.Si78H8	-0.335243
H	H.C7C778	4.23298C	-H.535978
H	2.0284C5	4.45H959	0.H93442
C	4.875C27	3.544074	-H.Si2585
H	4.998H07	4.35C780	-0.4H09H2
H	4.83H72H	4.00H397	-2.SiCC38
H	5.790220	2.9283C2	-H.H02C32
C	2.9257C0	H.C33039	-2.448588
H	H.9H82C0	H.200498	-2.4H222C
H	3.C2Si95	0.822400	-2.C92840
H	2.9C4999	2.37H024	-3.2C9742
Si	-3.7HC029	-3.23C009	0.753499
Si	-3.345430	-0.587792	2.545539

Si	-2.733802	2.8C5422	-H.423SiH
Si	-5.52CSi9	H.4287H9	-0.7H738H
C	-2.733C3C	-4.302547	-0.457902
H	-2.94C858	-5.3C2000	-0.23H74C
H	-H.C4C4H2	-4.H57039	-0.34830H
H	-2.995458	-4.H3CSi4	-H.5H22H7
C	-3.4C3HC2	-4.088975	2.422454
H	-3.7473C5	-5.Si9745	2.307889
H	-4.08C042	-3.CC87H5	3.22CH32
H	-2.4H38C9	-4.0C20H0	2.7554HC
C	-5.55H34C	-3.4545H3	0.37H789
H	-5.7C55HC	-4.53C98C	0.427229
H	-5.854924	-3.HHHH77	-0.C27038
H	-C.H99238	-2.955CH2	H.H08954
C	-2.324342	-H.375509	3.9304H5
H	-2.833CH0	-2.2HC770	4.422H24
H	-2.H2372C	-0.CHH53C	4.70H545
H	-H.3475H7	-H.735440	3.572422
C	-2.7C7093	H.202782	2.4977H9
H	-3.059282	H.7H5H38	3.430535
H	-3.H84H9H	H.773CH8	H.CCH340
H	-H.CC7HSi	H.2C5933	2.4353C0
C	-5.H58348	-0.C2900H	3.0C5598
H	-5.5384H9	-H.CC028C	3.Si2C44
H	-5.823424	-0.077784	2.3859C4
H	-5.250C54	-0.HC984C	4.0C55C2
C	-5.7C9434	2.5C4734	0.7C79C3
H	-5.329227	2.HC54C2	H.C92820
H	-C.849752	2.7030C5	0.948H5C
H	-5.334590	3.5C203H	0.593979
C	-C.2947H0	-0.2498C8	-0.377973
H	-C.3C24CH	-0.830353	-H.3H2089
H	-7.3H9050	-0.SiH049	0.0H7C03
H	-5.720H22	-0.843532	0.340009
C	-C.5H7303	2.H2H958	-2.H7H970

H	-7.590398	H.922799	-2.002892
H	-C.239579	H.C23828	-3.HH7259
H	-C.40HSi2	3.205279	-2.3H7987
C	-3.8H7070	4.H938CH	-2.2Si777
H	-4.C52843	4.5H2059	-H.573H73
H	-4.235447	3.8C2C5H	-3.H78C94
H	-3.H94278	5.084H39	-2.4H050H
C	-H.282898	2.CCC7H5	-2.CH9438
H	-0.5HH0H9	H.94H357	-2.3Si393
H	-0.772047	3.C394C4	-2.7HC482
H	-H.C2C8H3	2.3C80C2	-3.C22749
C	-2.05HC49	3.C2285C	0.HC4259
H	-H.3H5755	2.999547	0.C94888
H	-2.842778	3.8833CC	0.883759
H	-H.529955	4.55550H	-0.HHH74H

[Si*i*PrDis$_2$]-Al=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.H9C329	-0.079858	-0.374447
N	-0.582350	0.409090	-H.849939
Si	-2.3408C3	0.H0C7C0	0.3582H8
C	-3.370704	H.340977	-0.CSi475
H	-3.24HH2C	0.943234	-H.C35C97
C	-2.750458	-H.7CC575	0.2Si924
H	-H.7300CH	-2.H943C2	0.305H7C
C	-H.9H25C7	0.885HH8	2.09H808
H	-H.044979	H.5H547H	H.83435C

C	-H.45H2C2	-0.055285	3.2H3082
H	-2.30HH8C	-0.5849H0	3.CC5H2C
H	-0.9C3453	0.523C07	4.0HC907
H	-0.7355HH	-0.804544	2.8CHH9C
C	-2.985093	H.85HSi4	2.C35503
H	-2.5C7387	2.4HCC7C	3.4879HH
H	-3.8704C5	H.3Si980	3.007093
H	-3.32C3C4	2.577H2H	H.8900HC
Si	-3.H5C09C	-2.43H343	-H.575H9C
Si	-3.544979	-2.705H99	H.70399C
Si	-5.2C9540	H.3CC7C9	-0.49975C
Si	-2.C08353	3.093703	-0.858237
C	-H.793775	-3.C82200	-H.95HC39
H	-H.C72205	-4.42HH83	-H.SiHC42
H	-0.82C099	-3.H8275H	-2.H08533
H	-2.038C94	-4.235395	-2.87495H
C	-3.H30234	-H.HC3392	-2.9C0243
H	-4.027508	-0.52C095	-2.9849H7
H	-3.HH3528	-H.734389	-3.90C8HC
H	-2.225500	-0.532374	-2.92HH82
C	-4.7859C9	-3.38H2CC	-H.782825
H	-4.CC3757	-4.453H77	-H.5CCH98
H	-5.07483H	-3.290H37	-2.844705
H	-5.C25H90	-3.007580	-H.H84HH7
C	-4.497793	-4.270448	H.240707
H	-3.90477H	-4.953373	0.CH2087
H	-5.45H75C	-4.077752	0.732388
H	-4.722549	-4.803C03	2.H8H92H
C	-4.7438H2	-H.C549C2	2.7223HH
H	-5.753370	-H.CC5734	2.28H2C0
H	-4.43CSi4	-0.C048C5	2.8H5300
H	-4.829044	-2.0C7589	3.742538
C	-2.H5445H	-3.39H852	2.798929
H	-H.723858	-2.C7033H	3.5050H3
H	-H.3292HC	-3.789583	2.H83H3C

H	-2.5503H2	-4.235543	3.39HH33
C	-H.00075C	3.4C0332	0.0C2858
H	-0.CH093H	4.4SiCH2	-0.330275
H	-0.222999	2.702998	-0.H0399C
H	-H.Si7224	3.597007	H.Si4CH5
C	-2.29H097	3.2CHHH9	-2.70Si47
H	-H.838H94	4.238300	-2.94H933
H	-3.222H3C	3.HC2770	-3.2835H9
H	-H.598572	2.4CH925	-3.0H2923
C	-3.7H744H	4.5H792H	-0.27C23C
H	-4.7379C7	4.5H0990	-0.C83HCC
H	-3.239C34	5.458885	-0.C02387
H	-3.793750	4.5C5803	0.822C49
C	-5.9H858H	2.227490	-2.053793
H	-5.CHCC54	3.28020H	-2.H52033
H	-7.02H9CC	2.H92849	-2.0C5000
H	-5.5C3H87	H.C97C52	-2.95408H
C	-C.0H9380	-0.3C0HC9	-0.57C778
H	-5.884582	-0.8H0088	-H.570H89
H	-7.H05325	-0.293225	-0.3898HC
H	-5.597342	-H.0482H8	0.HCC787
C	-C.0HSi59	2.HC928C	H.038405
H	-5.594933	3.H5CSi3	H.28H87H
H	-5.895839	H.5222C3	H.92250H
H	-7.0954CC	2.29C52C	0.8C98H3
Si	2.448499	-0.Si4725	0.59C5C0
C	3.H9C774	H.5C9539	0.H77C94
H	4.2CC457	H.344C28	0.33C898
C	3.529399	-H.C4HH89	0.03C240
H	3.5H8202	-2.H97449	0.997570
C	2.20C97H	-0.43204H	2.484747
H	H.4C7385	0.3H7437	2.805005
C	3.488H02	-0.22C774	3.3H094C
H	3.27C537	-0.3277C4	4.390C09
H	3.934497	0.7C2C57	3.Si848H

H	4.2475C4	-0.984H5C	3.055392
C	H.CH57C5	-H.8H7778	2.8028CH
H	H.3H9H99	-H.877983	3.8C432H
H	2.349SiC	-2.C207CH	2.C2C494
H	0.73074C	-2.054748	2.H94909
Si	5.427C80	-H.47322C	-0.H5HC40
Si	2.724893	-3.00CH2H	-H.045883
Si	3.255200	2.0855CC	-H.C74803
Si	3.007335	3.0C0843	H.3C9402
C	C.H8C42C	-2.985844	0.705388
H	5.CC2295	-3.22H744	H.C47908
H	7.24HHH2	-2.78HC29	0.958378
H	C.HC4CC4	-3.888858	0.0787H7
C	C.228854	-0.00H849	0.734373
H	5.8350H8	0.HCCC35	H.747270
H	C.H5CH03	0.944594	0.H78937
H	7.305H5H	-0.227HC7	0.837357
C	C.052334	-H.403742	-H.932893
H	5.957385	-0.394009	-2.3C0592
H	5.53235H	-2.H02507	-2.C0C095
H	7.H2482C	-H.CC595H	-H.944HC7
C	3.89C095	-4.4CC579	-H.3H9C32
H	4.2048H7	-4.9353H3	-0.37H9CH
H	4.805H95	-4.203HC4	-H.88HC5H
H	3.357229	-5.23H292	-H.90C323
C	2.093785	-2.530H29	-2.7543C5
H	2.899345	-2.H920HC	-3.423CCH
H	H.3H08CH	-H.75C272	-2.74H99C
H	H.C5H974	-3.43824H	-3.202CC2
C	H.2795C4	-3.75H9C0	-0.08Si82
H	0.4C2283	-3.0383H9	0.H0593C
H	H.CH00CC	-4.Si4450	0.893205
H	0.848394	-4.589397	-0.C53544
C	H.704H08	2.89335H	2.730522
H	H.5H7524	3.8953HH	3.H53958

H	2.02H980	2.239H77	3.554C47
H	0.742832	2.52H9C2	2.34CH24
C	4.C94995	3.339774	2.H7943H
H	4.C53C57	4.203C05	2.8C53C2
H	5.45C704	3.5CH959	H.4H2850
H	5.05523H	2.473545	2.75555C
C	2.C0H5C5	4.705498	0.534437
H	3.328329	4.9903H9	-0.240C55
H	2.C28220	5.487024	H.3Si472
H	H.599H03	4.7H8C45	0.08CC94
C	4.9H9H27	2.95C7H0	-H.9H9297
H	5.042700	3.834424	-H.2C4C08
H	5.0H8744	3.304730	-2.9C2Si0
H	5.7C3H93	2.274573	-H.7H9277
C	3.207324	0.C0H7H7	-2.8244H8
H	2.HC4333	0.308297	-3.0H2397
H	3.C54943	0.875353	-3.795953
H	3.7420C3	-0.273354	-2.443CC9
C	H.875777	3.H9745H	-2.3H8HC9
H	H.999852	4.2C0H32	-2.0CC579
H	0.883C93	2.858783	-H.98C955
H	H.882HC4	3.HHH309	-3.4H957H

Al=N-[Si*i*PrDis$_2$]$_2$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Al	0.249405	0.907H03	H.80HC84
N	-0.0205HH	0.0C8CC2	0.HSi988

Si	-H.CC79C5	0.3C2HH0	-0.4920H5
Si	H.C2303H	-0.29733H	-0.509004
C	-2.CH7822	H.343705	0.904925
H	-3.585228	H.454378	0.3C9833
C	-2.80C749	-H.084497	-H.H54798
H	-2.442894	-H.0C8H0H	-2.20H094
C	-H.393389	H.47H053	-2.0807CH
H	-0.3390C2	H.7409HH	-H.909774
C	-2.H5985H	2.8020C5	-2.284287
H	-2.955420	2.C90477	-3.032327
H	-H.480305	3.587275	-2.C5CH7H
H	-2.C35829	3.H8598C	-H.3779H2
C	-H.442C02	0.7Si448	-3.428CH7
H	-H.0H9484	H.343505	-4.23HSi7
H	-2.48H907	0.488H07	-3.7Si825
H	-0.88C530	-0.23H2HC	-3.4305C9
C	H.49C772	-0.89C747	-2.3Si3HC
H	0.9C7032	-0.055739	-2.7840H5
C	0.C200H3	-2.H39943	-2.48989C
H	0.454499	-2.354228	-3.5C0393
H	-0.35794C	-2.009C77	-2.0H9932
H	H.080C42	-3.0375C4	-2.0489H7
C	2.80C050	-H.089453	-3.094H50
H	2.597757	-H.H57302	-4.H7700H
H	3.309009	-2.02H909	-2.80C484
H	3.5H9835	-0.274323	-2.943575
C	2.548359	H.440CC2	-0.5HH857
H	H.CCC577	2.0793CC	-0.2954C8
C	2.3C050C	-H.784727	0.5073H5
H	H.792835	-2.5C0H29	-0.0520H8
Si	-2.C3H928	-2.988C34	-0.9H0H50
Si	-4.C4HHSi	-0.C59CH0	-H.549748
Si	-2.247C25	3.208787	H.27C5H5
Si	-3.29303H	0.4C4082	2.484450
C	-4.097H20	-3.925285	-0.HC2223

H -3.839980 -4.999358 -0.207CH3
H -5.032870 -3.79445C -0.725370
H -4.288584 -3.C80H8C 0.89H8H3
C -2.4480C3 -3.7CH84C -2.C374C7
H -H.988949 -4.7CHC02 -2.54CHC8
H -H.8H80HC -3.H7H83C -3.3H8908
H -3.424443 -3.895954 -3.H27229
C -H.H38443 -3.523C52 0.HH240C
H -0.702343 -4.4335H2 -0.3323C3
H -H.423534 -3.7C8279 H.Si5CCH
H -0.35C483 -2.75895C 0.H52208
C -5.20077C -H.702395 -3.030589
H -5.352CH3 -2.7C4887 -2.787843
H -4.48C4C3 -H.C48884 -3.8C8C09
H -C.HC7Si8 -H.309277 -3.39239C
C -4.97702C H.HH235C -2.HH2938
H -C.0CC0C3 H.H9HC52 -2.279830
H -4.485994 H.3504CH -3.0CCH7H
H -4.70H087 H.887CC0 -H.384482
C -5.93C448 -0.930545 -0.20HH75
H -5.978827 -H.954H94 0.H9470H
H -C.9H8H88 -0.7HCH74 -0.CC0549
H -5.822850 -0.240384 0.C4588H
C -H.955483 3.C3937C 3.09C957
H -H.7C2548 4.72CC3H 3.H344H2
H -H.0798H2 3.H354HH 3.53H5H3
H -2.82C489 3.439282 3.738840
C -3.795572 4.204742 0.82CH39
H -4.H27275 4.07H85H -0.2H53C7
H -3.C05587 5.28HH94 0.98H0H9
H -4.C37H74 3.92HH98 H.479C9H
C -0.740942 3.9430H2 0.370833
H -H.054C97 4.C3492H -0.42CCC7
H -0.090078 3.H90C7C -0.098220
H -0.H23Si2 4.5H3235 H.084345

C	-2.297HC4	0.58487H	4.0995C0
H	-H.2Si274	0.740CC5	3.97C922
H	-2.425884	-0.3CH743	4.C50C39
H	-2.CC8723	H.40008H	4.738298
C	-4.9C933C	H.24C049	2.89H548
H	-4.84922C	2.2C4208	3.29C257
H	-5.4834CC	0.C4CC4H	3.CC3052
H	-5.C394C3	H.3H5223	2.020SiC
C	-3.533387	-H.380C38	2.2297H2
H	-2.5883CH	-H.883333	H.98C090
H	-4.250077	-H.C08937	H.438HC4
H	-3.9HH84C	-H.823C8C	3.HC7840
Si	3.07HHH2	2.37H5CH	-2.H2H7H5
Si	3.724435	2.020H33	0.9074CH
Si	H.8C2958	-2.44H7CH	2.255527
Si	4.Si8432	-2.375H07	0.088CHC
C	H.8C3H82	2.29H0C3	-3.574873
H	2.220293	3.020C9H	-4.32403H
H	0.84329C	2.59H077	-3.29489H
H	H.8H2832	H.3H3535	-4.072305
C	3.078337	4.223733	-H.7HH895
H	3.205577	4.785388	-2.C53979
H	3.890004	4.53H842	-H.03CCC2
H	2.H24752	4.545703	-H.2CH985
C	4.7740CC	H.9CCC87	-2.85C985
H	5.2H0307	2.905H37	-3.2422C3
H	4.C983C2	H.273750	-3.709HC7
H	5.49H927	H.5420HC	-2.Si5CCH
C	2.995H05	3.5C3809	H.722303
H	2.94CCSi	4.430252	H.04C582
H	3.CH7097	3.84C5CC	2.59020H
H	H.97C78C	3.3C973C	2.09972H
C	3.920383	0.7CHHC5	2.28240C
H	4.582728	H.H74C9H	3.0C2733
H	4.357408	-0.H83452	H.93859H

H	2.95CHH2	0.534377	2.75853C
C	5.499425	2.447305	0.40C735
H	5.585CH5	3.22730H	-0.3C2948
H	C.0C447H	H.5CC79H	0.0CC347
H	C.002848	2.824023	H.3H5H99
C	5.258474	-2.85CSi7	H.549033
H	5.577238	-H.992HC4	2.H52027
H	C.H7272H	-3.290C97	H.H05H50
H	4.833854	-3.C098C5	2.22C495
C	5.H95CC9	-H.H0H5H8	-0.842C72
H	5.388HH5	-H.4059HH	-H.88H830
H	C.H72809	-0.98CC20	-0.344020
H	4.723459	-0.HH3C59	-0.875404
C	4.0H5C54	-3.9CC47C	-0.9299H0
H	5.0HH843	-4.2C85H8	-H.29759H
H	3.352738	-3.87Si32	-H.8035C3
H	3.C2CH0H	-4.79H70H	-0.3HH770
C	H.92859H	-4.33Si7C	2.H00593
H	2.949H77	-4.72387C	H.97288C
H	H.32400H	-4.C8C052	H.250349
H	H.5H3HC8	-4.78728H	3.0HC38C
C	0.09CC5H	-2.0C025H	2.84HHCC
H	-0.5740C4	-H.727484	2.043CC2
H	0.09740C	-H.298852	3.C3C323
H	-0.340455	-2.97545H	3.27CC2H
C	2.885304	-H.98H3C3	3.780473
H	2.5C7923	-H.0H3340	4.H97022
H	3.972285	-H.95024H	3.C479C0
H	2.CC4479	-2.748508	4.545249

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Tbt_2-Al≡N-Tbt_2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.8H2CCH	H.293224	0.2H720H
C	3.548847	-H.4587HH	0.2280H5
C	3.9780C3	0.845708	-0.428C37
C	2.009573	0.307H30	0.8C8928
C	2.374Si2	-H.07H5H9	0.907993
C	4.352853	-0.5H5305	-0.450382
H	4.C23384	H.5C72C4	-0.932408
H	3.84C48H	-2.507453	0.2342H0
C	2.44H508	2.77CC32	0.2C9779
H	H.333843	2.8C344C	0.340750
C	5.CH8852	-0.90940C	-H.H7C533
H	C.03C74H	0.02Si83	-H.CH0299
C	H.5380H8	-2.08832H	H.C85989
H	0.585C95	-H.587903	H.985507
Si	0.908Si9	-3.C45838	0.750492
Si	2.342289	-2.477H98	3.377CCC
Si	C.9945C0	-H.475227	0.0H359C
Si	5.287923	-H.9C793H	-2.725C54
Si	3.H2234C	3.552C38	H.8878H0
Si	2.8H8972	3.8C927H	-H.2CH747
C	4.054049	-3.23H3C7	3.H857H5
H	4.042394	-4.H745C4	2.C20733
H	4.47H859	-3.44C055	4.H843C4
H	4.74H707	-2.5392H7	2.C78852
C	2.5HC8HC	-0.8C43HC	4.328553
H	3.22H85C	-0.H8C7H0	3.822804
H	2.89C9HC	-H.05H249	5.347H23
H	H.55HC85	-0.34Si05	4.4255HC
C	H.270C43	-3.C504C5	4.395893
H	0.22C980	-3.30CCC2	4.470295

H H.C7540C -3.70C447 5.42HC02
H H.2597Si -4.C75H55 3.99H777
C -0.C97453 -4.274C37 H.5H75C7
H -0.59C784 -4.5975C7 2.5C34H5
H -H.047555 -5.Si3802 0.9337H9
H -H.49C2H7 -3.5H9093 H.47340C
C 2.H52H8H -5.0C5292 0.74739C
H H.7797C9 -5.8C3584 0.08HC0H
H 2.288H59 -5.509747 H.74C200
H 3.SiH78C -4.7C3777 0.37H237
C 0.5H8228 -3.HC575C -H.0H0895
H H.4Si7C5 -2.845428 -H.5CHHH9
H -0.203447 -2.335358 -H.032552
H 0.0C53C2 -4.0H00H0 -H.55C925
C C.878C80 -0.448043 H.589873
H 5.909832 -0.57C3HH 2.09C587
H C.997544 0.C25C03 H.3C9243
H 7.C75398 -0.73C3C7 2.29720C
C C.884977 -3.30CHC2 0.448277
H 7.544783 -3.533048 H.303H2H
H 7.203979 -3.9397HH -0.395380
H 5.8C553C -3.C08292 0.730887
C 8.CC9H90 -H.H25075 -0.780820
H 9.472480 -H.2H29C5 -0.029348
H 8.708948 -0.H00C55 -H.H88973
H 8.90H857 -H.820500 -H.C0H834
C C.88842H -2.H30C8H -3.7HH88C
H 7.397794 -H.H59H92 -3.82C575
H C.C704H0 -2.5H33Si -4.723743
H 7.599954 -2.828H05 -3.24H305
C 4.C25924 -3.C90034 -2.344557
H 4.45C5C7 -4.23257H -3.290955
H 3.CCH757 -3.C474C8 -H.8HCCHC
H 5.32H923 -4.28835C -H.737787
C 4.0HH909 -H.0C879H -3.779CH2

H	3.84442C	-H.C0H793	-4.73H339
H	4.337H0C	-0.0437H2	-4.023829
H	3.043C22	-0.995954	-3.259933
C	2.882947	5.422352	H.95CC0C
H	3.H744C4	5.77C394	2.9CH055
H	H.829820	5.705754	H.800582
H	3.492809	5.9700HC	H.222354
C	2.H9HCC9	2.85335H	3.3C8324
H	H.H32C49	3.HC029H	3.3572HH
H	2.C2585H	3.2302C9	4.3H047H
H	2.2440HH	H.755797	3.404030
C	4.94H9H8	3.HH7C25	2.0C4889
H	5.072375	2.028C35	2.H57959
H	5.3C2042	3.59075H	2.9C8588
H	5.53C8C8	3.45Si55	H.20H54C
C	H.75772C	5.43930C	-H.20HHC0
H	H.35982H	5.C59938	-2.205800
H	2.347037	C.3H2C34	-0.880HH2
H	0.89440C	5.35CH98	-0.525384
C	2.4079CH	2.934CC2	-2.83C775
H	3.083C87	2.0835H9	-3.00C9H7
H	2.48494C	3.C08252	-3.707C32
H	H.38H0H2	2.5448C9	-2.80720C
C	4.C23825	4.425H59	-H.358920
H	5.335CC0	3.58508H	-H.37C399
H	4.9027H5	5.08509H	-0.52205H
H	4.7C9H8H	4.99988C	-2.290C38
C	-3.249H50	0.574875	0.907539
C	-3.380008	-0.3580C4	-H.749H2C
C	-2.H955H8	0.88C955	-0.0Si525
C	-4.2437H5	-0.333580	0.5005C2
C	-4.3H8C77	-0.83783C	-0.8H3493
C	-2.32072C	0.498755	-H.403904
H	-4.997754	-0.C32354	H.233HSi
H	-3.483054	-0.C77C24	-2.788222

C	-3.374H27	H.20C48H	2.30322H
H	-4.44793C	H.05H704	2.543529
C	-H.378H39	H.0C9902	-2.47HH39
H	-0.39H374	H.237474	-H.997H52
C	-5.420042	-H.78CCH2	-H.248405
H	-5.340C73	-H.892C83	-2.34933H
Si	-7.H5045C	-H.03C547	-H.00242H
Si	-5.H3325C	-3.559H7C	-0.C25C34
Si	-H.03C575	0.0C0570	-4.0C522C
Si	-2.0H59H2	2.8329H8	-2.9Si054
Si	-3.358C35	3.H2022H	2.3C4HC2
Si	-2.C409C2	0.350787	3.84C7HH
C	-3.50259C	-4.H8Si30	-H.343077
H	-3.5HC8H2	-4.H54C49	-2.44587C
H	-3.30C04H	-5.222952	-H.0342H9
H	-2.C57873	-3.5CH735	-H.005774
C	-C.5HCCC7	-4.C95C58	-H.228590
H	-C.C75H90	-4.5959C9	-2.3H5537
H	-7.47C748	-4.484C29	-0.730274
H	-C.2CH852	-5.750H78	-H.024C40
C	-5.02C058	-3.C73H78	H.25338H
H	-4.92Si2H	-4.728533	H.5C0998
H	-5.9H8942	-3.2C5H8C	H.75H2C8
H	-4.Si7775	-3.H270H0	H.C29802
C	-7.8C959H	-H.3C7CC7	0.7H3703
H	-8.050377	-2.44H347	0.88C258
H	-8.835747	-0.845338	0.82432H
H	-7.205CC5	-H.005HCC	H.5H5207
C	-8.3Si7Si	-H.7573C2	-2.302CH7
H	-8.54C532	-2.8H8347	-2.H22007
H	-7.8C7844	-H.C80H27	-3.308884
H	-9.2C802C	-H.20H894	-2.3H9592
C	-7.057483	0.82C537	-H.2C5507
H	-C.CH8250	H.0C4C7H	-2.248292
H	-C.433075	H.3H3837	-0.500C4C

H	-8.0C58CC	H.274H0C	-H.225745
C	0.547882	0.C5793C	-4.9HHH58
H	H.4SiC00	0.5899C3	-4.23C804
H	0.4993H0	H.C87H92	-5.29H580
H	0.75C705	-0.003500	-5.77HHH3
C	-0.732942	-H.77H270	-3.7C0099
H	-0.7H3850	-2.302444	-4.727907
H	-H.492508	-2.24CSiH	-3.H23589
H	0.248H32	-H.9H8852	-3.288Si8
C	-2.435H20	0.H72587	-5.335582
H	-2.58H282	H.H908HC	-5.72C8C3
H	-3.399840	-0.HC9447	-4.929HC7
H	-2.H8949H	-0.478C59	-C.H93320
C	-H.C49C77	4.025455	-H.50C7H2
H	-2.34H739	3.88CCHH	-0.CC8407
H	-H.7242C0	5.07SiH9	-H.850259
H	-0.C3CC5H	3.85742C	-H.HH84H5
C	-H.2003H3	3.C05C50	-4.44HC97
H	-H.39C82H	3.0C55C7	-5.3800C5
H	-0.H09390	3.703542	-4.3288C0
H	-H.C0C728	4.C2C403	-4.559738
C	-3.874828	2.77483H	-3.2HH272
H	-4.4058H0	2.43C775	-2.309H32
H	-4.Si4CH2	2.09H5H3	-4.03H030
H	-4.2502C2	3.779287	-3.473384
C	-4.524983	3.C9C983	H.00H357
H	-4.30425C	3.207CC3	0.042H20
H	-4.474073	4.789000	0.8553C4
H	-5.5C44H9	3.440822	H.270094
C	-4.H3HH78	3.C75075	4.004855
H	-3.480742	3.4875CC	4.874880
H	-5.H02C70	3.H90424	4.H9C972
H	-4.308208	4.7C4CSi	3.9C39Si
C	-H.C99520	4.0Si550	2.274974
H	-H.Si7338	3.75H70H	H.3C5HC0

H	-H.074399	3.7C2HCC	3.SiC988
H	-H.8CC80H	5.H0C2C7	2.295722
C	-3.983Si0	0.30H858	5.H79093
H	-4.2H9750	H.300CC3	5.57CCH0
H	-3.CC4528	-0.327257	C.0285Si
H	-4.9H7C9H	-0.H28C2H	4.779975
C	-H.Si35C4	H.H900C7	4.C5H054
H	-H.38048C	2.205427	5.0070H9
H	-0.2C9450	H.284848	3.9830H0
H	-0.8H2734	0.C00408	5.524294
C	-2.H85H33	-H.43943C	3.484H3C
H	-3.090409	-2.028243	3.2C8272
H	-H.C8C543	-H.89C329	4.3557H7
H	-H.5H94H3	-H.544322	2.CSi5H9
Al	0.2H8838	0.83495H	H.350324
N	-H.048572	H.5304C9	0.4H980C

Tbt_2-Al=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.CC0522	H.320970	-0.HH3879
C	3.H750C2	-H.388054	0.482C53
C	3.872H04	0.C90447	-0.49H897
C	H.C0747H	0.53CH97	0.507H32
C	H.953435	-0.8Si439	0.90873H
C	4.Si28HH	-0.C7500H	-0.2C3H5C
H	4.C52Si0	H.2908H7	-0.975083
H	3.392738	-2.4H8355	0.77530C

C	2.592HC7	2.83023H	-0.3H9595
H	H.537272	3.H8H028	-0.Si5995
C	5.4CH899	-H.255790	-0.742703
H	C.0797CH	-0.387823	-H.0CH59C
C	H.H33790	-H.52237C	H.974049
H	0.2C4432	-0.87H247	2.H8C283
Si	0.3CSi28	-3.222795	H.5397HC
Si	2.H59999	-H.553C59	3.C0740H
Si	C.5444HC	-2.049979	0.CHH57C
Si	5.28H098	-2.245C97	-2.370C30
Si	3.39559H	3.7HH7H3	H.209220
Si	3.H7229H	3.573057	-H.979470
C	3.34740C	-3.0209HC	3.C5CC70
H	2.82C203	-3.99H72C	3.CC0850
H	3.9509H7	-2.9C4858	4.580029
H	4.050755	-3.020448	2.8HH9C5
C	3.H5C347	0.034543	3.8002H3
H	3.5932C0	0.39HSi9	2.855CH3
H	3.978H53	-0.H2H743	4.5H997H
H	2.525909	0.839257	4.200509
C	H.055899	-H.C5H29H	5.H339CC
H	0.3C2342	-0.80Si2H	5.H78525
H	H.C95879	-H.C028C9	C.03HC05
H	0.4C70C0	-2.57C0HC	5.H92H7C
C	-H.2HH7C8	-2.94255C	0.5527C4
H	-2.044H34	-2.C474HC	H.2H2740
H	-H.5H2303	-3.87H9H7	0.0402H9
H	-H.HH5H79	-2.Si5555	-0.H985H5
C	-0.H8309C	-4.H89499	3.0737CH
H	-0.C9H772	-5.H08829	2.728504
H	-0.90935H	-3.C2C004	3.C80H8C
H	0.C44305	-4.50H77H	3.729775
C	H.538994	-4.3408C3	0.582025
H	2.48H993	-4.52HH98	H.H2C225
H	H.7925C7	-3.937772	-0.409795

H	H.055729	-5.323350	0.428H87
C	C.37SiC4	-H.048740	2.H95339
H	5.34H834	-H.0572H0	2.578278
H	C.C50C82	0.005499	2.0H9094
H	7.035532	-H.4440C7	2.984437
C	C.099H53	-3.8CHH33	0.909542
H	C.C2H5C9	-4.25H572	H.80H03C
H	C.394CH5	-4.487439	0.050452
H	5.0H88Si	-4.0H32Si	H.0C754H
C	8.35C358	-H.943544	0.079588
H	9.0HC72H	-2.H2C458	0.94C2H3
H	8.599850	-0.938084	-0.3087Si
H	8.C2H998	-2.C75903	-0.C98879
C	C.8C7H34	-3.H70H99	-2.82C49H
H	7.733C7C	-2.4909C9	-2.90HC44
H	C.73HH77	-3.C38049	-3.8H8909
H	7.H2C959	-3.973734	-2.HH78H8
C	3.8C8027	-3.483C40	-2.27C929
H	3.8H80H2	-4.074999	-3.209338
H	2.898C27	-2.973980	-2.H5HH72
H	3.990534	-4.H9Si43	-H.4399H3
C	4.959494	-H.02C5H3	-3.770H74
H	4.784C87	-H.5539HH	-4.725H55
H	5.8H89C8	-0.3473H0	-3.9H5HC2
H	4.072400	-0.4083H7	-3.5C9427
C	3.405C08	5.588320	0.9C7H34
H	3.7HSi85	C.0C48H8	H.9SiCC3
H	2.3908H7	5.945537	0.732249
H	4.087770	5.945273	0.H80CC8
C	2.373344	3.4H8257	2.7C4980
H	H.535442	4.HH9474	2.8035H9
H	3.005273	3.5C989H	3.C5C50C
H	H.97H284	2.403772	2.79C287
C	5.H5H078	3.08H795	H.509C30
H	5.Si9700	2.004223	H.745290

H	5.588575	3.CH5775	2.372C03
H	5.8H7345	3.23C805	0.C4493C
C	2.245588	5.H85H95	-2.325H7C
H	2.448700	5.497874	-3.3C34C4
H	2.573475	5.999450	-H.CC4424
H	H.HCSi53	5.090332	-2.2H79H7
C	2.85H3H8	2.375530	-3.3909H2
H	3.C00023	H.5C885H	-3.4H0399
H	2.897209	2.897942	-4.3CH582
H	H.8C590H	H.904897	-3.30C092
C	5.02C580	3.97CCHH	-2.028C74
H	5.C5C720	3.082955	-H.8C7795
H	5.3234Si	4.733525	-H.283585
H	5.28040C	4.3805H3	-3.027HH3
C	-3.094907	0.555C0H	0.853398
C	-3.H20059	-0.C90587	-H.C8CC7H
C	-H.9HH77H	0.C0243C	0.04H788
C	-4.H98445	-0.2HH582	0.408HC8
C	-4.23495C	-0.8C9C29	-0.8384H7
C	-H.9840C7	0.044922	-H.28C040
H	-5.073459	-0.282303	H.0CH58C
H	-3.HC5H59	-H.HH38H8	-2.C94887
C	-3.340493	H.324C54	2.H55228
H	-4.299989	0.908700	2.532CCC
C	-0.9H9792	0.408H92	-2.3085C7
H	0.007307	0.CC0903	-H.750233
C	-5.43C394	-H.C92028	-H.2C2CH3
H	-5.274050	-H.9875HC	-2.3228HH
Si	-7.0CH375	-0.C9H252	-H.32C547
Si	-5.4933H2	-3.3C5837	-0.333582
Si	-0.4348H0	-0.953977	-3.5C5038
Si	-H.5H794H	2.057H85	-3.H27554
Si	-3.935H58	3.SiHH7H	H.9237C0
Si	-2.28HC50	0.9Si88C	3.CCH548
C	-4.HC542C	-4.4C23C5	-H.H04C57

H -4.4755Si -4.79CH22 -2.HH2000
H -3.97305C -5.3C538C -0.497028
H -3.2H5099 -3.9H3874 -H.208553
C -7.Si745H -4.255H92 -0.550225
H -7.4H3838 -4.387579 -H.CH2C48
H -7.98270C -3.732057 -0.0550C3
H -7.07CC54 -5.2C2080 -0.099H07
C -5.H9CC39 -3.HC8433 H.5H8C0H
H -5.28H2H3 -4.H53HH5 2.0Si4H3
H -5.94059H -2.49858C H.984H29
H -4.H9C70H -2.7C20H7 H.7374H9
C -7.800H29 -0.3825H2 0.38C409
H -7.9CC459 -H.320095 0.944394
H -8.779727 0.HH9427 0.288383
H -7.H58529 0.2C9927 H.0024H7
C -8.329708 -H.CHH342 -2.385203
H -8.853384 -2.4H0827 -H.838H98
H -7.85850H -2.0CC8H8 -3.274404
H -9.0933C9 -0.90009C -2.747588
C -C.730705 0.958H54 -2.H70773
H -C.3CH753 0.8093C8 -3.200374
H -5.97835H H.55H90H -H.C3H7CH
H -7.C5C87H H.557352 -2.228933
C H.237384 -0.548H95 -4.32H2HH
H H.983930 -0.39H309 -3.527455
H H.232482 0.345073 -4.9CH89H
H H.58Si84 -H.399979 -4.934237
C -0.234297 -2.C3Si5C -2.73H8C0
H 0.HC7H04 -3.3599C9 -3.4C0548
H -H.H83333 -3.03HC2H -2.34HH78
H 0.47C9Si -2.573HC9 -H.89H024
C -H.C73C70 -H.H7H02H -4.982789
H -H.832880 -0.247043 -5.5C0273
H -2.CCH22H -H.527224 -4.C45HC5
H -H.277385 -H.930593 -5.C8H539

C	-H.283344	3.4C0Si5	-H.90C57C
H	-H.5C8834	4.408089	-2.3734H9
H	-0.25H385	3.548005	-H.583258
H	-H.907537	3.3H844H	-H.023C8H
C	-0.C20499	2.50C235	-4.723498
H	-0.7500C2	H.747097	-5.508998
H	0.452374	2.C80CH2	-4.5943H9
H	-H.0C3H2C	3.442307	-5.099237
C	-3.33454H	H.922988	-3.587390
H	-3.9793H0	H.832245	-2.70422C
H	-3.532H58	H.053853	-4.2339H5
H	-3.C38HC4	2.825930	-4.Si07H2
C	-4.7C0802	3.257SiH	0.234843
H	-4.HH3988	2.8C88CH	-0.5CCCC0
H	-5.02204H	4.3022CH	-0.00455C
H	-5.C92045	2.CCC492	0.2255H3
C	-5.2C090H	3.5007C5	3.227928
H	-4.82203H	3.730790	4.2H0852
H	-5.978289	2.C739C2	3.3C2305
H	-5.83254H	4.39H584	2.9HH972
C	-2.C74280	4.52447H	2.HH8842
H	-3.2H9238	5.488748	2.H05H0C
H	-H.9SiC8H	4.532C70	H.3H999H
H	-2.H3H940	4.47003H	3.0734H8
C	-3.Si20CC	H.57779H	5.20254C
H	-3.0C0372	2.CC8702	5.29CCC7
H	-2.C934C5	H.H293C2	C.H02837
H	-4.2H329C	H.320C92	5.20237H
C	-0.5C5879	H.C799C7	3.C4H77H
H	-0.C55C7C	2.750H03	3.50534H
H	0.HC3H89	H.3H084C	2.9H09CH
H	-0.H00054	H.50C280	4.CH88H2
C	-2.27HH88	-0.958H84	3.803H38
H	-3.3H0403	-H.3287H7	3.784420
H	-H.809C2H	-H.299CHC	4.74037C

H	-H.74H705	-H.429027	2.9C5H75
N	-0.H23907	3.28C7H0	0.80C0C4
Al	-0.H8H004	H.402770	0.C00C77

Al=N-Tbt_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.2C5C24	H.25797H	0.33C84C
C	-2.87C224	-H.302CH2	-0.C8C249
C	-3.53H977	0.C55443	0.5HCH24
C	-H.200592	0.4C99HH	-0.2458HC
C	-H.590Si8	-0.75C45H	-0.924054
C	-3.8C3333	-0.C35H97	0.0C9H80
H	-4.3HH8C0	H.243785	H.0005H7
H	-3.H33504	-2.2400C7	-H.H77C44
C	-2.HC90H3	2.743743	0.C9H542
H	-H.HHH9Si	3.055Si7	0.C39459
C	-5.259H02	-H.H79C9C	0.340380
H	-5.824938	-0.343435	0.799990
C	-0.779909	-H.3454Si	-2.0808C2
H	0.HCH758	-0.774C50	-2.HCC8C3
Si	-0.H53740	-3.Si909C	-H.93C25C
Si	-H.7070C9	-H.082H82	-3.759775
Si	-C.340240	-H.C07053	-H.H745C0
Si	-5.282954	-2.47937C	H.7395H2
Si	-3.H58083	3.90C27C	-0.5H22CC
Si	-2.705497	3.2Si07C	2.487C53
C	-2.9H3770	-2.483279	-4.H5C359

H -2.40727C -3.4443H7 -4.335250
H -3.4C0508 -2.2237C3 -5.080042
H -3.CC53C2 -2.C4050C -3.37007H
C -2.C82285 0.53HC42 -3.793053
H -3.H93545 0.753897 -2.84C435
H -3.44H579 0.49Si28 -4.593592
H -2.00C84H H.37H527 -4.02H08C
C -0.502HCC -0.95330C -5.208C93
H 0.H87422 -0.H05453 -5.084009
H -H.084374 -0.7C9074 -C.H29328
H 0.099847 -H.85C328 -5.3737CC
C H.273H73 -3.H93802 -0.7374C0
H 2.H29030 -2.C30927 -H.H35H08
H H.59C484 -4.2332HC -0.5734H8
H H.029549 -2.743052 0.228435
C 0.5CCH53 -3.78797H -3.5C5598
H H.0H8284 -4.7748C7 -3.359248
H H.3C93Si -3.H38578 -3.947C92
H -0.H7459C -3.9304HH -4.3CCC78
C -H.480922 -4.3805C9 -H.4HH005
H -2.3CC070 -4.3C5C5H -2.0C4C70
H -H.8H5825 -4.2Si99H -0.378545
H -H.055945 -5.398C99 -H.4598H2
C -5.9CC055 -0.44H949 -2.C0H075
H -4.9C284C -0.C05CC7 -3.0H2C24
H -C.032827 0.CH255H -2.287233
H -C.C9CH85 -0.59CC54 -3.4Si488
C -C.H24784 -3.388089 -H.7C2C85
H -C.CH333C -3.5253CC -2.742823
H -C.58532C -4.H03728 -H.0C2H00
H -5.0CCCH8 -3.CC925H -H.87C770
C -8.H55732 -H.3479H3 -0.7H39CC
H -8.775839 -H.35435C -H.C274CH
H -8.3H0C45 -0.373C4H -0.2H9Si8
H -8.545820 -2.H28289 -0.044003

C	-7.05C094	-2.935859	2.20457C
H	-7.C88472	-2.045905	2.358332
H	-7.04827H	-3.504H38	3.H5H320
H	-7.544030	-3.5C9934	H.447HC8
C	-4.358473	-4.05478C	H.29944C
H	-4.322880	-4.722259	2.H782CC
H	-3.322592	-3.83877H	H.0073C7
H	-4.83C088	-4.C09474	0.478225
C	-4.477Si2	-H.C8H085	3.23C8C4
H	-4.43C7H8	-2.373724	4.094HH2
H	-5.0337C7	-0.783CC5	3.55C589
H	-3.449H7H	-H.3724CH	3.0033C9
C	-3.048779	5.C9397C	0.H030H5
H	-3.435305	C.35H985	-0.C9479C
H	-2.004724	5.99H8C7	0.293250
H	-3.C29798	5.904553	H.0HH399
C	-2.589775	4.054553	-2.30C330
H	-H.58H3H8	4.478959	-2.4H8848
H	-3.29C993	4.75CC2H	-2.788075
H	-2.C34838	3.HH3232	-2.8C8404
C	-4.9C30C7	3.380223	-0.C85907
H	-5.0302C2	2.409059	-H.200493
H	-5.479CH3	4.H250C7	-H.3HC92H
H	-5.5H7527	3.300824	0.257729
C	-H.74CC80	4.752029	3.039978
H	-H.53274C	4.C94328	4.H20878
H	-2.3254C9	5.C7243H	2.870893
H	-0.785H94	4.8C2829	2.5H7HC5
C	-2.393C9C	H.794H34	3.CC948C
H	-3.05288H	0.945SiH	3.439205
H	-2.C048CC	2.HHC778	4.703322
H	-H.3C0C37	H.4374C3	3.C3H995
C	-4.542002	3.C0984C	2.732950
H	-5.H99H5C	2.75884H	2.493323
H	-4.89CH98	4.4832C0	2.HCCC43

H	-4.C8C94C	3.834930	3.805025
C	2.587392	0.78CCHH	-0.C49355
C	2.705C32	-H.02HH5H	H.47CC78
C	H.35590C	0.4890C4	0.0C40CC
C	3.75H22C	0.038950	-0.3C0758
C	3.847097	-0.909C34	0.CC9538
C	H.50273H	-0.304829	H.270H95
H	4.C4284C	0.254CC0	-0.953237
H	2.780C59	-H.C30894	2.374807
C	2.8C7H25	H.958747	-H.C30CC8
H	3.978939	H.977783	-H.574978
C	0.5C2020	-0.23224C	2.4828H0
H	-0.38H943	0.252C70	2.H8525C
C	5.Si0597	-H.C4932C	H.00H885
H	5.05H0H9	-H.98982C	2.053498
Si	C.7237C3	-0.580839	H.03H722
Si	5.308874	-3.285477	0.02955H
Si	0.0HC490	-H.8C0700	3.337533
Si	H.4235HH	0.982244	3.730H99
Si	2.8H39CH	3.75H594	-0.93097C
Si	2.927H53	H.C48H22	-3.55H029
C	4.0940C9	-4.5H9749	0.777Si7
H	4.5H00C3	-4.932008	H.7H2855
H	3.90H283	-5.3CC9CC	0.09C928
H	3.H30538	-4.048CSi	H.0H35Si
C	7.0HC224	-4.07987H	0.20835H
H	7.284989	-4.235H8H	H.2C5940
H	7.823554	-3.499779	-0.2C53HH
H	C.998C92	-5.073384	-0.274242
C	5.005238	-3.005898	-H.808938
H	5.0C5743	-3.9CH570	-2.3579C4
H	5.7C4973	-2.32980C	-2.234833
H	4.0H8C43	-2.5C4208	-2.00C4H7
C	7.48C380	-0.33277H	-0.C8H8C7
H	7.78HC23	-H.287225	-H.SiC308

H	8.395C55	0.288234	-0.597432
H	C.8039H5	0.H79243	-H.379474
C	8.0H3307	-H.403H34	2.Si5303
H	8.542555	-2.232037	H.C53579
H	7.553948	-H.798009	3.0C78H5
H	8.7C9554	-0.C58H38	2.448357
C	C.375407	H.HH3200	H.773527
H	C.H0H935	H.028HCH	2.837444
H	5.554843	H.C295H9	H.2579C0
H	7.27C3CC	H.7483H5	H.709C29
C	-H.2H7C88	-H.529257	4.73C080
H	-H.89C85H	-0.C88440	4.549897
H	-0.709589	-H.340795	5.C92579
H	-H.839377	-2.430745	4.8C7308
C	-0.835497	-3.030293	2.H2973C
H	-H.559H93	-3.C55344	2.C77285
H	-0.H24820	-3.707H9H	H.C3CH58
H	-H.38097C	-2.480834	H.348C55
C	H.428H3H	-2.808045	4.H73892
H	2.030HC4	-2.HC53HC	4.83C74H
H	2.H090CH	-3.2987H7	3.4CH39C
H	0.988937	-3.C0SiH8	4.804729
C	H.22C58H	2.74C554	3.0897Si
H	2.HH5087	3.35H875	3.333322
H	0.3C2H02	3.23HH34	3.5C2388
H	H.0840C8	2.775H52	2.000HC2
C	0.752CC4	0.9589C0	5.502775
H	H.03C078	0.040CH0	C.04H248
H	-0.33C448	H.0750C5	5.580400
H	H.2H79C8	H.804777	C.0409H3
C	3.2C7C77	0.C48583	3.943H05
H	3.832774	0.8447HH	3.02340C
H	3.48C70C	-0.3833H3	4.2579HH
H	3.C478C7	H.322C57	4.732449
C	3.77HC73	3.73024H	0.C8982C

H	3.442930	2.924274	H.3593C0
H	3.C5H880	4.C88C05	H.22345C
H	4.848H32	3.590525	0.498290
C	3.777758	4.872357	-2.H09885
H	3.309294	4.978084	-3.H0HH73
H	4.8H0983	4.5H9784	-2.258HC3
H	3.837207	5.88HH28	-H.CC4389
C	H.H7H754	4.C3357C	-0.C22204
H	H.409042	5.C208C0	-0.H83CH5
H	0.5H8793	4.H09935	0.090389
H	0.C003Si	4.820023	-H.545H72
C	4.CC8290	2.H34C85	-4.H22H5C
H	4.800HC3	3.225457	-4.H90328
H	4.838209	H.7227H9	-5.H32523
H	5.458900	H.735894	-3.4C4H39
C	H.783C82	2.C35539	-4.C995C0
H	H.CHC7CC	3.C5799H	-4.322738
H	0.792CC5	2.H8H299	-4.8397C7
H	2.2C7855	2.7HC582	-5.C9097H
C	2.77C503	-0.203900	-3.838H03
H	3.C505H2	-0.7H9229	-3.4H038C
H	2.745797	-0.425388	-4.9H7950
H	H.880284	-0.C3838H	-3.37530H
Al	-0.020388	2.0573C3	-2.02C9C8
N	0.H32884	H.042445	-0.42C848

Ar*-Al≡N-Ar*

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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C	2.99059C	2.853894	-0.007440
C	4.52H058	H.237408	-H.C90342
C	2.3C0933	2.2H2032	-H.HH9252
C	4.379878	2.73H295	0.H758H8
C	5.H7C39H	H.9C2394	-0.C8439C
C	3.H379H9	H.34C39H	-H.9430H4
H	4.852003	3.28H734	0.9905C4
H	5.HH3780	0.584434	-2.339987
C	2.2H8239	3.77C22C	0.937378
H	H.H557HC	3.504905	0.87C782
C	2.343534	5.244530	0.4825H0
H	H.748737	5.907472	H.H33075
H	3.39C300	5.5C9994	0.528CH8
H	H.993293	5.3C7407	-0.552CC4
C	2.C42488	3.C28477	2.4H2088
H	3.C50C9C	4.035285	2.59HH0C
H	2.C43478	2.57C274	2.73HC97
H	H.948C08	4.H8C078	3.0CH594
C	2.C49CH8	0.552429	-3.HCHH54
H	3.3089H8	-0.3334H0	-3.H9H348
C	2.9H9353	H.347897	-4.458958
H	3.970245	H.C74277	-4.5H4H40
H	2.280299	2.243H7C	-4.50803C
H	2.70H432	0.72C32C	-5.343775
C	H.2H0820	0.0H8975	-3.H34878
H	0.98H929	-0.49447H	-2.H90043
H	H.08H299	-0.70449H	-3.957H0C
H	0.4729CH	0.8H7C45	-3.28424C
C	C.C99535	H.97380C	-0.C22C80
H	7.0490H3	0.98785H	-0.9C995C
C	7.243459	3.030409	-H.CH3884
H	C.9022C3	4.038880	-H.3248C5
H	C.88C995	2.835CH2	-2.C37532
H	8.34C799	3.030585	-H.C2H973

C	7.277C24	2.2HC8CC	0.78H475
H	7.095HC8	3.250C34	H.HH88C3
H	8.3C9320	2.0C5H24	0.772989
H	C.838C80	H.534CC3	H.5249H7
C	-5.H73779	2.HC5H33	H.H48H32
C	-2.707953	2.458529	-0.278C42
C	-4.985522	H.58C043	-0.HH59C3
C	-4.07982H	2.8344H3	H.7H8C33
C	-2.8CH049	2.999H42	H.03553H
C	-3.782543	H.709093	-0.843C93
H	-5.803570	H.03040H	-0.579249
H	-4.200428	3.28245H	2.709483
C	-C.5244C5	2.H8H933	H.858929
H	-C.320H77	2.30498H	2.937832
C	-7.35C900	0.900CC5	H.C8H797
H	-C.7985C7	0.00C0H4	H.995750
H	-7.CC507H	0.7CH9C2	0.C3334H
H	-8.27C48C	0.9C08C7	2.28C792
C	-7.33485C	3.4H5837	H.39C29H
H	-C.770488	4.347HH0	H.5CH982
H	-8.29052H	3.4847H8	H.943283
H	-7.5CH427	3.345788	0.3H9HH5
C	-3.80579H	H.05H04H	-2.227H05
H	-4.474798	0.H83540	-2.H05995
C	-2.4850H0	0.488552	-2.7C7C7C
H	-H.959CH4	-0.HHH22H	-2.0HHC04
H	-H.8H0778	H.277704	-3.H24983
H	-2.707937	-0.H7H9H5	-3.C2HH92
C	-4.47H2H3	H.99H384	-3.258H09
H	-5.45740C	2.3345C2	-2.90C3C8
H	-4.C08720	H.470797	-4.220770
H	-3.84C857	2.879C28	-3.44HH85
C	-H.77C53C	3.844303	H.702H52
H	-0.892H29	3.83C293	H.0527HH
C	-2.227445	5.3H4032	H.823C43

H	-2.5HH00H	5.7H42C2	0.837C88
H	-H.4H349H	5.93C05H	2.23H783
H	-3.098C5H	5.4HH703	2.492H50
C	-H.354H09	3.273997	3.070255
H	-0.9959H8	2.234800	2.983280
H	-2.H92383	3.2C7952	3.785C08
H	-0.543083	3.877894	3.507H24
C	-H.472872	2.82C732	-H.0C2787
C	0.838400	3.CC7298	-2.4C2329
C	-0.208H42	2.2275CH	-0.808885
C	-H.555785	3.848408	-2.02770H
C	-0.4H0H43	4.249300	-2.734858
C	0.9C5803	2.CC2838	-H.480998
H	-2.5HCC2H	4.334CH4	-2.207803
H	-0.4833C3	5.045940	-3.479C7H
H	H.7348C8	4.0H4470	-2.980CH7
C	3.22307C	-2.74H904	0.044384
C	4.77H890	-H.0C3H94	H.C4H502
C	2.CH740H	-2.HH8C07	H.H7CCHC
C	4.5883C8	-2.5434H5	-0.22884C
C	5.39C384	-H.728030	0.57C005
C	3.4H0807	-H.245C09	H.973H83
H	5.0373C9	-3.08H290	-H.0C59H9
H	5.37705C	-0.409H5C	2.280048
C	2.4C7935	-3.7C2422	-0.804772
H	H.40038C	-3.C73232	-0.573H4H
C	2.904522	-5.H89997	-0.4HH823
H	2.3H7548	-5.945295	-0.9C0CC0
H	3.97H537	-5.349257	-0.C42884
H	2.7C287H	-5.35774C	0.CCC8HH
C	2.C32983	-3.5349C0	-2.3H8HH8
H	3.C7C0C3	-3.C7828H	-2.C4509C
H	2.3224C4	-2.520403	-2.C02328
H	2.0H38H5	-4.2552H5	-2.877549
C	2.987390	-0.558755	3.27782H

H	3.C3C7H5	0.3320HH	3.35C882
C	3.33C073	-H.4C3954	4.483302
H	4.385732	-H.79300C	4.42727H
H	2.C97575	-2.35999C	4.495047
H	3.H90938	-0.924222	5.434C27
C	H.543539	-0.052535	3.3923C3
H	H.293734	0.CH5808	2.545C00
H	H.428857	0.5432C5	4.3H3780
H	0.8HH853	-0.870075	3.4H7234
C	C.9HHH2C	-H.C53C75	0.409279
H	7.229889	-0.C50284	0.737597
C	7.58C488	-2.C80294	H.349505
H	7.283H54	-3.705C53	H.078347
H	7.2949C5	-2.5H08H3	2.397899
H	8.C8C205	-2.CH7433	H.278723
C	7.4028H8	-H.859228	-H.033947
H	7.25989C	-2.90HC20	-H.3C29C9
H	8.48H370	-H.C4H387	-H.H037C7
H	C.87H05C	-H.20C920	-H.743424
C	-4.922CH9	-2.494390	-H.H83904
C	-2.43H8H8	-2.45C2H8	0.240898
C	-4.82792H	-H.9C3C5C	0.H09282
C	-3.727900	-2.9HH747	-H.792203
C	-2.4925C7	-2.890485	-H.H20C70
C	-3.CH4955	-H.92C939	0.833083
H	-5.728883	-H.58C79C	0.C00840
H	-3.773885	-3.30454C	-2.8HH257
C	-C.2CHH79	-2.C992HH	-H.88C7H0
H	-C.0392HH	-2.95238C	-2.938889
C	-7.HC0478	-H.449299	-H.887H24
H	-C.C49440	-0.58C755	-2.34H940
H	-7.4575H2	-H.H70HCC	-0.8C3707
H	-8.08505C	-H.C4049C	-2.457228
C	-7.007928	-3.902H7C	-H.2CC7CH
H	-C.382984	-4.809047	-H.289H25

H	-7.94400C	-4.H09450	-H.8H343C
H	-7.2CCH94	-3.C9770C	-0.2H4HC7
C	-3.74C9HH	-H.33H834	2.24H482
H	-4.54C795	-0.578352	2.H43297
C	-2.5333C8	-0.574C98	2.79738H
H	-2.H75539	0.HC8080	2.0CH83C
H	-H.70384C	-H.243200	3.0C0494
H	-2.828250	-0.0H49C4	3.70H085
C	-4.25C9C7	-2.3829H5	3.253C33
H	-5.H39793	-2.909H08	2.85C470
H	-4.54H405	-H.900CCC	4.204529
H	-3.48225C	-3.H32378	3.47H499
C	-H.2C4027	-3.45H757	-H.83C004
H	-0.38079C	-2.992C57	-H.377343
C	-H.H83574	-4.9783H7	-H.C2C27C
H	-H.H5889H	-5.22957H	-0.5559HC
H	-0.27772H	-5.389CCH	-2.H0H597
H	-2.0CH38H	-5.4734H9	-2.07C050
C	-H.207278	-3.HH47C0	-3.33833H
H	-H.288707	-2.033350	-3.5H3894
H	-2.00C274	-3.CHC808	-3.90872C
H	-0.247320	-3.455H9H	-3.757778
C	-H.H984C2	-2.775C49	H.0473H4
C	H.H0H430	-3.C34H24	2.4C4C07
C	0.055480	-2.09498H	0.872375
C	-H.2C8450	-3.839329	H.9C2C59
C	-0.H43H9H	-4.2459HH	2.700455
C	H.23H240	-2.585999	H.5409C2
H	-2.2H9790	-4.3CH737	2.084C92
H	-0.224030	-5.0C547C	3.4H8HH0
H	H.99C950	-3.993228	2.977825
Al	-0.H2H5H7	0.CC8C53	0.338437
N	0.H3028H	-0.9957C2	0.0C5803

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Ar^*_2-Al=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.3H87HH	-0.8045CC	-0.035987
N	-H.7C3258	-H.9807H7	0.HH4HH3
H	2.793499	-0.899C87	-4.232C04
C	H.880343	-0.474CC8	-3.8H2CH4
C	-0.4057C5	0.C40225	-2.C720HC
C	H.C40H25	-0.C52592	-2.429H72
C	H.000H9H	0.23H387	-4.C339C0
C	-0.HH5498	0.824H55	-4.04H3C0
C	0.4H8C98	-0.H84278	-H.830C7H
H	H.20H532	0.350HC5	-5.702232
H	-0.7843CH	H.45HC85	-4.C32434
C	2.822847	-H.308900	-H.753304
C	5.252C0H	-2.CH97C2	-H.024089
C	2.8C2382	-2.7H8820	-H.58CC78
C	4.029H54	-0.559HH2	-H.59537H
C	5.2HH4H4	-H.2349C2	-H.2385C2
C	4.0C2359	-3.342H7H	-H.H975H0
H	C.H3C270	-0.CC37C5	-H.H22473
H	4.078800	-4.42C902	-H.08H30C
C	-H.599930	H.4448C0	-2.224928
C	-3.9H7H42	3.0505H8	-H.782499
C	-2.903HC5	0.88C079	-2.358508
C	-H.4C3332	2.84HH27	-H.959938
C	-2.C272C2	3.59557H	-H.708378
C	-4.03HH4C	H.C9CH37	-2.H325C7
H	-2.505529	4.C597H2	-H.485972

H	-5.028829	H.2CHH9C	-2.23H8C9
C	H.C88953	-3.59H309	-2.0HCHC8
H	0.7704H7	-2.98H247	-H.995C5C
C	H.480C22	-4.80223H	-H.H0H932
H	2.3490H2	-5.479C33	-H.H09H99
H	0.CH552C	-5.384382	-H.443H92
H	H.304828	-4.488C37	-0.0C278C
C	H.899H72	-4.057574	-3.475249
H	2.03H990	-3.203093	-4.H5484H
H	H.033330	-4.C45990	-3.822524
H	2.798C0C	-4.C92987	-3.5447CC
C	4.HH3028	0.94H505	-H.8792C8
H	3.09000H	H.334532	-H.874H04
C	4.9H2493	H.7H2C94	-0.8H4045
H	5.983503	H.450C95	-0.838003
H	4.530C87	H.52H357	0.H93785
H	4.8405HH	2.794874	-H.004548
C	4.728990	H.22C90C	-3.2C779C
H	4.H35572	0.792C90	-4.083225
H	5.7499HH	0.8H3392	-3.330020
H	4.792983	2.3H55C9	-3.435530
C	C.5C2HH8	-3.3H9875	-0.C843C9
H	7.3HH93C	-2.53H94C	-0.49H774
C	C.453272	-4.H87727	0.58447H
H	5.74H9H0	-5.0H7CH5	0.440C00
H	C.H0C988	-3.593284	H.443949
H	7.43H772	-4.C29H3C	0.837599
C	7.058442	-4.H55922	-H.884CH8
H	7.HC5378	-3.528875	-2.78432C
H	C.345035	-4.9C30C3	-2.H20C98
H	8.034792	-4.CH9874	-H.CC4H39
C	-3.092885	-0.529498	-2.897937
H	-2.HC3252	-H.089374	-2.7H9CC0
C	-3.328CH2	-0.472239	-4.424829
H	-4.244CHH	0.H00004	-4.C4882H

H	-3.4502H8	-H.489399	-4.833C8H
H	-2.49HH3H	0.0H03C9	-4.9485HC
C	-4.229CH3	-H.297747	-2.2H437C
H	-4.H07229	-H.29735H	-H.H2CH72
H	-4.223973	-2.345894	-2.55H857
H	-5.2H7220	-0.87C52H	-2.4C49H7
C	-5.H58C27	3.9HHC35	-H.577534
H	-C.0H4C29	3.222793	-H.4C3CCH
C	-5.4H9329	4.782289	-2.82C877
H	-5.4982H9	4.HC0H34	-3.732559
H	-4.593027	5.49C7H4	-2.98002C
H	-C.353HHH	5.359CH9	-2.7HCH84
C	-5.084593	4.78C95C	-0.3HHC9H
H	-4.28H408	5.537834	-0.389239
H	-4.893947	4.H79C07	0.585427
H	-C.03HC25	5.332804	-0.HC5842
C	-0.H84H24	3.C82940	-2.0925H2
H	-0.35H974	4.55507C	-H.43925H
C	-0.070238	4.2C2074	-3.52444C
H	0.732254	5.0H8590	-3.5CH77C
H	-H.0H2328	4.7400C0	-3.8357C8
H	0.H7CH2C	3.475783	-4.253079
C	H.H50C2H	3.058H29	-H.CC9023
H	H.9H2C37	3.849C38	-H.5837C2
H	H.499544	2.339550	-2.4H8HC8
H	H.090H4H	2.54CH4H	-0.C99534
H	H.H4C045	0.5C5343	4.935H52
C	0.492720	0.0H8455	4.2509C0
C	-H.2H5828	-H.27H772	2.489324
C	0.C24320	0.253C02	2.8C2200
C	-0.49277C	-0.83CHC9	4.7CH979
C	-H.39270H	-H.438592	3.872829
C	-0.H84HH3	-0.45C772	H.93C72C
H	-0.588483	-0.98C397	5.84H203
H	-2.245C70	-2.0H0074	4.24C282

C	H.549743	H.359705	2.47822C
C	3.29C494	3.537872	2.0H3C82
C	H.008954	2.C39088	2.H52332
C	2.947437	H.H837H3	2.CH897H
C	3.7975H3	2.2808C8	2.3828H7
C	H.90H395	3.C983H0	H.9HC258
H	4.8792CH	2.H537H3	2.4878H4
H	H.5008CH	4.C80325	H.CC2H03
C	-2.25939H	-H.7C37H5	H.523590
C	-4.74257H	-3.H00037	0.824704
C	-2.227CC2	-3.H5C22H	0.935724
C	-3.59245H	-H.090992	H.70CH24
C	-4.732928	-H.73CC93	H.332384
C	-3.5C2542	-3.7508C3	0.C27942
H	-5.C9250C	-H.22C28H	H.449957
H	-3.592787	-4.80059H	0.327C90
C	-0.50CH24	2.88558C	2.H5H287
H	-0.9795CC	2.03423H	H.C38393
C	-0.93888C	4.HCC3H8	H.423H57
H	-0.CC93HC	5.0CC824	2.000H37
H	-2.03H38H	4.HC8H50	H.294889
H	-0.4859C7	4.248358	0.430047
C	-H.0C9739	2.93809H	3.590733
H	-0.93053C	H.9943HH	4.H30277
H	-2.H49C8C	3.H594H2	3.5C3399
H	-0.57H2C2	3.739328	4.HCH832
C	3.532309	-0.H5H9HC	3.07C229
H	2.C92C53	-0.844938	3.227CH2
C	4.448HC0	-0.790092	2.020837
H	5.325049	-0.HC0272	H.80HC78
H	3.9H3740	-0.954097	H.07C740
H	4.8H8392	-H.7C5834	2.375C5H
C	4.25399H	-0.003380	4.430830
H	3.590058	0.44H293	5.H89235
H	5.H4HC48	0.C44704	4.342C05

H	4.58938H	-0.987584	4.7988C9
C	4.24H878	4.7HH593	H.79H4H3
H	5.2CH203	4.2944C7	H.70C387
C	3.940530	5.48C500	0.494229
H	2.952H47	5.972284	0.537042
H	3.947353	4.8H9007	-0.380884
H	4.C9H073	C.2783HH	0.333C0C
C	4.2H7035	5.C53840	3.0H4539
H	4.950209	C.470285	2.900909
H	4.447577	5.H00897	3.939H99
H	3.2H7C5C	C.H04787	3.H33340
C	-H.22494H	-4.20834C	H.4C8388
H	-0.230073	-3.733492	H.47C95H
C	-H.H88HC8	-5.4C9532	0.580C47
H	-2.043575	-C.H25899	0.80C000
H	-0.27C80C	-C.05H738	0.783770
H	-H.2H85H8	-5.22724C	-0.489C29
C	-H.5C5H24	-4.CCC3CH	2.903789
H	-H.438H44	-3.8C7802	3.C43004
H	-0.90C324	-5.502880	3.H95043
H	-2.C05895	-5.02827C	2.957728
C	-C.077327	-3.790250	0.5C5503
H	-5.855829	-4.85459H	0.3C93C3
C	-C.77H707	-3.2HC543	-0.C8C904
H	-C.H38C2H	-3.3432H8	-H.57C897
H	-C.973390	-2.H39H90	-0.5C9729
H	-7.734554	-3.724C30	-0.8C5752
C	-7.0HC784	-3.727382	H.788803
H	-C.530HC7	-4.H3240H	2.C9H043
H	-7.93344C	-4.3H05HC	H.597038
H	-7.32C584	-2.C92443	2.008497
C	-3.C38485	0.320390	2.28572C
H	-2.C38050	0.5C2027	2.CC4302
C	-4.C07732	0.450C38	3.473882
H	-4.352927	-0.2C789H	4.2C880H

H	-5.C5H25H	0.2C5H95	3.H7H338
H	-4.55573H	H.4C7502	3.897978
C	-3.952C50	H.34H3HH	H.H8043H
H	-3.92808C	2.3C5974	H.583457
H	-4.948398	H.HCC298	0.74309H
H	-3.224088	H.28H359	0.3C20H5

Al=N-Ar*$_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	3.438898	H.94H347	-0.89284H
C	4.427443	0.0372C4	-2.C744CC
C	2.5HH32H	H.08445C	-H.5CC890
C	4.8257H8	H.7C7CC7	-H.08H9C0
C	5.3508C3	0.837522	-H.98450H
C	3.0350H9	0.H5H9HH	-2.5082H5
H	5.503070	2.43828H	-0.5539HH
H	4.7973HC	-0.C79793	-3.4H5283
C	3.03C827	3.20H444	-0.HH7847
H	H.953574	3.H585C8	0.08C837
C	3.27797C	4.4CC493	-0.973579
H	2.93H078	5.3C337H	-0.433HCH
H	4.352848	4.590735	-H.H87320
H	2.744534	4.4H3852	-H.932807
C	3.7C8CC7	3.34839H	H.232335
H	4.830C93	3.C03705	H.087H83
H	3.720H87	2.422C8H	H.825CC8
H	3.308C35	4.H5C749	H.823875

C	2.202070	-0.C54C07	-3.503899
H	2.85H28C	-H.4930H5	-3.80C5C8
C	H.92C494	0.H47737	-4.79CC22
H	2.854878	0.589534	-5.H93277
H	H.205730	0.957884	-4.CHC458
H	H.50H574	-0.5HC472	-5.5C85H9
C	0.9HC237	-H.27H853	-2.954039
H	H.059975	-H.C534H0	-H.93C348
H	0.CH2534	-2.H05354	-3.59989C
H	0.09H240	-0.55H253	-2.928H50
C	C.835C2C	0.75820H	-2.333222
H	7.H24827	-0.308C34	-2.304984
C	7.0CH858	H.257439	-3.78037C
H	C.7C4900	2.3HC2H0	-3.8C543C
H	C.4C7838	0.C82287	-4.50C777
H	8.H25CH9	H.H73947	-4.0C0478
C	7.7543C9	H.5297H4	-H.37283H
H	7.5998CC	2.CH7C2C	-H.4CC444
H	8.8H0240	H.32522C	-H.CH202H
H	7.583390	H.253H02	-0.3229C9
C	-5.0872H7	2.32H427	H.H34935
C	-2.5C274C	H.87CC77	-0.H34HH7
C	-4.994245	H.C7982H	-0.H0C945
C	-3.897759	2.80H988	H.700593
C	-2.C50H79	2.C23240	H.079232
C	-3.7C7828	H.47275C	-0.77303C
H	-5.90C030	H.33C727	-0.C0050H
H	-3.952799	3.37H42H	2.C32455
C	-C.42C4C7	2.5944H3	H.809025
H	-C.205C4H	2.97C442	2.82H800
C	-7.2895H4	H.328043	H.9C4022
H	-C.7520C3	0.54H877	2.5HC907
H	-7.57303C	0.9H859H	0.98H379
H	-8.220C22	H.558573	2.508043
C	-7.H97297	3.C97295	H.05H098

H	-C.59H093	4.CH3C4C	0.9C845H
H	-8.H39HH8	3.947H99	H.5C87C7
H	-7.44C829	3.3C5CH7	0.02952C
C	-3.927244	0.925C00	-2.20H2C3
H	-4.C5H547	0.H035C4	-2.098550
C	-2.7H7C59	0.33C785	-2.9422C0
H	-2.H023C8	-0.285389	-2.287H98
H	-2.08H4H0	H.HHH703	-3.388H99
H	-3.09H959	-0.3025C9	-3.757C99
C	-4.59H950	2.000273	-3.097908
H	-5.52CH02	2.383907	-2.CC0539
H	-4.823234	H.57C587	-4.090037
H	-3.9H4705	2.8558H3	-3.2494C0
C	-H.47C05H	3.425740	H.C30403
H	-0.553C73	3.0C4898	H.H4H838
C	-H.C258H8	4.9HH4C9	H.230377
H	-H.734904	5.02H758	0.H40430
H	-0.7434H9	5.490440	H.552409
H	-2.5H7CHH	5.352C47	H.708H35
C	-H.278C59	3.298CH5	3.H509H7
H	-H.203C27	2.24753C	3.4C483H
H	-2.HH074C	3.7C053H	3.707053
H	-0.34789H	3.80C38H	3.45H803
C	-H.272375	H.89CH34	-0.920C44
C	0.897358	2.5208C7	-2.580378
C	-0.0799C2	H.07993H	-0.792005
C	-H.3223C9	2.959724	-H.85HC33
C	-0.273HHC	3.2C2473	-2.7H4H80
C	H.045822	H.49C097	-H.CH7H39
H	-2.2350C3	3.55C47C	-H.879247
H	-0.34989H	4.077357	-3.438748
H	H.7C5599	2.7C4CHC	-3.H94279
C	3.28252H	-H.98H49C	0.74H289
C	4.3C875C	-0.28834C	2.C7C4C0
C	2.407455	-H.340CH0	H.C77574

C	4.CC2793	-H.72905H	0.78CC7C
C	5.232H5H	-0.8C0772	H.73240H
C	2.982597	-0.572883	2.737830
H	5.30CH89	-2.253578	0.0820H9
H	4.78883H	0.3C55CH	3.44503C
C	2.789997	-3.HH7HC3	-0.HC4C42
H	H.7H82H3	-2.9C7075	-0.35377C
C	2.954HCH	-4.473547	0.5C42H3
H	2.575273	-5.2934H4	-0.0C9379
H	4.02H508	-4.CC3987	0.7C8H57
H	2.4H3798	-4.50337C	H.5H8H99
C	3.5H8557	-3.2H5078	-H.5HC458
H	4.528587	-3.C4H8H9	-H.398CC4
H	3.C23372	-2.23C202	-H.990C37
H	2.9C2H75	-3.88207C	-2.H94748
C	2.333CC7	-0.H42078	4.085093
H	2.540CC4	0.94044H	4.H8HH73
C	3.0C4970	-0.853408	5.254450
H	4.H4483H	-0.C474C9	5.2C505H
H	2.9302H8	-H.945774	5.H84375
H	2.C42C93	-0.5H7535	C.2HC794
C	0.825753	-0.335795	4.3H80HH
H	0.H902H7	0.0334H9	3.4997C4
H	0.535373	0.222H30	5.22309H
H	0.5CC543	-H.392399	4.4C3829
C	C.7405CC	-0.C2338H	H.835525
H	C.908948	0.4C2839	H.709HH2
C	7.2C2728	-H.0HC957	3.237938
H	7.077430	-2.088070	3.42478H
H	C.77H380	-0.447284	4.040504
H	8.348705	-0.8387C4	3.3H0377
C	7.5C2034	-H.3C3588	0.7C8H29
H	7.49984H	-2.45534C	0.9H3H30
H	8.C23C7H	-H.078C02	0.842CH9
H	7.2208C8	-H.H37037	-0.2509H0

C	-5.237970	-2.H52334	-H.HH3C70
C	-2.C00C2C	-H.78040C	-0.0CCH25
C	-5.02H958	-H.508C59	0.HH08C5
C	-4.HH2247	-2.C43057	-H.79H422
C	-2.808775	-2.49HCH0	-H.287975
C	-3.73784C	-H.342CC5	0.CC94CH
H	-5.878253	-H.H48335	0.C852H4
H	-4.2CC225	-3.H922C8	-2.7233C4
C	-C.C39524	-2.404798	-H.C5CHHH
H	-C.522700	-2.8H3723	-2.C75C44
C	-7.479982	-H.HH7720	-H.7C0HCC
H	-C.97CC05	-0.3C0502	-2.38H553
H	-7.C55425	-0.C780C8	-0.7C5458
H	-8.4C534H	-H.33220H	-2.20C558
C	-7.3C4954	-3.4C9345	-0.804350
H	-C.772357	-4.39C425	-0.7470HC
H	-8.352C5C	-3.7HH745	-H.232455
H	-7.5H975H	-3.H04775	0.224793
C	-3.758H7C	-0.820979	2.HH4CCC
H	-4.4C8533	0.0H939C	2.094479
C	-2.4CCH80	-0.284358	2.74334H
H	-H.9070C8	0.348H05	2.04C72C
H	-H.8H4H08	-H.09CC98	3.08C022
H	-2.729427	0.33H28C	3.CH9H84
C	-4.35C7H9	-H.902258	3.0494C2
H	-5.3345CC	-2.2CH34C	2.C93583
H	-4.48C878	-H.495738	4.0C70C0
H	-3.C8HHH8	-2.7C9247	3.HH8H88
C	-H.C80789	-3.25HHC3	-H.988H43
H	-0.728597	-2.809595	-H.CC7H38
C	-H.C73400	-4.73539C	-H.55059H
H	-H.545H94	-4.8422H0	-0.4C55C4
H	-0.848473	-5.274H3H	-2.047450
H	-2.C20C44	-5.223883	-H.83542C
C	-H.7C0037	-3.H9C940	-3.52C259

H	-H.79229C	-2.HC7599	-3.905500
H	-2.C49592	-3.727C43	-3.900977
H	-0.883H99	-3.700H9H	-3.9C427C
C	-H.28700C	-H.9C2H89	0.CC5203
C	0.72HC02	-2.88C302	2.40874C
C	-0.0804C3	-H.HCH825	0.7CH888
C	-H.4H4707	-3.H5H7HH	H.429CH5
C	-0.4C70H3	-3.C0744H	2.3402H5
C	0.95240H	-H.747C35	H.CH7H82
H	-2.353C42	-3.C97C92	H.327534
H	-0.C385HC	-4.499494	2.947HH3
H	H.529999	-3.2HC250	3.0C4532
Al	H.H33H57	H.3H4C9C	H.580945
N	0.H9C298	0.H7798H	0.3H9554

M062X/Def2-TZVP

F-Al≡N-F

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
Al	0.562558	-0.161030	0.000446
N	-1.010979	0.487323	0.000160
F	-2.204662	-0.190055	-0.000328
F	2.178395	0.043625	-0.000441

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F2-Al=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.000723	-0.033672	0.000499
N	-0.527436	-1.793075	-0.000277
F	1.581589	0.347328	-0.000257
F	-1.172405	1.095923	-0.000249

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Al=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.616118	-0.000149	-0.000839
N	-0.244733	-0.000088	0.005063
F	-1.071731	1.088943	-0.001363
F	-1.072314	-1.088659	-0.001363

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F-Al≡N-F-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.179207	0.728014	-0.004125
Al	-0.485961	0.199429	0.004706
F	1.829440	-0.587095	-0.000065
F	-2.044657	-0.267202	-0.003524

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F-Al≡N-F-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.500576	-0.104878	-0.065419
N	-0.354217	-0.027372	0.493091
F	-0.767909	1.162344	-0.132635
F	-1.124088	-0.989564	-0.156387

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HO-Al≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Al	-0.577081	-0.302242	0.003701
N	0.986332	0.343434	-0.097597
O	2.271736	-0.010208	0.157830
H	2.695975	-0.104053	-0.704399
O	-2.203383	0.099807	-0.018254
H	-2.645076	0.912367	0.222867

(OH)2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.229159	0.213448	-0.002138
N	-1.361723	0.907796	0.002658
O	1.879874	-0.011804	0.029519
H	2.415047	-0.792525	-0.098181
O	-1.158066	-0.883083	-0.100808
H	-1.636525	-1.177772	0.677684

Al≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.596676	0.000045	-0.000003

N	-0.230360	0.000023	0.000022
O	-1.023092	1.137834	-0.109876
H	-1.388128	1.295469	0.771987
O	-1.022937	-1.137912	0.109865
H	-1.387913	-1.295583	-0.772017

HO-Al≡N-OH-TS1

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Al	0.173419	0.126817	0.000448
N	-1.247180	1.175758	0.005302
O	1.818264	-0.146946	0.017427
H	2.557333	0.456169	-0.018094
O	-1.120725	-0.986844	-0.100476
H	-1.661826	-1.264780	0.639536

HO-Al≡N-OH-TS2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Al	-1.429577	-0.393302	-0.027318
N	0.378864	-0.150308	0.307476
O	1.559486	-0.606010	-0.194400
H	2.230803	-0.451122	0.481293
O	0.115216	1.211067	-0.164443
H	0.304038	1.775759	0.592260

H-Al≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.559668	0.000920	0.000110
N	1.048016	-0.002894	-0.000029
H	2.045825	0.010935	-0.000380
H	-2.106260	-0.002639	-0.000852

H2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.005759	-0.518837	0.000000
N	0.005759	1.294097	-0.000000
H	-1.482818	-1.019456	0.000000

H	1.367641	-1.294342	0.000000

Al≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.787959	0.000014	0.000007
N	1.006878	0.000044	-0.000054
H	1.598041	0.821909	0.000142
H	1.597281	-0.822405	0.000142

H-Al≡N-H-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.014577	-0.518592	0.000000
N	0.014577	1.284228	0.000000
H	1.252035	-1.474404	0.000000
H	-1.543573	-0.773492	-0.000000

H-Al≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.518933	-0.009744	0.000425
N	-1.279095	0.081908	-0.000209
H	0.629691	-1.586143	-0.001763
H	1.577846	1.139461	-0.002302

3HC-Al≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.865230	-0.746801	-0.701041
C	-2.487970	0.001193	-0.002895
H	-2.871761	0.976008	-0.301750
H	-2.872733	-0.231585	0.990205
Al	-0.560442	-0.001347	0.006353
N	1.052609	0.002631	-0.011311
C	2.468731	-0.000518	0.001441
H	2.884231	0.993743	-0.207434
H	2.888511	-0.683451	-0.748213
H	2.869899	-0.312873	0.973544

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(CH3)2-Al≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.121910	1.901995	0.000146
Al	-0.010096	0.084643	-0.000305
C	-1.801254	-0.679045	0.000844
H	-1.977154	-1.229403	-0.926059
H	-2.578628	0.078718	0.094042
H	-1.914706	-1.385223	0.826011
C	1.725366	-0.803825	-0.000662
H	2.552608	-0.104382	-0.118196
H	1.779513	-1.533276	-0.811465
H	1.871578	-1.343539	0.937516

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Al≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-0.369362	2.093305	0.000269
C	-1.005165	1.202471	-0.000020
H	-1.652215	1.256407	0.884709
H	-1.651498	1.256492	-0.885275
N	-0.199950	-0.000056	0.000157
Al	1.600994	-0.000179	-0.000019

C	-1.005689	-1.202221	-0.000019
H	-1.653155	-1.255159	-0.884451
H	-0.370295	-2.093231	-0.001319
H	-1.651619	-1.256596	0.885456

3HC-Al≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.336683	-1.863916	-0.000889
Al	0.030305	-0.081030	0.001634
C	-1.660455	0.894196	-0.000874
H	-1.748990	1.500455	0.903042
H	-2.519997	0.225612	-0.043584
H	-1.711601	1.567111	-0.859322
C	1.867263	0.558261	0.000323
H	2.583851	-0.246148	0.164636
H	2.014251	1.309107	0.779201
H	2.104452	1.029922	-0.955691

3HC-Al≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Al	-0.948543	-0.913033	0.002794
N	0.626202	-0.286842	-0.006688
C	-1.163816	1.211756	0.001223
H	-1.485438	1.412810	-1.016950
H	-0.318553	1.828006	0.278563
H	-1.985663	1.341722	0.701629
C	1.957396	0.170462	-0.005486
H	1.952405	1.227438	0.304526
H	2.456404	0.117207	-0.978963
H	2.567009	-0.343173	0.747262

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3HSi-Al≡N-SiH3

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Al	-0.500356	-0.005243	-0.006704
N	1.135749	-0.007877	-0.011300
Si	-2.923765	0.002780	0.003882
Si	2.822593	0.003332	0.004308
H	-3.405923	-1.105703	-0.840553
H	-3.391759	1.294366	-0.532590
H	-3.392028	-0.171776	1.390985
H	3.385588	1.233979	-0.613238
H	3.402356	-1.147220	-0.736920
H	3.372562	-0.065912	1.383913

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(SiH3)2-Al≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.008634	2.100932	-0.014488
Al	0.000839	0.325167	0.026070
Si	2.301761	-0.521377	-0.005159
H	3.278967	0.574790	0.145523
H	2.538210	-1.217735	-1.288604
H	2.484388	-1.489752	1.098552
Si	-2.299453	-0.524589	-0.004285
H	-2.459624	-1.547048	1.053218
H	-3.283056	0.556424	0.201376
H	-2.541657	-1.166850	-1.315344

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Al≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.592167	0.257811	0.158105
Si	-1.500412	-0.735200	0.000185
H	-1.573616	-1.703708	1.116853
H	-1.717981	-1.474288	-1.262816
N	-0.000040	0.124986	-0.000035
Al	-0.005023	1.956568	0.000033

Si	1.504096	-0.728701	-0.000179
H	1.570128	-1.715416	-1.101192
H	2.590367	0.265952	-0.184025
H	1.737272	-1.446020	1.272802

3HSi-Al≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.022274	2.098288	0.002709
Al	-0.002925	0.333902	-0.005272
Si	-2.319117	-0.521731	0.000969
H	-3.294833	0.593264	0.041611
H	-2.508184	-1.391153	1.192808
H	-2.538593	-1.331185	-1.227241
Si	2.312545	-0.531016	0.000678
H	2.486276	-1.469989	-1.139607
H	3.291170	0.575832	-0.114251
H	2.538286	-1.267052	1.273187

3HSi-Al≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Al	-0.703742	1.383558	-0.025545
N	0.673396	0.449844	0.108734
Si	-1.932085	-0.734870	-0.000558
H	-3.386925	-0.541883	-0.184023
H	-1.681606	-1.362868	1.305719
H	-1.401067	-1.518819	-1.127238
Si	2.152507	-0.384648	-0.015942
H	1.841779	-1.812915	-0.289965
H	2.969194	-0.335184	1.220739
H	3.007593	0.109758	-1.123279

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F-Al≡N-F

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Al	-0.566044	-0.198655	-0.003439
N	1.014611	0.496985	-0.001925
F	2.213049	-0.175594	0.002918
F	-2.184572	0.075996	0.003547

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F2-Al=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.000463	-0.024989	-0.000013
N	-0.043032	-1.864425	0.000007
F	1.461914	0.713092	0.000007
F	-1.429113	0.773112	0.000006

Al=N-F2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.622487	-0.000049	-0.000193
N	-0.246828	-0.000029	0.001166
F	-1.075711	1.100182	-0.000314
F	-1.075904	-1.100088	-0.000314

F-Al≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z

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N	1.181656	0.730918	0.005256
Al	-0.491556	0.191766	-0.006106
F	1.856331	-0.581851	0.000155
F	-2.065372	-0.263636	0.004577

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F-Al≡N-F-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.529145	0.088360	-0.063125
N	-0.341834	0.028522	0.459402
F	-1.122852	1.025197	-0.143097
F	-0.820042	-1.175012	-0.123035

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HO-Al≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.586172	-0.376601	-0.001259
N	0.978811	0.347968	-0.096385
O	2.259711	0.021923	0.158338

H	2.694060	-0.069183	-0.702220
O	-2.190312	0.161529	-0.002485
H	-2.480700	1.061593	0.146449

(OH)2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.230115	0.217153	-0.000724
N	-1.364171	0.919101	-0.000370
O	1.890202	-0.012236	0.029053
H	2.387894	-0.816828	-0.103765
O	-1.164006	-0.897585	-0.100945
H	-1.639750	-1.161295	0.690903

Al≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.599565	-0.000000	0.000000
N	-0.234529	0.000000	-0.000001
O	-1.024821	1.145626	-0.110929
H	-1.377754	1.310076	0.776041

O	-1.024821	-1.145626	0.110930
H	-1.377755	-1.310075	-0.776040

HO-Al≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z

Al	0.088332	0.070922	0.017872
N	-0.984248	1.528927	-0.011580
O	1.745625	-0.210888	0.022635
H	2.442298	0.427790	-0.115857
O	-1.101998	-1.140149	-0.089240
H	-1.849896	-1.243958	0.497425

HO-Al≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z

Al	-1.489103	-0.336299	-0.017910
N	0.329981	-0.135847	0.238715
O	1.494100	-0.738901	-0.172805

H	2.106614	-0.675567	0.573470
O	0.305747	1.268875	-0.158547
H	0.543083	1.758594	0.639170

H-Al≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.562067	0.035537	-0.000010
N	1.056506	-0.069752	-0.000007
H	2.018208	0.201425	0.000085
H	-2.106876	-0.175144	0.000091

H2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.000063	-0.515576	-0.000000
N	0.000063	1.293706	-0.000000
H	-1.440129	-1.175260	0.000000
H	1.438870	-1.178198	-0.000000

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Al≡N-H2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.789723	-0.000002	0.000000
N	1.009546	-0.000007	-0.000001
H	1.599728	0.822464	0.000002
H	1.599853	-0.822383	0.000002

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H-Al≡N-H-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.014577	-0.518592	-0.000000
N	0.014577	1.284228	0.000000
H	1.252035	-1.474404	0.000000
H	-1.543573	-0.773492	-0.000000

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H-Al≡N-H-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.000994	-0.516280	0.000000
N	-0.000994	1.296310	0.000000
H	-1.427101	-1.203751	0.000000
H	1.446980	-1.158770	-0.000000

3HC-Al≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.878946	0.170978	-1.008552
C	-2.496872	0.000826	-0.000329
H	-2.878885	0.789562	0.650383
H	-2.881217	-0.956426	0.356569
Al	-0.559043	-0.001411	0.000533
N	1.059426	0.001206	-0.000368
C	2.468980	0.000152	-0.000097
H	2.886305	0.751435	0.686191
H	2.886206	0.218595	-0.993963
H	2.885466	-0.970116	0.307575

(CH3)2-Al≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.000238	1.907366	0.001351
Al	0.000030	0.097287	-0.002278
C	-1.773257	-0.751848	0.001093
H	-1.898515	-1.343898	-0.910061
H	-2.584871	-0.026124	0.055934
H	-1.853637	-1.428239	0.856986
C	1.773385	-0.751814	0.000895
H	2.584531	-0.025918	-0.059319
H	1.854221	-1.432761	-0.851366
H	1.898780	-1.337370	0.916062

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Al≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-0.360136	2.092856	0.000031
C	-1.003346	1.205284	-0.000003
H	-1.651639	1.270865	0.885669
H	-1.651577	1.270880	-0.885719
N	-0.207040	-0.000014	0.000013
Al	1.601363	-0.000055	-0.000002
C	-1.003507	-1.205204	-0.000002
H	-1.651781	-1.270690	-0.885697
H	-0.360413	-2.092859	-0.000013

H	-1.651781	-1.270710	0.885688

3HC-Al≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.051440	-1.898069	0.003000
Al	-0.002892	-0.090033	-0.006020
C	-1.796174	0.718264	0.001016
H	-1.963030	1.223533	0.956612
H	-2.582971	-0.023390	-0.138513
H	-1.867412	1.464589	-0.795003
C	1.761808	0.770766	0.001991
H	2.574246	0.055473	-0.126203
H	1.909285	1.297311	0.949173
H	1.813593	1.505215	-0.806848

3HC-Al≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.948345	-0.923012	-0.002520
N	0.623245	-0.269086	0.011092

C	-1.162135	1.224371	0.000828
H	-1.624123	1.392509	-0.970210
H	-0.304296	1.869632	0.143188
H	-1.880028	1.347435	0.810591
C	1.950988	0.180310	-0.012492
H	2.138586	0.945232	0.756308
H	2.293276	0.554578	-0.987084
H	2.609240	-0.654716	0.272312

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3HSi-Al≡N-SiH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.500005	0.000349	0.000526
N	1.141861	0.000619	0.001104
Si	-2.931012	-0.000220	-0.000311
Si	2.828479	-0.000218	-0.000394
H	-3.413983	-1.022727	0.960045
H	-3.412777	-0.320901	-1.366387
H	-3.413517	1.343070	0.404568
H	3.392683	-0.381674	-1.330813
H	3.394477	-0.962129	0.993789
H	3.395602	1.341625	0.334097

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(SiH3)2-Al≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.005303	2.118733	0.001674
Al	0.000437	0.356007	-0.002874
Si	2.305408	-0.536371	0.000870
H	3.303674	0.559173	-0.005573
H	2.489656	-1.384950	-1.206699
H	2.492832	-1.375142	1.214588
Si	-2.303370	-0.538849	0.000523
H	-2.483664	-1.401145	1.198914
H	-3.302045	0.556126	0.028911
H	-2.497535	-1.360193	-1.223993

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Al≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.578476	0.353355	0.003814
Si	-1.533446	-0.713869	0.000036
H	-1.728869	-1.566237	1.203746
H	-1.733502	-1.562069	-1.206118
N	-0.000046	0.087892	-0.000803
Al	0.004884	1.925689	0.000036
Si	1.529842	-0.720124	0.000130
H	1.728911	-1.566053	-1.210615
H	2.580138	0.345087	0.008898

H	1.719083	-1.577375	1.203099

3HSi-Al≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.022274	2.098288	0.002709
Al	-0.002925	0.333902	-0.005272
Si	-2.319117	-0.521731	0.000969
H	-3.294833	0.593264	0.041611
H	-2.508184	-1.391153	1.192808
H	-2.538593	-1.331185	-1.227241
Si	2.312545	-0.531016	0.000678
H	2.486276	-1.469989	-1.139607
H	3.291170	0.575832	-0.114251
H	2.538286	-1.267052	1.273187

3HSi-Al≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.721890	1.415787	-0.006795
N	0.621908	0.401282	0.027321

Si	-1.890539	-0.757050	-0.000747
H	-3.359380	-0.546911	-0.134499
H	-1.629418	-1.410101	1.301705
H	-1.429934	-1.570451	-1.147110
Si	2.146804	-0.369524	-0.002953
H	1.941117	-1.805153	-0.356665
H	2.858505	-0.330725	1.307026
H	3.062601	0.221168	-1.021570

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B3LYP/LANL2DZ+dp

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F-Al≡N-F

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Al	0.556956	-0.181546	0.000198
N	-1.041501	0.536748	0.000074
F	-2.225518	-0.208050	-0.000150
F	2.231082	0.052813	-0.000194

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F2-Al=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.000037	-0.034730	-0.000005
N	0.003172	-1.889993	0.000003
F	1.480985	0.762272	0.000003
F	-1.483398	0.757889	0.000003

Al=N-F2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.655636	0.000054	-0.000390
N	-0.253823	0.000020	0.002366
F	-1.097130	1.112937	-0.000638
F	-1.096927	-1.113030	-0.000638

F-Al≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.203199	0.739689	0.000611

Al	-0.487969	0.203503	-0.000694
F	1.874674	-0.597726	0.000013
F	-2.105651	-0.271537	0.000515

F-Al≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.590161	0.077243	-0.058371
N	-0.314866	0.035215	0.394259
F	-1.166777	1.036441	-0.120088
F	-0.885228	-1.175403	-0.102244

HO-Al≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.583456	-0.359891	-0.008275
N	1.000980	0.380729	-0.133220
O	2.278737	-0.002993	0.182821
H	2.740918	-0.096497	-0.668975
O	-2.231288	0.139377	-0.000707
H	-2.542436	1.018896	0.252174

(OH)2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.230344	0.220093	0.001444
N	-1.373451	0.952510	-0.001503
O	1.916668	-0.011992	0.024627
H	2.388730	-0.845949	-0.083411
O	-1.178981	-0.926029	-0.101902
H	-1.670539	-1.178648	0.693351

Al≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	1.628092	-0.000008	-0.000000
N	-0.239112	-0.000004	0.000001
O	-1.043852	1.159098	-0.111675
H	-1.394751	1.321364	0.783686
O	-1.043882	-1.159084	0.111674
H	-1.394783	-1.321340	-0.783687

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HO-Al≡N-OH-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.108059	0.093089	0.013276
N	-1.092853	1.459793	-0.007975
O	1.793379	-0.180550	0.019843
H	2.478473	0.490755	-0.078130
O	-1.101199	-1.145926	-0.097125
H	-1.770708	-1.307665	0.579622

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HO-Al≡N-OH-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-1.535923	-0.265081	-0.023819
N	0.318200	-0.092204	0.294038
O	1.373756	-0.888436	-0.183009
H	2.050082	-0.863881	0.515549
O	0.482964	1.287632	-0.174500
H	0.835762	1.761801	0.595904

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H-Al≡N-H

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.568540	0.051668	0.000240
N	1.072760	-0.105717	0.000133
H	1.989127	0.322163	-0.001897
H	-2.107425	-0.253825	-0.002159

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H2-Al≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.000055	-0.521169	0.000000
N	0.000055	1.308377	-0.000000
H	-1.448028	-1.190458	0.000000
H	1.446922	-1.192977	0.000000

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Al≡N-H2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.802628	-0.000002	0.000000
N	1.025723	-0.000007	-0.000000
H	1.626992	0.826757	0.000000
H	1.627106	-0.826684	0.000000

H-Al≡N-H-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.000152	-0.521589	0.000000
N	-0.000152	1.309958	-0.000000
H	1.447768	-1.191049	0.000000
H	-1.444719	-1.197998	-0.000000

H-Al≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	0.521691	-0.000191	-0.000001

N	-1.310430	0.002270	0.000000
H	1.182319	-1.452411	0.000004
H	1.208710	1.438997	0.000004

3HC-Al≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.901543	0.388595	-0.953259
C	-2.515551	0.002147	-0.000412
H	-2.901778	0.636005	0.809094
H	-2.907432	-1.013876	0.142102
Al	-0.565386	-0.004377	0.000775
N	1.066721	0.006104	-0.000890
C	2.493166	-0.000538	0.000012
H	2.911168	0.582765	0.840852
H	2.911482	0.433591	-0.926559
H	2.905387	-1.022559	0.086318

(CH3)2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z

N	0.002584	1.942702	0.000970
Al	-0.000106	0.114503	-0.002113
C	-1.773433	-0.771165	0.000702
H	-1.889827	-1.365564	-0.918877
H	-2.615963	-0.072496	0.071531
H	-1.827528	-1.466897	0.852803
C	1.770669	-0.774389	0.000231
H	2.612169	-0.075829	-0.086589
H	1.825879	-1.487485	-0.837131
H	1.895145	-1.345858	0.933338

Al≡N-(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-0.382343	2.110175	0.000065
C	-1.020708	1.212054	-0.000003
H	-1.673356	1.270219	0.890458
H	-1.673251	1.270270	-0.890538
N	-0.207688	-0.000012	0.000012
Al	1.627801	-0.000041	-0.000002
C	-1.020829	-1.211994	-0.000001
H	-1.673460	-1.270084	-0.890482
H	-0.382552	-2.110176	-0.000053
H	-1.673409	-1.270143	0.890511

3HC-Al≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.026324	-1.931086	0.000033
Al	0.002064	-0.103273	-0.000046
C	-1.772976	0.777168	0.000034
H	-1.869872	1.420528	0.888063
H	-2.603734	0.060539	0.002523
H	-1.871844	1.416548	-0.890626
C	1.789367	0.749897	0.000011
H	2.608839	0.020310	-0.001336
H	1.898377	1.388842	0.889819
H	1.897313	1.390997	-0.888339

3HC-Al≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.976239	-0.932816	-0.002215
N	0.625468	-0.284940	0.010464
C	-1.145846	1.260395	0.000486
H	-1.559534	1.451672	-0.994780
H	-0.273599	1.884516	0.192153
H	-1.901134	1.394533	0.782766
C	1.971989	0.165057	-0.013013

H	2.113210	1.028596	0.664838
H	2.349905	0.433205	-1.015433
H	2.627131	-0.624048	0.401172

3HSi-Al≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.513124	0.000221	-0.000013
N	1.142141	-0.000261	-0.000161
Si	-2.936283	-0.000062	0.000020
Si	2.843933	0.000003	0.000044
H	-3.418014	-1.399908	-0.035735
H	-3.418464	0.730778	-1.194228
H	-3.418285	0.668768	1.230101
H	3.407825	0.664853	-1.210866
H	3.407923	-1.381056	0.029800
H	3.407553	0.716350	1.181321

(SiH3)2-Al≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z

N	-0.002674	2.169782	-0.001047
Al	0.000254	0.386906	0.001863
Si	2.282906	-0.556927	-0.000286
H	3.309634	0.508472	0.003459
H	2.443956	-1.401090	-1.211111
H	2.443614	-1.408782	1.205125
Si	-2.282059	-0.558084	-0.000181
H	-2.424566	-1.458202	1.172051
H	-3.310044	0.504266	0.061923
H	-2.459035	-1.352769	-1.241798

Al≡N-(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.606038	0.294914	-0.022795
Si	-1.528136	-0.735855	-0.000104
H	-1.709649	-1.576868	1.214833
H	-1.689914	-1.611361	-1.193076
N	-0.000009	0.108577	0.000238
Al	0.001689	1.974578	-0.000037
Si	1.526888	-0.738051	0.000069
H	1.708040	-1.577608	-1.216668
H	2.606263	0.291844	0.024791
H	1.686887	-1.615790	1.192225

3HSi-Al≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.002282	2.157439	0.000674
Al	-0.000207	0.375510	-0.001209
Si	-2.289874	-0.550938	0.000237
H	-3.305950	0.524557	0.007463
H	-2.456204	-1.402367	1.205236
H	-2.462183	-1.392025	-1.211159
Si	2.289124	-0.551938	0.000169
H	2.452431	-1.416582	-1.195776
H	3.305645	0.522904	-0.020734
H	2.463475	-1.379925	1.220291

3HSi-Al≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Al	-0.758622	1.452011	-0.014928
N	0.605629	0.426623	0.057814
Si	-1.846176	-0.799243	-0.001421
H	-3.295876	-0.624328	-0.284095
H	-1.694213	-1.357338	1.358972
H	-1.268305	-1.676815	-1.038726
Si	2.136744	-0.364878	-0.007351
H	1.916073	-1.773105	-0.442211
H	2.838748	-0.407816	1.304687
H	3.058309	0.274592	-0.986460

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b97d3/LANL2DZ+dp

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$SiMe(SitBu_3)_2$-Ga≡N-$SiMe(SitBu_3)_2$

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.549007	0.059447	-0.143399
N	1.134145	-0.090053	0.085475
Si	2.689742	0.402443	-0.477005
Si	3.704511	-1.576375	-1.556796
Si	3.578673	1.772386	1.466005
C	2.404815	1.593498	-1.955663
H	1.995360	1.012958	-2.797432
H	3.297059	2.124339	-2.320234
H	1.641745	2.338473	-1.683604
C	5.419790	-1.221022	-2.458771
C	5.874490	-2.369042	-3.394844
H	5.974550	-3.327918	-2.866337
H	6.869431	-2.118236	-3.810170
H	5.200072	-2.520906	-4.247661
C	6.558792	-1.017104	-1.437616
H	6.332658	-0.222100	-0.720389
H	7.482734	-0.723908	-1.971405
H	6.785090	-1.934221	-0.875688
C	5.348793	0.074469	-3.304559
H	6.327249	0.245061	-3.792561
H	5.137179	0.956230	-2.686516
H	4.588197	0.033043	-4.093619
C	3.915811	-2.913759	-0.138942

C	4.606602	-2.245811	1.068072
H	4.108440	-1.309297	1.345179
H	5.663696	-2.020327	0.876798
H	4.564941	-2.916232	1.946912
C	4.749318	-4.163527	-0.503000
H	4.785931	-4.842985	0.370424
H	5.789380	-3.905343	-0.753118
H	4.330384	-4.731905	-1.343832
C	2.520630	-3.368751	0.353724
H	1.997498	-3.993694	-0.384524
H	1.878599	-2.508410	0.591026
H	2.634334	-3.975017	1.272568
C	2.441041	-2.264257	-2.936040
C	2.709067	-3.762595	-3.229750
H	2.060224	-4.086582	-4.066136
H	2.466157	-4.400748	-2.368881
H	3.748044	-3.966839	-3.520505
C	0.962410	-2.153895	-2.505512
H	0.325822	-2.680982	-3.242332
H	0.637626	-1.104742	-2.470738
H	0.771330	-2.588980	-1.519608
C	2.538155	-1.510913	-4.284494
H	2.370593	-0.429634	-4.173826
H	1.755466	-1.896865	-4.965340
H	3.502061	-1.655084	-4.788775
C	2.516057	3.459152	1.413540
C	3.235698	0.859561	3.209426
C	5.475084	2.239003	1.213227
C	5.921787	3.451530	2.060610
H	5.726898	3.300388	3.134948
H	5.428880	4.382702	1.749752
H	7.011809	3.602738	1.941280
C	5.712157	2.577574	-0.277801
H	6.786437	2.778751	-0.447757
H	5.153391	3.459087	-0.614156

H	5.430813	1.739142	-0.927213
C	6.437028	1.076172	1.565570
H	7.413437	1.247963	1.076512
H	6.068029	0.098413	1.237189
H	6.622955	1.014272	2.644418
C	2.093967	-0.167987	3.056376
H	2.357536	-1.001032	2.394460
H	1.188703	0.282635	2.633577
H	1.846959	-0.590149	4.049164
C	4.456207	0.111900	3.800848
H	4.919289	-0.602277	3.112084
H	4.119030	-0.459250	4.686476
H	5.232154	0.811408	4.145828
C	2.795030	1.834287	4.328325
H	1.813361	2.286599	4.132074
H	3.523843	2.639609	4.503191
H	2.699611	1.263633	5.271487
C	1.016231	3.102393	1.357658
H	0.782901	2.500208	0.473819
H	0.409545	4.027101	1.320574
H	0.693218	2.524544	2.236274
C	2.686687	4.449235	2.602716
H	2.263780	5.425725	2.298901
H	2.138424	4.134438	3.496767
H	3.730850	4.623411	2.890178
C	2.854058	4.291752	0.150236
H	2.904973	3.701977	-0.769584
H	3.810322	4.822594	0.266141
H	2.074351	5.064305	0.008840
Si	-2.882451	0.327986	0.428066
Si	-3.896445	1.649619	-1.412641
Si	-3.306555	-1.867918	1.521110
C	-2.708602	1.677383	1.798025
H	-2.294285	2.600949	1.371115
H	-2.047523	1.371416	2.615639

H	-3.689883	1.920584	2.235805
C	-2.440646	2.692382	-2.241959
C	-2.993371	3.825530	-3.145677
H	-2.145631	4.321375	-3.653835
H	-3.520732	4.599150	-2.571366
H	-3.673749	3.458320	-3.925135
C	-1.534037	1.810340	-3.131877
H	-1.141994	0.924712	-2.602892
H	-0.656982	2.396681	-3.458398
H	-2.048205	1.456430	-4.035694
C	-1.521964	3.354081	-1.193785
H	-0.735607	3.938093	-1.704620
H	-0.999367	2.612551	-0.573747
H	-2.053313	4.033831	-0.517388
C	-4.696350	0.462810	-2.740570
C	-3.740716	-0.718064	-3.025838
H	-2.828879	-0.411728	-3.552878
H	-4.252540	-1.467364	-3.656856
H	-3.436621	-1.224429	-2.103300
C	-5.010913	1.136967	-4.098873
H	-4.103865	1.487529	-4.610333
H	-5.702704	1.985766	-4.009196
H	-5.488462	0.392317	-4.762552
C	-6.015993	-0.136051	-2.201833
H	-6.807354	0.619332	-2.096774
H	-5.883395	-0.619725	-1.226704
H	-6.386987	-0.904177	-2.905573
C	-5.238879	2.884891	-0.651589
C	-6.178854	3.431796	-1.756141
H	-6.883162	4.152096	-1.299447
H	-6.783210	2.641659	-2.221605
H	-5.638401	3.961927	-2.551790
C	-6.132118	2.192823	0.401353
H	-6.855731	2.926058	0.803546
H	-5.549971	1.813047	1.252061

H	-6.713156	1.360382	-0.014585
C	-4.612260	4.115693	0.049721
H	-4.051582	4.760230	-0.639594
H	-3.948956	3.839421	0.878351
H	-5.426735	4.731275	0.474421
C	-1.900483	-2.157197	2.882167
C	-5.067507	-1.760404	2.377436
C	-3.237341	-3.326964	0.214295
C	-3.120097	-4.719198	0.889011
H	-3.946040	-4.920848	1.585355
H	-2.175904	-4.853240	1.432289
H	-3.155459	-5.496032	0.102808
C	-2.019836	-3.176319	-0.728523
H	-2.017375	-3.998519	-1.467478
H	-1.064495	-3.219158	-0.193285
H	-2.036876	-2.238953	-1.301832
C	-4.514637	-3.376234	-0.655720
H	-5.386348	-3.719862	-0.080549
H	-4.365026	-4.094932	-1.482002
H	-4.766404	-2.409895	-1.104888
C	-6.115619	-1.226720	1.379258
H	-5.773769	-0.314369	0.881070
H	-7.049830	-0.978928	1.916087
H	-6.368236	-1.961672	0.604970
C	-5.605699	-3.114061	2.901567
H	-5.744927	-3.841787	2.089183
H	-6.598660	-2.946859	3.359482
H	-4.965947	-3.572712	3.665704
C	-5.028211	-0.764002	3.561332
H	-4.691384	0.235886	3.251121
H	-4.376482	-1.101558	4.378360
H	-6.046779	-0.653583	3.976898
C	-2.377467	-3.198312	3.928347
H	-1.532735	-3.429148	4.602943
H	-2.707639	-4.144391	3.479880

H	-3.193305	-2.812405	4.554902
C	-0.572679	-2.683959	2.289063
H	-0.667067	-3.672999	1.824749
H	0.166882	-2.779020	3.103678
H	-0.127108	-1.998357	1.554602
C	-1.526110	-0.877252	3.664727
H	-0.940657	-0.187232	3.043831
H	-2.394285	-0.339049	4.065748
H	-0.878862	-1.153542	4.515959

$[SiMe(SitBu_3)_2]_2$-Ga=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.149946	0.145031	0.352384
Ga	-0.512164	0.152618	-0.052247
Si	2.677562	-0.281635	-0.345253
Si	3.726146	-1.819881	1.321378
Si	3.445978	1.886180	-1.383066
C	2.422750	-1.507364	-1.808118
H	2.472057	-2.544353	-1.456242
H	3.148967	-1.403302	-2.626356
H	1.421700	-1.360509	-2.230369
C	5.311296	-2.780914	0.609070
C	5.663513	-4.059944	1.408979
H	5.863340	-3.850260	2.469691
H	6.584989	-4.501070	0.982778
H	4.884905	-4.832012	1.353625
C	6.587691	-1.910847	0.617994

H	6.481243	-1.022325	-0.011339
H	7.427369	-2.500177	0.202687
H	6.884040	-1.590005	1.625829
C	5.103120	-3.195766	-0.867998
H	5.988943	-3.759984	-1.216955
H	4.997280	-2.317070	-1.519655
H	4.224593	-3.836472	-1.020336
C	4.200529	-0.797695	2.918001
C	4.919708	0.488860	2.469426
H	4.272263	1.070845	1.802885
H	5.864441	0.298681	1.942887
H	5.148668	1.122484	3.347358
C	5.120290	-1.531808	3.922347
H	5.307807	-0.874135	4.792898
H	6.100735	-1.776277	3.487103
H	4.680692	-2.463736	4.302822
C	2.925292	-0.334247	3.662873
H	2.417972	-1.162471	4.177581
H	2.204533	0.140366	2.978713
H	3.204217	0.407271	4.435923
C	2.370712	-3.195424	1.825578
C	2.768898	-3.928126	3.134572
H	2.040233	-4.740260	3.322193
H	2.730005	-3.258225	4.004746
H	3.765772	-4.383878	3.101989
C	0.961609	-2.612202	2.079794
H	0.285380	-3.433252	2.387868
H	0.557349	-2.148959	1.175235
H	0.941790	-1.848856	2.866197
C	2.181003	-4.274672	0.731197
H	1.815248	-3.847140	-0.211754
H	1.418976	-5.001946	1.071690
H	3.095372	-4.842527	0.516371
C	2.130069	2.268272	-2.833321
C	3.409679	3.416716	-0.121122

C	5.244359	1.732988	-2.146646
C	5.810503	3.024387	-2.785944
H	5.778548	3.879745	-2.095238
H	5.284979	3.312977	-3.705515
H	6.871973	2.858367	-3.052808
C	5.284249	0.619224	-3.218791
H	6.318364	0.506867	-3.595864
H	4.643067	0.846430	-4.082972
H	4.979235	-0.356975	-2.812850
C	6.223398	1.321415	-1.021798
H	7.126477	0.854197	-1.455154
H	5.765703	0.603411	-0.332941
H	6.552604	2.179969	-0.424322
C	2.254756	3.225236	0.885375
H	2.369876	2.315796	1.490488
H	1.282998	3.146288	0.386387
H	2.214387	4.093456	1.571267
C	4.712628	3.592630	0.697292
H	5.043374	2.681633	1.203275
H	4.537247	4.358364	1.476253
H	5.541045	3.955673	0.072381
C	3.205955	4.788454	-0.816601
H	2.254737	4.872350	-1.354680
H	4.016447	5.022423	-1.523088
H	3.210911	5.578750	-0.041909
C	0.785773	2.774322	-2.262985
H	0.389377	2.067713	-1.518410
H	0.043622	2.854895	-3.079724
H	0.847458	3.756938	-1.781425
C	2.650861	3.325648	-3.839769
H	1.816211	3.633169	-4.499057
H	3.050930	4.231352	-3.368444
H	3.431592	2.906185	-4.490761
C	1.762305	1.025692	-3.677173
H	1.139105	0.326444	-3.110407

H	2.632140	0.470890	-4.051794
H	1.170387	1.350682	-4.554027
Si	-2.894571	0.323166	-0.454596
Si	-3.551156	-1.910542	-1.341545
Si	-3.566713	1.808673	1.436308
C	-2.930591	1.369135	-2.072359
H	-2.335519	0.883660	-2.857678
H	-2.541060	2.382393	-1.939433
H	-3.961437	1.452384	-2.446588
C	-1.966938	-2.670195	-2.235943
C	-2.341656	-3.881615	-3.128136
H	-1.413607	-4.318104	-3.541158
H	-2.974243	-3.602491	-3.980423
H	-2.855030	-4.674138	-2.567371
C	-0.919373	-3.183022	-1.227405
H	-0.570803	-2.401540	-0.536082
H	-0.025843	-3.529722	-1.774014
H	-1.279657	-4.024961	-0.622706
C	-1.248681	-1.638003	-3.135144
H	-0.383711	-2.117398	-3.625821
H	-0.848493	-0.790852	-2.555814
H	-1.890493	-1.224900	-3.921890
C	-4.104545	-3.045596	0.141610
C	-3.137614	-2.843352	1.328659
H	-2.114050	-3.174942	1.114995
H	-3.495551	-3.414014	2.205062
H	-3.091612	-1.791039	1.628148
C	-4.134681	-4.559132	-0.178628
H	-3.136902	-4.954420	-0.414563
H	-4.806912	-4.811355	-1.010173
H	-4.495525	-5.104507	0.713208
C	-5.516165	-2.635104	0.619523
H	-6.296963	-2.911754	-0.102353
H	-5.593524	-1.554978	0.797778
H	-5.750626	-3.146710	1.571065

C	-4.993509	-1.703953	-2.676991
C	-5.696740	-3.061782	-2.940531
H	-6.457791	-2.918974	-3.730261
H	-6.221660	-3.440715	-2.053055
H	-5.008279	-3.842900	-3.288599
C	-6.090369	-0.714524	-2.226648
H	-6.873074	-0.667536	-3.006392
H	-5.702877	0.305475	-2.099627
H	-6.580830	-1.015322	-1.292478
C	-4.484198	-1.188652	-4.046156
H	-3.808798	-1.897571	-4.541631
H	-3.971955	-0.220376	-3.975069
H	-5.353229	-1.050571	-4.715544
C	-2.338126	3.360557	1.452995
C	-5.400481	2.383901	1.053498
C	-3.441775	0.893737	3.165731
C	-3.550084	1.882036	4.355884
H	-4.488970	2.453304	4.341337
H	-2.719357	2.597351	4.394263
H	-3.530145	1.305580	5.299174
C	-2.103093	0.127965	3.318346
H	-2.125577	-0.464862	4.250905
H	-1.236308	0.795479	3.376573
H	-1.915870	-0.579881	2.499220
C	-4.597748	-0.118060	3.339777
H	-5.563325	0.389841	3.475333
H	-4.420385	-0.727084	4.244939
H	-4.694633	-0.806755	2.494699
C	-6.283626	1.158984	0.733299
H	-5.800026	0.489157	0.014665
H	-7.237437	1.491494	0.283277
H	-6.528557	0.571808	1.627596
C	-6.095388	3.150084	2.205034
H	-6.219315	2.524139	3.100358
H	-7.109532	3.442577	1.872992

H	-5.569798	4.067347	2.498870
C	-5.415608	3.290262	-0.201979
H	-4.977182	2.792857	-1.077656
H	-4.879201	4.236227	-0.046971
H	-6.461388	3.543465	-0.456175
C	-2.995982	4.566318	2.172857
H	-2.243424	5.370178	2.273497
H	-3.354085	4.323855	3.182532
H	-3.836876	4.984165	1.601669
C	-1.013034	3.059959	2.189928
H	-1.151530	2.856246	3.258348
H	-0.355990	3.942756	2.112181
H	-0.454980	2.218521	1.751399
C	-1.929991	3.845932	0.044894
H	-1.292101	3.113480	-0.466024
H	-2.786199	4.074537	-0.603298
H	-1.331074	4.769566	0.141803

Ga=N-[SiMe(SitBu$_3$)$_2$]$_2$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	0.087132	-0.993037	-1.408038
N	0.032717	0.045352	0.302514
Si	1.784757	0.451572	0.536932
Si	2.909082	1.832025	-1.712482
Si	3.215462	-1.649005	1.747981
C	2.079883	1.818066	1.811141
H	1.716965	2.789421	1.459965

H	3.161590	1.904739	1.974975
H	1.621505	1.607751	2.780934
C	4.335829	3.103316	-1.108193
C	4.710986	4.099578	-2.239761
H	4.985065	3.617762	-3.185281
H	5.586494	4.687442	-1.905192
H	3.904740	4.817595	-2.440617
C	5.624518	2.369490	-0.682622
H	5.453654	1.776662	0.222026
H	6.405697	3.113868	-0.438692
H	6.035831	1.706391	-1.455492
C	3.949732	3.976709	0.112367
H	4.728387	4.750341	0.249510
H	3.917288	3.390764	1.036113
H	2.989240	4.493612	0.003180
C	3.668912	0.563626	-3.036529
C	4.370038	-0.585886	-2.290005
H	3.679511	-1.076629	-1.592358
H	5.245157	-0.249327	-1.719181
H	4.719112	-1.348083	-3.011762
C	4.704868	1.205452	-3.992820
H	5.069988	0.430726	-4.693525
H	5.582291	1.597845	-3.461352
H	4.277956	2.017257	-4.599038
C	2.593804	-0.102281	-3.928272
H	2.063005	0.607029	-4.576785
H	1.842812	-0.650017	-3.335376
H	3.086138	-0.841379	-4.587737
C	1.503520	2.901856	-2.599503
C	1.893706	3.372270	-4.024036
H	1.064234	3.980130	-4.433383
H	2.054577	2.537161	-4.717989
H	2.794264	3.999271	-4.035824
C	0.210290	2.074137	-2.726376
H	-0.569570	2.669471	-3.234261

H	-0.179671	1.789538	-1.740351
H	0.357682	1.162629	-3.320831
C	1.154770	4.167939	-1.786534
H	0.955510	3.940545	-0.734479
H	0.243850	4.635515	-2.204006
H	1.953773	4.920568	-1.825471
C	2.069822	-2.027530	3.308145
C	3.439125	-3.328303	0.699244
C	5.008796	-1.064038	2.332233
C	5.800383	-2.178084	3.065224
H	5.904282	-3.091314	2.463501
H	5.357195	-2.453216	4.030923
H	6.822727	-1.804630	3.267311
C	4.944478	0.145249	3.293484
H	5.969110	0.398435	3.624231
H	4.347460	-0.055078	4.195035
H	4.534688	1.037853	2.803439
C	5.855795	-0.635125	1.110659
H	6.681523	0.023898	1.435544
H	5.258861	-0.088605	0.373658
H	6.309080	-1.491691	0.596310
C	2.252457	-3.498645	-0.269138
H	2.244717	-2.703977	-1.032826
H	1.284803	-3.484687	0.243699
H	2.328429	-4.463504	-0.804674
C	4.724260	-3.382021	-0.163259
H	4.843457	-2.518689	-0.823318
H	4.676098	-4.282275	-0.804311
H	5.631756	-3.474986	0.449193
C	3.514848	-4.590596	1.599307
H	2.602283	-4.778914	2.176354
H	4.356808	-4.546464	2.304674
H	3.676966	-5.473567	0.952753
C	0.834489	-2.820872	2.833630
H	0.344141	-2.304034	2.000715

H	0.101710	-2.896540	3.657311
H	1.070435	-3.840624	2.510325
C	2.771405	-2.812904	4.442419
H	2.013002	-3.108779	5.192269
H	3.273313	-3.727086	4.101197
H	3.511973	-2.189504	4.964979
C	1.514687	-0.734772	3.945173
H	0.840635	-0.214483	3.256165
H	2.299202	-0.031829	4.255961
H	0.925311	-0.997444	4.843248
Si	-1.688955	-0.010475	0.778957
Si	-3.049244	2.149766	1.429189
Si	-3.012713	-2.137480	-1.281879
C	-1.970599	-1.036718	2.356247
H	-1.346983	-0.652080	3.178068
H	-1.750508	-2.102924	2.235174
H	-3.022504	-0.938863	2.661035
C	-1.667158	3.271639	2.234282
C	-2.160176	4.542624	2.963686
H	-1.278942	5.127657	3.288567
H	-2.739288	4.307619	3.867425
H	-2.770072	5.197453	2.326996
C	-0.715392	3.715612	1.109794
H	-0.354109	2.856862	0.528799
H	0.161302	4.230445	1.542329
H	-1.188854	4.421571	0.416133
C	-0.842613	2.453125	3.250519
H	0.025820	3.048244	3.583192
H	-0.457228	1.528741	2.804572
H	-1.413969	2.180900	4.144515
C	-3.808043	3.015083	-0.163933
C	-2.865096	2.789773	-1.366373
H	-1.897751	3.286806	-1.237865
H	-3.326896	3.198926	-2.284509
H	-2.669696	1.721056	-1.541833

C	-4.010397	4.542117	-0.000502
H	-3.068962	5.082435	0.166690
H	-4.698399	4.792186	0.819351
H	-4.451683	4.942441	-0.932582
C	-5.179277	2.425699	-0.560677
H	-5.949286	2.572297	0.208963
H	-5.116883	1.356727	-0.779077
H	-5.535372	2.928620	-1.479441
C	-4.449449	1.863785	2.815032
C	-5.302284	3.153639	2.952067
H	-6.006790	3.022360	3.795010
H	-5.906691	3.348399	2.055890
H	-4.706676	4.050589	3.160365
C	-5.446640	0.723555	2.529850
H	-6.185713	0.686085	3.352044
H	-4.963279	-0.261202	2.486087
H	-6.004793	0.872300	1.599238
C	-3.849651	1.564345	4.210797
H	-3.314976	2.424526	4.633787
H	-3.168344	0.702282	4.204555
H	-4.675474	1.327022	4.906859
C	-2.074500	-3.919173	-1.232365
C	-4.793958	-2.404484	-0.415951
C	-3.331697	-1.534771	-3.167536
C	-3.779251	-2.711535	-4.073419
H	-4.687405	-3.210308	-3.709190
H	-2.996491	-3.473774	-4.187683
H	-4.000759	-2.319683	-5.084465
C	-2.078597	-0.910405	-3.817718
H	-2.315450	-0.607944	-4.855421
H	-1.226052	-1.602694	-3.861045
H	-1.763967	-0.000624	-3.282218
C	-4.427080	-0.444354	-3.247079
H	-5.426937	-0.834754	-3.017114
H	-4.465006	-0.045424	-4.277800

H	-4.221629	0.400406	-2.575842
C	-5.441701	-1.034124	-0.166275
H	-4.730895	-0.337136	0.289517
H	-6.300251	-1.142466	0.518900
H	-5.821914	-0.580590	-1.087644
C	-5.815200	-3.214286	-1.256943
H	-6.052316	-2.717985	-2.208189
H	-6.761011	-3.278705	-0.685293
H	-5.496984	-4.240060	-1.476979
C	-4.670810	-3.092454	0.966027
H	-3.988701	-2.556486	1.637910
H	-4.330550	-4.134466	0.900188
H	-5.666297	-3.106601	1.447770
C	-3.047606	-5.103630	-1.463292
H	-2.470073	-6.046859	-1.439685
H	-3.547189	-5.049422	-2.441010
H	-3.818516	-5.180952	-0.687871
C	-0.951813	-4.096156	-2.280206
H	-1.319303	-4.022661	-3.313119
H	-0.500842	-5.097952	-2.155787
H	-0.141359	-3.362275	-2.165418
C	-1.434453	-4.088505	0.164382
H	-0.741230	-3.265893	0.386579
H	-2.179563	-4.114723	0.970706
H	-0.858648	-5.031435	0.209929

Si*i*PrDis$_2$-Ga≡N-Si*i*PrDis$_2$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Ga	-0.337462	0.267543	-0.136413
N	1.300018	-0.162359	-0.267856
Si	2.812940	-0.368822	0.512682
Si	-2.632739	-0.330338	-0.638024
C	3.584068	1.370281	0.769627
H	4.680361	1.236184	0.773808
C	3.940664	-1.575122	-0.503975
H	4.038476	-2.411563	0.221893
C	2.478598	-1.485002	2.063558
H	2.055067	-2.360771	1.531900
C	1.378360	-1.021916	3.030791
H	1.072386	-1.847284	3.699510
H	0.478817	-0.690621	2.484085
H	1.697371	-0.188052	3.670973
C	3.711458	-2.000050	2.836517
H	3.405074	-2.686740	3.646989
H	4.290572	-1.187497	3.295620
H	4.401658	-2.558545	2.185258
C	-2.327985	-1.443110	-2.176222
H	-1.764637	-2.310286	-1.798563
C	-1.470709	-0.790235	-3.275618
H	-1.294872	-1.507874	-4.095672
H	-0.483858	-0.474211	-2.905662
H	-1.967921	0.089985	-3.712034
C	-3.653338	-1.946701	-2.786215
H	-3.451269	-2.664390	-3.600828
H	-4.231079	-1.114901	-3.223473
H	-4.298820	-2.448967	-2.053410
C	-2.976496	-1.434114	0.919343
H	-1.915015	-1.681416	1.154515
C	-3.665885	1.159407	-1.256518
H	-3.734508	0.872597	-2.328877
Si	3.002385	-2.522627	-1.864358
Si	5.783727	-1.199394	-0.742203

Si	3.270890	2.261329	2.415250
Si	3.296298	2.555670	-0.703129
C	4.014131	-3.969863	-2.554300
H	3.337975	-4.622782	-3.135169
H	4.470055	-4.585551	-1.762257
H	4.817707	-3.644605	-3.233489
C	1.465091	-3.346862	-1.125598
H	0.916208	-3.891955	-1.913773
H	0.794915	-2.597540	-0.681820
H	1.736474	-4.079274	-0.345301
C	2.478018	-1.518931	-3.368370
H	1.993869	-2.192212	-4.098118
H	3.336272	-1.046177	-3.872982
H	1.764611	-0.728787	-3.103202
C	6.766079	-2.768671	-1.148100
H	6.638081	-3.106574	-2.186643
H	6.493869	-3.609232	-0.487649
H	7.840782	-2.564640	-0.995806
C	6.598881	-0.614246	0.869060
H	7.690695	-0.559333	0.711573
H	6.422315	-1.335115	1.684047
H	6.273739	0.372452	1.227952
C	6.176569	0.045667	-2.102893
H	5.812551	1.057573	-1.877758
H	5.742282	-0.260484	-3.069295
H	7.270811	0.109342	-2.236536
C	4.074357	3.978256	2.452865
H	3.950666	4.406835	3.463442
H	3.637801	4.689718	1.736988
H	5.157221	3.918940	2.251042
C	4.097300	1.397353	3.882145
H	4.152918	2.108430	4.725502
H	5.130699	1.098811	3.636424
H	3.567802	0.505186	4.239981
C	1.426512	2.506245	2.775144

H	1.257949	2.638133	3.858030
H	0.822673	1.648272	2.445939
H	1.036952	3.401140	2.266429
C	1.811850	3.708907	-0.470183
H	0.891824	3.137604	-0.275687
H	1.654136	4.276264	-1.403930
H	1.934664	4.438117	0.344135
C	4.842579	3.636503	-0.912167
H	4.887337	4.454029	-0.176804
H	4.853179	4.091291	-1.918205
H	5.771704	3.051257	-0.807392
C	2.978248	1.742558	-2.369471
H	1.982087	1.283189	-2.382421
H	3.703608	0.962175	-2.626059
H	3.021998	2.517010	-3.156103
Si	-3.590276	-3.256172	0.824281
Si	-3.449807	-0.544962	2.550941
Si	-2.747765	2.836090	-1.439110
Si	-5.524953	1.306533	-0.854847
C	-2.509285	-4.301130	-0.320082
H	-2.673355	-5.364488	-0.072331
H	-1.435663	-4.095152	-0.176378
H	-2.737358	-4.177603	-1.388303
C	-3.363431	-4.057161	2.522899
H	-3.574586	-5.136055	2.420488
H	-4.048144	-3.661799	3.288518
H	-2.334118	-3.956335	2.901701
C	-5.397748	-3.563282	0.377884
H	-5.567639	-4.653013	0.442274
H	-5.678286	-3.246880	-0.636365
H	-6.093698	-3.082708	1.082988
C	-2.457935	-1.228335	4.008818
H	-2.915749	-2.113782	4.472103
H	-2.387555	-0.446754	4.785338
H	-1.428471	-1.492349	3.721231

C	-2.976406	1.272968	2.465726
H	-3.371052	1.808765	3.346116
H	-3.360831	1.773876	1.571165
H	-1.881119	1.399950	2.478278
C	-5.280747	-0.689709	2.979729
H	-5.594361	-1.741710	3.072616
H	-5.942733	-0.206068	2.247776
H	-5.457491	-0.207023	3.956862
C	-5.902575	2.448714	0.597002
H	-5.540877	2.059010	1.558759
H	-6.995990	2.576737	0.681774
H	-5.463159	3.449105	0.454988
C	-6.262931	-0.392578	-0.542899
H	-6.250903	-0.987200	-1.470514
H	-7.315193	-0.306175	-0.221135
H	-5.725438	-0.961442	0.222404
C	-6.447648	1.951758	-2.375921
H	-7.515864	1.684486	-2.287790
H	-6.071140	1.484703	-3.302994
H	-6.389218	3.042394	-2.502957
C	-3.857217	4.131706	-2.251090
H	-4.725083	4.414143	-1.635640
H	-4.230285	3.799209	-3.232918
H	-3.259034	5.045202	-2.415172
C	-1.278958	2.672193	-2.617104
H	-0.493874	1.970947	-2.294516
H	-0.796005	3.659255	-2.715134
H	-1.603757	2.358919	-3.622637
C	-2.112649	3.620810	0.153707
H	-1.388683	3.005016	0.707602
H	-2.922987	3.887667	0.849285
H	-1.590053	4.552533	-0.124085

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[Si*i*PrDis$_2$]-Ga=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.149914	-0.428251	0.682656
Ga	-0.531814	-0.490324	0.381069
Si	-2.721794	0.256722	-0.380827
Si	2.516228	-0.412365	-0.380968
C	-3.469011	1.319125	1.015353
H	-4.536917	1.438181	0.746954
C	-3.891562	-1.079259	-1.077553
H	-3.593507	-1.026555	-2.143550
C	-1.883010	1.133293	-1.916546
H	-0.900467	1.461678	-1.529534
C	-2.532277	2.381379	-2.539387
H	-1.915052	2.731982	-3.385356
H	-2.607863	3.209728	-1.825106
H	-3.539014	2.175886	-2.928883
C	-1.579028	0.099408	-3.024503
H	-0.864545	0.523444	-3.748414
H	-2.490804	-0.167359	-3.584093
H	-1.138339	-0.834241	-2.639277
C	2.025772	-1.040516	-2.137757
H	1.313324	-0.282236	-2.504141
C	1.288031	-2.388763	-2.135664
H	0.889541	-2.627522	-3.138824
H	0.443122	-2.397508	-1.429444
H	1.952575	-3.217042	-1.841467
C	3.198691	-1.118392	-3.131123
H	2.845210	-1.357684	-4.150968
H	3.907202	-1.912385	-2.840846

H	3.767241	-0.181718	-3.186089
C	2.890836	1.498914	-0.526016
H	1.834987	1.785123	-0.315803
C	3.816615	-1.715856	0.199474
H	3.710024	-2.443489	-0.634917
Si	-3.623712	-2.963997	-0.818648
Si	-5.721659	-0.580721	-1.264872
Si	-2.835815	3.119174	1.198674
Si	-3.507667	0.414901	2.701683
C	-5.034285	-3.851916	0.071436
H	-4.823968	-4.935673	0.047609
H	-6.014792	-3.700391	-0.404180
H	-5.119239	-3.557893	1.128004
C	-3.462366	-3.706906	-2.548627
H	-3.283004	-4.794232	-2.488644
H	-2.608244	-3.261881	-3.087915
H	-4.364878	-3.549437	-3.159588
C	-2.034422	-3.468470	0.071319
H	-1.146234	-3.325845	-0.562990
H	-2.089702	-4.549445	0.291441
H	-1.846521	-2.966592	1.033055
C	-6.522695	-1.678143	-2.579287
H	-6.570069	-2.742204	-2.305034
H	-5.972107	-1.604511	-3.532915
H	-7.555124	-1.337008	-2.769249
C	-5.886153	1.172166	-1.946701
H	-6.957237	1.419717	-2.051227
H	-5.435336	1.253042	-2.949287
H	-5.431187	1.942820	-1.307129
C	-6.747175	-0.655835	0.314259
H	-6.777792	-1.661842	0.757925
H	-7.785359	-0.367213	0.072887
H	-6.384333	0.043667	1.082868
C	-2.985408	3.824062	2.947938
H	-2.589486	4.854932	2.919809

H	-2.416978	3.276504	3.713673
H	-4.033571	3.886408	3.277824
C	-3.936014	4.268070	0.169372
H	-4.301906	3.822446	-0.766273
H	-3.401049	5.198091	-0.090418
H	-4.819878	4.555997	0.765388
C	-1.012359	3.284816	0.749007
H	-0.675972	4.306134	0.995410
H	-0.792281	3.115496	-0.313805
H	-0.385514	2.589181	1.331309
C	-1.809717	0.437361	3.535966
H	-1.282138	1.399222	3.462970
H	-1.132735	-0.335907	3.131210
H	-1.929424	0.204583	4.608613
C	-4.823939	1.201007	3.814505
H	-4.414635	1.969874	4.485907
H	-5.288736	0.422175	4.442967
H	-5.629644	1.669987	3.224534
C	-3.993215	-1.397171	2.569139
H	-3.296845	-1.984999	1.958692
H	-5.000991	-1.523333	2.153677
H	-3.992088	-1.838418	3.581497
Si	3.109656	2.502382	-2.130346
Si	3.704570	2.327753	0.986413
Si	3.244815	-2.827841	1.644215
Si	5.688661	-1.427895	0.094126
C	1.759069	2.144630	-3.412976
H	1.796315	2.929916	-4.188652
H	0.756668	2.186326	-2.955837
H	1.862535	1.175181	-3.919632
C	2.846650	4.345442	-1.764922
H	2.857268	4.895019	-2.722947
H	3.628328	4.783840	-1.126681
H	1.874852	4.538440	-1.282587
C	4.767138	2.437123	-3.037919

H	4.715401	3.160240	-3.871834
H	5.011502	1.456146	-3.469276
H	5.609785	2.736644	-2.396153
C	2.761353	3.902535	1.491232
H	3.258760	4.823276	1.146314
H	2.696666	3.952110	2.592615
H	1.732843	3.915708	1.100759
C	3.615310	1.219444	2.497785
H	4.122262	1.700294	3.352820
H	4.076640	0.239739	2.337967
H	2.563980	1.040766	2.770134
C	5.503527	2.841229	0.707297
H	5.603556	3.565183	-0.117857
H	6.168544	1.993601	0.490783
H	5.880650	3.333313	1.621452
C	6.498833	-0.884314	1.713314
H	6.231651	0.143733	1.997244
H	7.596269	-0.919590	1.593942
H	6.236688	-1.542820	2.556818
C	6.125769	-0.171100	-1.239042
H	6.013851	-0.613636	-2.241616
H	7.176142	0.152405	-1.136764
H	5.494229	0.721880	-1.201454
C	6.545586	-3.019423	-0.477872
H	7.561852	-2.781478	-0.839735
H	5.998895	-3.479024	-1.320363
H	6.642565	-3.779052	0.310895
C	4.533585	-4.167513	2.027951
H	5.497097	-3.764574	2.377556
H	4.734770	-4.813187	1.157160
H	4.136944	-4.814026	2.831233
C	1.698976	-3.807950	1.170530
H	0.835358	-3.140186	1.048147
H	1.466269	-4.537578	1.966852
H	1.832020	-4.371198	0.231455

C	2.878768	-1.977656	3.284823
H	2.079645	-1.231744	3.170557
H	3.759160	-1.481090	3.721845
H	2.541943	-2.747017	4.003112

Ga=N-[Si$_i$PrDis$_2$]$_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.255296	-0.985310	-1.704259
N	-0.027887	-0.050879	-0.020938
Si	-1.684194	-0.313058	0.563109
Si	1.617283	0.345461	0.562959
C	-2.649032	-1.334144	-0.796482
H	-3.614815	-1.407748	-0.251507
C	-2.813175	1.166769	1.174765
H	-2.432104	1.198183	2.214613
C	-1.434928	-1.375107	2.189763
H	-0.385988	-1.669595	2.027691
C	-2.227614	-2.685287	2.436719
H	-2.965334	-2.556315	3.240522
H	-1.552359	-3.497509	2.752899
H	-2.779678	-3.044505	1.562519
C	-1.463387	-0.568218	3.508552
H	-1.045745	-1.174189	4.331389
H	-2.495781	-0.310734	3.792865
H	-0.889587	0.366173	3.470937
C	1.488663	1.021635	2.342294
H	0.951969	0.199164	2.836066

C	0.608175	2.269573	2.456931
H	0.426616	2.525122	3.515666
H	-0.362348	2.120147	1.977407
H	1.075502	3.149923	1.988867
C	2.784688	1.247641	3.135651
H	2.557086	1.352410	4.211819
H	3.286823	2.173390	2.823735
H	3.506636	0.432461	3.027249
C	2.557205	-1.384748	0.635783
H	1.687437	-2.041118	0.423190
C	2.350935	1.793962	-0.514944
H	1.768990	2.586662	0.004294
Si	-2.640654	3.056728	0.836127
Si	-4.645973	0.776233	1.613915
Si	-2.303836	-3.216997	-1.088193
Si	-3.316544	-0.520692	-2.412866
C	-4.110511	3.958638	0.053636
H	-3.845967	5.031839	0.033791
H	-5.038898	3.866721	0.636757
H	-4.319518	3.656026	-0.981894
C	-2.443042	3.918066	2.520878
H	-1.930418	4.885589	2.381769
H	-1.856519	3.336459	3.246991
H	-3.419618	4.130033	2.982084
C	-1.155704	3.540632	-0.222554
H	-0.731733	4.483881	0.159900
H	-1.446044	3.712314	-1.268724
H	-0.364269	2.784739	-0.213642
C	-5.180029	1.906199	3.040649
H	-5.348197	2.950337	2.736956
H	-4.443673	1.911299	3.861101
H	-6.132546	1.528758	3.452395
C	-5.003026	-0.955053	2.280890
H	-6.087849	-0.994997	2.485468
H	-4.488511	-1.158434	3.229682

H	-4.772472	-1.773150	1.584229
C	-5.946728	0.979562	0.258935
H	-5.982355	1.978130	-0.196755
H	-6.928269	0.800847	0.733772
H	-5.841650	0.239009	-0.546203
C	-1.993668	-3.729973	-2.884259
H	-1.778047	-4.813443	-2.867477
H	-1.128586	-3.230388	-3.343939
H	-2.868269	-3.581503	-3.535221
C	-3.869003	-4.177847	-0.622069
H	-4.214863	-4.004654	0.408461
H	-3.689162	-5.261243	-0.735650
H	-4.697544	-3.909480	-1.297975
C	-0.810696	-3.926579	-0.142893
H	-1.140607	-4.607854	0.656596
H	-0.174907	-3.163575	0.329087
H	-0.176907	-4.506714	-0.833654
C	-2.309234	-0.703850	-4.011231
H	-1.216718	-0.678356	-3.883390
H	-2.577653	0.142846	-4.666206
H	-2.549826	-1.630937	-4.549879
C	-4.993387	-1.310918	-2.804408
H	-4.881016	-2.340018	-3.182544
H	-5.503725	-0.728421	-3.591263
H	-5.665428	-1.351617	-1.932579
C	-3.570085	1.331195	-2.242237
H	-2.633170	1.855435	-2.014909
H	-4.297492	1.585363	-1.468171
H	-3.946746	1.726098	-3.202412
Si	3.059764	-2.249791	2.289056
Si	3.775309	-2.000662	-0.728132
Si	1.867548	2.367544	-2.294834
Si	4.126527	2.432624	-0.108832
C	1.812200	-2.142695	3.705059
H	2.175536	-2.821864	4.497269

H	0.812440	-2.494444	3.412392
H	1.712190	-1.145427	4.152530
C	3.120375	-4.116371	1.953415
H	3.194673	-4.636198	2.924947
H	3.984150	-4.432770	1.349850
H	2.207063	-4.478110	1.453522
C	4.739765	-1.784729	3.047397
H	5.263926	-2.714986	3.327531
H	4.610922	-1.196164	3.969476
H	5.409304	-1.223525	2.384785
C	3.122741	-3.621325	-1.458651
H	3.232997	-4.479743	-0.779783
H	3.681518	-3.852294	-2.382774
H	2.057020	-3.542639	-1.731912
C	3.938280	-0.830073	-2.182810
H	4.648859	-1.259935	-2.910556
H	4.309099	0.161280	-1.898402
H	2.979305	-0.696867	-2.703486
C	5.555257	-2.321056	-0.171004
H	5.650881	-3.061100	0.636364
H	6.073084	-1.403768	0.146122
H	6.102470	-2.715598	-1.046018
C	5.256888	2.830986	-1.579107
H	5.590890	1.932560	-2.120846
H	6.161534	3.296654	-1.147159
H	4.841978	3.538761	-2.309811
C	5.180826	1.242772	0.919596
H	5.356926	1.628803	1.934473
H	6.165357	1.107654	0.441513
H	4.722553	0.253391	1.021043
C	3.959634	4.077396	0.815597
H	4.951221	4.421744	1.158155
H	3.306686	4.011133	1.699818
H	3.545929	4.859946	0.159298
C	1.939902	4.263078	-2.245386

H	2.960104	4.661094	-2.134823
H	1.329825	4.668482	-1.422233
H	1.531964	4.664189	-3.189657
C	0.101210	1.961448	-2.865050
H	-0.560510	1.620501	-2.062846
H	0.108350	1.200174	-3.660370
H	-0.351308	2.869987	-3.297586
C	2.900219	1.826736	-3.785714
H	2.593679	0.834298	-4.148678
H	3.986747	1.811872	-3.644431
H	2.680033	2.547485	-4.594475

Tbt_2-Ga≡N-Tbt_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.942153	1.309574	-0.128880
C	-3.706814	-1.424227	-0.267061
C	-4.121005	0.846203	0.485136
C	-2.129837	0.346339	-0.798508
C	-2.526114	-1.018875	-0.923641
C	-4.495126	-0.513243	0.468754
H	-4.763175	1.552014	1.013685
H	-4.010856	-2.469528	-0.319192
C	-2.567198	2.784821	-0.115598
H	-1.463970	2.872425	-0.234889
C	-5.728742	-0.955098	1.223063
H	-6.154332	-0.049197	1.700568
C	-1.710853	-2.007517	-1.744931

H	-0.763948	-1.502794	-2.045475
Si	-1.086131	-3.559192	-0.812423
Si	-2.533365	-2.314220	-3.441999
Si	-7.116231	-1.512498	0.040837
Si	-5.289998	-2.043494	2.727120
Si	-3.267983	3.631639	-1.688404
Si	-2.867543	3.740443	1.512469
C	-4.247022	-3.071315	-3.273041
H	-4.225305	-4.050846	-2.772486
H	-4.688476	-3.216869	-4.274095
H	-4.922373	-2.415201	-2.705345
C	-2.694361	-0.650045	-4.304449
H	-3.364004	0.017551	-3.739879
H	-3.108726	-0.766696	-5.320196
H	-1.718157	-0.146506	-4.397985
C	-1.457880	-3.449056	-4.496134
H	-0.415616	-3.096146	-4.549797
H	-1.852083	-3.480677	-5.526724
H	-1.443222	-4.483565	-4.117029
C	0.517751	-4.182868	-1.579680
H	0.409884	-4.487274	-2.630838
H	0.869295	-5.060971	-1.010634
H	1.314805	-3.426326	-1.529734
C	-2.329607	-4.978082	-0.821413
H	-1.952444	-5.797139	-0.184416
H	-2.470647	-5.390161	-1.833957
H	-3.318193	-4.690304	-0.433079
C	-0.696471	-3.032926	0.941367
H	-1.582565	-2.654532	1.472386
H	0.055330	-2.226918	0.935277
H	-0.275115	-3.867498	1.525264
C	-7.014087	-0.429821	-1.498974
H	-6.035455	-0.521413	-1.994759
H	-7.149295	0.632956	-1.237346
H	-7.795398	-0.700091	-2.229397

C	-6.981985	-3.331134	-0.436955
H	-7.674576	-3.563279	-1.264178
H	-7.244808	-3.985334	0.410651
H	-5.969563	-3.603482	-0.770671
C	-8.781861	-1.213949	0.873488
H	-9.605339	-1.339153	0.149255
H	-8.846525	-0.187471	1.273823
H	-8.962037	-1.909273	1.708668
C	-6.837956	-2.276536	3.779763
H	-7.349696	-1.318178	3.970474
H	-6.578100	-2.716255	4.758135
H	-7.563537	-2.951664	3.297117
C	-4.599326	-3.737235	2.274646
H	-4.375564	-4.297789	3.199329
H	-3.659538	-3.656916	1.709562
H	-5.303793	-4.340522	1.682412
C	-3.976506	-1.127966	3.720692
H	-3.697434	-1.691285	4.627896
H	-4.326785	-0.132343	4.040845
H	-3.062629	-0.981021	3.122642
C	-3.073919	5.505688	-1.628182
H	-3.392982	5.931081	-2.595719
H	-2.022749	5.796401	-1.470625
H	-3.677020	5.982212	-0.840293
C	-2.286520	3.036588	-3.180830
H	-1.232353	3.353367	-3.109316
H	-2.693126	3.464612	-4.113437
H	-2.311824	1.942388	-3.281674
C	-5.078644	3.162666	-1.885832
H	-5.187502	2.077611	-2.036291
H	-5.521911	3.673795	-2.757336
H	-5.671166	3.434706	-0.997704
C	-1.800871	5.303763	1.511837
H	-1.382478	5.476592	2.517357
H	-2.386007	6.194914	1.235936

H	-0.950598	5.238103	0.816811
C	-2.350428	2.649976	2.951082
H	-2.987985	1.759360	3.050879
H	-2.394480	3.207735	3.902058
H	-1.315115	2.301827	2.818305
C	-4.665193	4.279711	1.736815
H	-5.373333	3.436995	1.775735
H	-4.990495	4.952393	0.926473
H	-4.763948	4.837056	2.684941
C	3.399252	0.570726	-0.901374
C	3.569183	-0.429119	1.724945
C	2.330766	0.814159	0.022089
C	4.429791	-0.308613	-0.519150
C	4.514599	-0.859449	0.775291
C	2.482009	0.399933	1.399310
H	5.196713	-0.555907	-1.257604
H	3.686867	-0.772520	2.754307
C	3.492591	1.237169	-2.273382
H	4.553588	1.084085	-2.563767
C	1.541567	0.919424	2.484618
H	0.544503	1.073546	2.029008
C	5.601946	-1.841976	1.164488
H	5.535116	-1.988593	2.261853
Si	7.343233	-1.118932	0.914628
Si	5.209110	-3.569273	0.472009
Si	1.270755	-0.148886	4.046231
Si	2.146501	2.690355	2.940604
Si	3.468315	3.148458	-2.265571
Si	2.648322	0.405708	-3.766409
C	3.548698	-4.120861	1.181901
H	3.572940	-4.163940	2.283926
H	3.273218	-5.124252	0.812781
H	2.745999	-3.423626	0.894143
C	6.540525	-4.803157	0.994278
H	6.708858	-4.781196	2.084302

H	7.505425	-4.593913	0.503331
H	6.246019	-5.831805	0.722480
C	5.060177	-3.585087	-1.406354
H	4.877474	-4.613994	-1.763235
H	5.966016	-3.209241	-1.906356
H	4.212119	-2.963555	-1.730482
C	8.026063	-1.419968	-0.820886
H	8.151916	-2.495635	-1.027578
H	9.014810	-0.941434	-0.930084
H	7.369813	-1.002541	-1.601629
C	8.511495	-1.906411	2.171410
H	8.668026	-2.980019	1.979649
H	8.109366	-1.805428	3.194516
H	9.498981	-1.413525	2.152933
C	7.263232	0.736173	1.235571
H	6.835247	0.944137	2.230564
H	6.622390	1.240719	0.495899
H	8.266623	1.193569	1.193094
C	-0.326506	0.366063	4.915695
H	-1.196129	0.256986	4.249298
H	-0.321012	1.398363	5.292028
H	-0.492627	-0.302606	5.778997
C	1.050596	-1.985448	3.689234
H	1.118452	-2.547734	4.637447
H	1.796921	-2.395923	2.994976
H	0.053810	-2.176951	3.268343
C	2.682852	-0.003957	5.298483
H	2.829886	1.023644	5.663799
H	3.646113	-0.350918	4.892239
H	2.449253	-0.635037	6.174388
C	1.699473	3.905189	1.577475
H	2.301136	3.750052	0.675850
H	1.846769	4.944141	1.920649
H	0.646822	3.782935	1.287756
C	1.346055	3.398263	4.504727

H	1.546474	2.818983	5.418200
H	0.253984	3.495717	4.397604
H	1.749435	4.414545	4.663206
C	4.014923	2.669993	3.177969
H	4.526679	2.345016	2.260068
H	4.320154	1.985164	3.984050
H	4.381358	3.678956	3.435312
C	4.588062	3.690599	-0.848490
H	4.328309	3.180487	0.089760
H	4.535584	4.778431	-0.673764
H	5.637036	3.435950	-1.079310
C	4.276621	3.726356	-3.879292
H	3.645981	3.526837	-4.761534
H	5.255122	3.246799	-4.050041
H	4.443516	4.817285	-3.840758
C	1.802536	4.032222	-2.193588
H	1.246629	3.793061	-1.279042
H	1.176763	3.756516	-3.056579
H	1.969211	5.123666	-2.239830
C	3.944749	0.265271	-5.136858
H	4.265213	1.255278	-5.499512
H	3.552119	-0.296276	-6.002481
H	4.844619	-0.263031	-4.776696
C	1.172324	1.315217	-4.524246
H	1.450768	2.310579	-4.905703
H	0.336123	1.458876	-3.820594
H	0.785896	0.731346	-5.378581
C	2.093009	-1.338003	-3.326560
H	2.955961	-1.981155	-3.095924
H	1.543647	-1.800004	-4.164544
H	1.437259	-1.348357	-2.441715
Ga	-0.260398	0.783714	-1.091619
N	1.164166	1.447782	-0.388224

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Tbt_2-Ga=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.641803	1.277356	0.165416
C	3.305259	-1.455086	0.193366
C	3.910717	0.839356	-0.272277
C	1.664307	0.314938	0.578661
C	2.059133	-1.051805	0.719582
C	4.234723	-0.528184	-0.339794
H	4.660998	1.566045	-0.584775
H	3.583255	-2.506455	0.242716
C	2.282220	2.764810	0.272078
H	0.425204	3.785375	0.214198
C	5.558447	-0.958731	-0.952391
H	6.185280	-0.047477	-1.034433
C	1.264321	-1.994110	1.622704
H	0.389900	-1.427522	1.988706
Si	0.473174	-3.553009	0.854496
Si	2.310365	-2.326354	3.198849
Si	6.621352	-2.107400	0.129048
Si	5.299529	-1.464096	-2.777533
Si	3.155492	3.449298	1.874511
Si	2.760995	3.801061	-1.279574
C	3.548355	-3.727813	2.938452
H	3.059714	-4.669519	2.643447
H	4.090767	-3.916953	3.881429
H	4.300316	-3.487646	2.175871
C	3.247763	-0.768871	3.702343
H	3.667993	-0.229212	2.842200

H	4.076976	-1.024748	4.383960
H	2.585138	-0.075355	4.241314
C	1.230093	-2.797841	4.674051
H	0.447789	-2.048604	4.864876
H	1.865724	-2.848265	5.575898
H	0.741429	-3.774774	4.556455
C	-1.182024	-3.065368	0.108205
H	-1.951694	-3.036217	0.892106
H	-1.506917	-3.811529	-0.631797
H	-1.177310	-2.080101	-0.373584
C	0.041184	-4.877347	2.134371
H	-0.474599	-5.701617	1.609892
H	-0.652157	-4.496696	2.900629
H	0.913883	-5.309990	2.646247
C	1.588665	-4.366955	-0.422909
H	2.528254	-4.724348	0.029235
H	1.848359	-3.689754	-1.246889
H	1.075092	-5.242801	-0.856061
C	6.508990	-1.525827	1.916040
H	5.481455	-1.552635	2.299048
H	6.864010	-0.484005	1.999140
H	7.136696	-2.149333	2.575845
C	6.129499	-3.925187	-0.026253
H	6.707679	-4.543833	0.681787
H	6.337908	-4.302719	-1.040846
H	5.063176	-4.104836	0.176156
C	8.429638	-1.940821	-0.392257
H	9.082607	-2.436420	0.347437
H	8.732878	-0.880354	-0.438627
H	8.637871	-2.393489	-1.373483
C	6.806301	-2.325403	-3.522499
H	7.709998	-1.696954	-3.462843
H	6.614906	-2.526177	-4.591512
H	7.032552	-3.290736	-3.042502
C	3.807778	-2.590282	-2.970158

H	3.670634	-2.864513	-4.030349
H	2.886768	-2.096533	-2.627667
H	3.924580	-3.521906	-2.394652
C	5.024515	0.121837	-3.756353
H	4.769797	-0.085657	-4.809456
H	5.927617	0.756172	-3.745056
H	4.202778	0.709372	-3.322604
C	3.100264	5.337198	1.945114
H	3.428533	5.658960	2.949301
H	2.077103	5.719222	1.796932
H	3.759124	5.827768	1.212057
C	2.219923	2.840114	3.378194
H	1.249790	3.350366	3.466890
H	2.799978	3.034623	4.296470
H	2.033826	1.762371	3.316476
C	4.956381	2.900283	2.021698
H	5.031640	1.806607	2.119339
H	5.404432	3.352138	2.924383
H	5.569584	3.201889	1.158830
C	1.912287	5.494563	-1.257341
H	1.953205	5.912936	-2.278547
H	2.418732	6.205965	-0.589149
H	0.849919	5.470407	-0.969378
C	2.189872	2.887538	-2.809916
H	2.795747	1.989510	-2.983548
H	2.262016	3.523439	-3.707839
H	1.147592	2.564496	-2.704600
C	4.607787	4.167056	-1.460042
H	5.215719	3.262616	-1.614742
H	5.017990	4.709413	-0.594145
H	4.750508	4.810851	-2.346284
C	-2.999763	0.390559	1.002555
C	-3.233327	-0.376704	-1.695358
C	-1.914768	0.673908	0.110577
C	-4.127635	-0.311952	0.522860

C	-4.270185	-0.724047	-0.814740
C	-2.082786	0.327222	-1.277844
H	-4.936097	-0.523239	1.223650
H	-3.347079	-0.625265	-2.751041
C	-3.142147	0.918112	2.432873
H	-4.157209	0.589272	2.741056
C	-1.130230	0.808166	-2.375067
H	-0.165167	1.119350	-1.925293
C	-5.505351	-1.455473	-1.307828
H	-5.441869	-1.495317	-2.414290
Si	-7.129424	-0.506262	-1.001536
Si	-5.442308	-3.294680	-0.795460
Si	-0.614479	-0.458348	-3.723391
Si	-1.876369	2.435618	-3.100838
Si	-3.414733	2.811180	2.490021
Si	-2.165036	0.077136	3.828174
C	-4.134379	-4.097854	-1.889525
H	-4.514080	-4.212503	-2.919679
H	-3.843839	-5.097554	-1.525036
H	-3.228272	-3.476509	-1.934085
C	-7.075217	-4.189315	-1.104831
H	-7.411992	-4.088870	-2.149418
H	-7.884480	-3.826828	-0.450781
H	-6.944064	-5.266638	-0.900790
C	-5.016643	-3.485509	1.027854
H	-4.941609	-4.554521	1.291480
H	-5.791486	-3.035468	1.670411
H	-4.059432	-3.006144	1.274281
C	-7.743662	-0.646101	0.779385
H	-7.867406	-1.694662	1.096227
H	-8.726709	-0.152844	0.876059
H	-7.060279	-0.156123	1.491434
C	-8.467816	-1.165800	-2.160728
H	-8.877163	-2.135093	-1.837897
H	-8.081515	-1.288819	-3.187553

H	-9.306462	-0.449121	-2.208944
C	-6.866191	1.309199	-1.423174
H	-6.638574	1.433634	-2.494899
H	-6.033351	1.743914	-0.852015
H	-7.774620	1.896563	-1.202915
C	1.023133	0.071303	-4.488090
H	1.819347	0.070208	-3.729259
H	1.002346	1.066301	-4.952953
H	1.310549	-0.659227	-5.264037
C	-0.310247	-2.163785	-3.002935
H	0.147030	-2.812409	-3.769567
H	-1.235036	-2.645855	-2.660633
H	0.381657	-2.114728	-2.149907
C	-1.890502	-0.640499	-5.108265
H	-2.137725	0.314741	-5.595714
H	-2.833311	-1.092569	-4.760790
H	-1.478542	-1.308445	-5.885278
C	-1.674397	3.823090	-1.841698
H	-2.315758	4.680687	-2.107891
H	-0.633655	4.175734	-1.820543
H	-1.946036	3.501756	-0.826178
C	-1.049679	3.017722	-4.697342
H	-1.152950	2.298627	-5.524030
H	0.020173	3.234228	-4.569170
H	-1.540814	3.955063	-5.013853
C	-3.710614	2.232071	-3.464749
H	-4.284528	2.040750	-2.548377
H	-3.916285	1.409528	-4.166975
H	-4.094295	3.163248	-3.917500
C	-4.330647	3.306556	0.919767
H	-3.839203	2.931822	0.011832
H	-4.417026	4.403801	0.839242
H	-5.352375	2.891771	0.938608
C	-4.561150	3.228588	3.933723
H	-4.064237	3.148637	4.912918

H	-5.446995	2.570182	3.952446
H	-4.924281	4.266524	3.830255
C	-1.846359	3.831325	2.704836
H	-2.078023	4.902645	2.569975
H	-1.042903	3.572537	1.999068
H	-1.438474	3.711695	3.722739
C	-3.000601	0.475572	5.473903
H	-2.818141	1.513643	5.793940
H	-2.598990	-0.186218	6.260955
H	-4.092085	0.323191	5.434383
C	-0.383399	0.644059	3.974928
H	-0.327128	1.737427	4.063151
H	0.253673	0.347529	3.127885
H	0.081450	0.221075	4.880642
C	-2.263505	-1.782006	3.567891
H	-3.310320	-2.101372	3.435971
H	-1.847299	-2.331348	4.427274
H	-1.709364	-2.089262	2.672152
N	0.802293	2.873258	0.455610
Ga	-0.062488	1.248266	0.548355

Ga=N-Tbt_2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

C	-2.267556	1.152321	0.528531
C	-2.877571	-1.250785	-0.822693
C	-3.531652	0.526857	0.630242
C	-1.200385	0.452160	-0.155611

C	-1.591109	-0.678312	-0.984892
C	-3.865346	-0.691015	0.013778
H	-4.311004	1.043761	1.190898
H	-3.134808	-2.114274	-1.435047
C	-2.181769	2.578865	1.079406
H	-1.128641	2.907518	1.067716
C	-5.262973	-1.264612	0.207466
H	-5.832442	-0.489972	0.761034
C	-0.782653	-1.121102	-2.206891
H	0.168027	-0.559088	-2.217386
Si	-0.180169	-2.936584	-2.296181
Si	-1.700759	-0.640854	-3.841533
Si	-6.336734	-1.509643	-1.352604
Si	-5.296025	-2.724565	1.438697
Si	-3.185097	3.878988	0.041125
Si	-2.733559	2.805489	2.918814
C	-2.886752	-1.985515	-4.444312
H	-2.368433	-2.908237	-4.746797
H	-3.426016	-1.606405	-5.330205
H	-3.644958	-2.256197	-3.695847
C	-2.701212	0.949295	-3.657432
H	-3.195754	1.041829	-2.680585
H	-3.478384	0.992670	-4.439981
H	-2.048749	1.825682	-3.798968
C	-0.476812	-0.292608	-5.237784
H	0.169189	0.565481	-4.995968
H	-1.044913	-0.028416	-6.147661
H	0.171411	-1.142857	-5.487805
C	1.218904	-3.166128	-1.087263
H	2.094540	-2.577523	-1.393064
H	1.515447	-4.225590	-1.051423
H	0.962221	-2.836678	-0.076847
C	0.568074	-3.351739	-3.984640
H	1.006789	-4.363120	-3.909287
H	1.386030	-2.665035	-4.254721

H	-0.154424	-3.371735	-4.814301
C	-1.524232	-4.216549	-1.963294
H	-2.403713	-4.105841	-2.614928
H	-1.866578	-4.193108	-0.920118
H	-1.104955	-5.221291	-2.148612
C	-5.961159	-0.184920	-2.632384
H	-4.973063	-0.323729	-3.087608
H	-5.989040	0.824250	-2.190412
H	-6.713813	-0.219231	-3.439280
C	-6.114640	-3.206405	-2.149922
H	-6.600754	-3.225678	-3.140651
H	-6.574028	-4.002790	-1.541994
H	-5.055086	-3.468083	-2.294207
C	-8.154691	-1.309707	-0.871696
H	-8.770702	-1.203895	-1.781835
H	-8.312557	-0.403697	-0.261552
H	-8.547701	-2.166352	-0.304563
C	-7.071467	-3.228676	1.843383
H	-7.702615	-2.361708	2.099526
H	-7.065901	-3.903796	2.717201
H	-7.559632	-3.769168	1.016743
C	-4.377455	-4.238762	0.810787
H	-4.326511	-5.000719	1.608155
H	-3.346735	-3.989084	0.527884
H	-4.868508	-4.698812	-0.059401
C	-4.493184	-2.117669	3.024436
H	-4.457105	-2.910278	3.790340
H	-5.049517	-1.265061	3.449784
H	-3.464095	-1.785150	2.833563
C	-3.116884	5.571388	0.888564
H	-3.521308	6.320824	0.185847
H	-2.080770	5.867635	1.119950
H	-3.701983	5.642938	1.815618
C	-2.586613	4.269406	-1.705607
H	-1.577389	4.707401	-1.737232

H	-3.282177	5.031240	-2.104704
H	-2.622016	3.413308	-2.392232
C	-4.980840	3.357343	-0.220915
H	-5.032513	2.470453	-0.871158
H	-5.508664	4.178477	-0.737710
H	-5.535409	3.132816	0.699056
C	-1.799965	4.271666	3.673510
H	-1.589153	4.074503	4.738439
H	-2.391524	5.198090	3.624479
H	-0.838102	4.463704	3.175418
C	-2.414394	1.250733	3.913192
H	-3.058020	0.430234	3.566061
H	-2.644800	1.435437	4.976359
H	-1.375815	0.915763	3.847099
C	-4.577741	3.140225	3.202921
H	-5.220461	2.315854	2.855135
H	-4.947708	4.072883	2.753386
H	-4.727037	3.223146	4.294679
C	2.604864	0.811530	-0.471482
C	2.650913	-1.293367	1.363943
C	1.346503	0.431923	0.159161
C	3.745210	-0.002755	-0.281488
C	3.807384	-1.095004	0.596081
C	1.466448	-0.528475	1.246396
H	4.652319	0.280103	-0.819475
H	2.700496	-2.020742	2.171286
C	2.957612	2.116849	-1.242005
H	4.062609	2.103584	-1.117364
C	0.522922	-0.598422	2.458724
H	-0.418408	-0.075463	2.224967
C	5.084555	-1.896574	0.837534
H	4.981281	-2.365897	1.837034
Si	6.692261	-0.877966	1.007536
Si	5.231301	-3.398334	-0.334822
Si	-0.027040	-2.316374	3.113943

Si	1.395984	0.448366	3.844871
Si	2.891721	3.784300	-0.291941
Si	3.127172	2.093813	-3.176721
C	3.996183	-4.700728	0.246296
H	4.411920	-5.247625	1.110348
H	3.779954	-5.440550	-0.543294
H	3.044685	-4.249092	0.557101
C	6.923206	-4.241500	-0.257669
H	7.182013	-4.541491	0.770867
H	7.744839	-3.620432	-0.646973
H	6.889004	-5.161663	-0.867941
C	4.941985	-2.877267	-2.122942
H	4.965288	-3.757026	-2.789158
H	5.729455	-2.183928	-2.461783
H	3.974592	-2.373969	-2.259834
C	7.476156	-0.440754	-0.657980
H	7.762242	-1.336609	-1.231699
H	8.393024	0.152290	-0.492984
H	6.806996	0.161187	-1.293739
C	7.950936	-1.861793	2.021373
H	8.463027	-2.639156	1.436140
H	7.474022	-2.352775	2.887067
H	8.723307	-1.178706	2.415836
C	6.382701	0.725516	1.942809
H	6.072949	0.524438	2.980611
H	5.597796	1.331682	1.471251
H	7.307970	1.326991	1.979205
C	-1.249001	-2.158137	4.553310
H	-1.926061	-1.298623	4.481894
H	-0.732510	-2.095192	5.521822
H	-1.873368	-3.067128	4.574486
C	-0.892568	-3.327370	1.778381
H	-1.627195	-4.000670	2.248326
H	-0.190087	-3.953354	1.210883
H	-1.427272	-2.683520	1.064907

C	1.383003	-3.367045	3.822005
H	2.007678	-2.806118	4.536296
H	2.043173	-3.792439	3.050465
H	0.940285	-4.214412	4.375401
C	1.172494	2.280504	3.454462
H	2.042482	2.861797	3.801066
H	0.288628	2.675715	3.971720
H	1.050568	2.459953	2.377108
C	0.757885	0.185392	5.610571
H	1.045610	-0.798060	6.015176
H	-0.329140	0.293877	5.723133
H	1.236909	0.949637	6.249430
C	3.245419	0.104614	3.978107
H	3.788664	0.415435	3.077348
H	3.475249	-0.957178	4.156560
H	3.640639	0.677803	4.836683
C	3.778464	3.514020	1.347679
H	3.447486	2.599403	1.856625
H	3.611673	4.365141	2.029357
H	4.865202	3.431701	1.181483
C	3.932442	5.048667	-1.240617
H	3.532559	5.307570	-2.233366
H	4.970072	4.701207	-1.372592
H	3.975311	5.980826	-0.649817
C	1.234716	4.621463	0.052171
H	1.436930	5.543758	0.626584
H	0.555232	4.002249	0.655212
H	0.707538	4.923698	-0.867285
C	4.933102	2.511556	-3.564481
H	5.166743	3.572774	-3.386930
H	5.134495	2.305845	-4.630463
H	5.638063	1.904928	-2.971140
C	2.109446	3.338581	-4.184360
H	1.964622	4.288178	-3.644002
H	1.110606	2.965412	-4.455099

H	2.651372	3.568123	-5.119621
C	2.837474	0.335103	-3.775465
H	3.638635	-0.324306	-3.406922
H	2.840423	0.293838	-4.877680
H	1.883361	-0.080315	-3.422438
Ga	0.002393	2.289864	-1.799293
N	0.129308	1.045943	-0.271312

Ar*-Ga≡N-Ar*

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.969776	2.975071	-0.023550
C	4.476986	1.293829	-1.668538
C	2.354735	2.366760	-1.157590
C	4.338550	2.766621	0.220511
C	5.123154	1.958169	-0.612749
C	3.115441	1.483956	-1.975796
H	4.803680	3.274773	1.066558
H	5.060571	0.621002	-2.305355
C	2.212277	3.930870	0.897631
H	1.144153	3.860840	0.658188
C	2.632340	5.392516	0.639650
H	2.043266	6.081953	1.267776
H	3.699463	5.545264	0.871219
H	2.471672	5.663819	-0.415378
C	2.374303	3.555459	2.383410
H	3.421010	3.644778	2.715878
H	2.051895	2.519949	2.571250

H	1.769145	4.226306	3.014101
C	2.616888	0.774745	-3.239767
H	3.309540	-0.074561	-3.376877
C	2.782414	1.691207	-4.474120
H	3.806058	2.094975	-4.533986
H	2.079872	2.538518	-4.429075
H	2.575234	1.128527	-5.400159
C	1.201450	0.181381	-3.191011
H	1.047717	-0.438731	-2.294969
H	1.041607	-0.462224	-4.071330
H	0.431452	0.962576	-3.214218
C	6.638288	1.881241	-0.479566
H	6.947284	0.882432	-0.824498
C	7.283069	2.915637	-1.432511
H	6.992701	3.939132	-1.140828
H	6.952670	2.755465	-2.470828
H	8.383737	2.846371	-1.400176
C	7.158931	2.077403	0.954220
H	7.009585	3.114356	1.298229
H	8.241118	1.872791	0.996898
H	6.652460	1.408353	1.666617
C	-5.060847	2.042633	1.292556
C	-2.653601	2.443191	-0.185187
C	-4.905249	1.527196	-0.003147
C	-3.958494	2.694678	1.867467
C	-2.762534	2.906320	1.160752
C	-3.728352	1.707477	-0.758181
H	-5.723840	0.974474	-0.465550
H	-4.051317	3.081533	2.886276
C	-6.394255	2.024940	2.033014
H	-6.168653	2.098658	3.112279
C	-7.237763	0.758494	1.812052
H	-6.692569	-0.151228	2.104591
H	-7.536983	0.654441	0.757166
H	-8.162486	0.810156	2.409642

C	-7.200850	3.284015	1.635882
H	-6.619850	4.200875	1.823489
H	-8.144773	3.343802	2.203681
H	-7.446831	3.255485	0.560914
C	-3.759973	1.115940	-2.169793
H	-4.444029	0.256598	-2.090848
C	-2.440752	0.553140	-2.711931
H	-1.955808	-0.107518	-1.979061
H	-1.738593	1.346545	-2.996638
H	-2.647334	-0.048524	-3.611058
C	-4.390738	2.106987	-3.173375
H	-5.357478	2.485870	-2.804778
H	-4.560311	1.611191	-4.144207
H	-3.728287	2.969361	-3.347508
C	-1.651875	3.710615	1.834670
H	-0.748840	3.620360	1.218581
C	-2.018031	5.208599	1.879829
H	-2.223913	5.589972	0.867294
H	-1.192054	5.798625	2.311817
H	-2.917416	5.376308	2.495313
C	-1.303277	3.173140	3.235738
H	-1.007571	2.113521	3.195954
H	-2.155097	3.254715	3.929670
H	-0.468235	3.746898	3.666734
C	-1.459997	2.883555	-0.985978
C	0.791940	3.923083	-2.348515
C	-0.184975	2.273036	-0.847056
C	-1.587579	4.001655	-1.834999
C	-0.475395	4.499104	-2.533887
C	0.959091	2.818917	-1.487753
H	-2.561812	4.486328	-1.931725
H	-0.589010	5.362892	-3.195518
H	1.669486	4.348715	-2.841136
C	3.167700	-2.850373	-0.006291
C	4.691434	-1.227493	1.678774

C	2.566546	-2.303349	1.163552
C	4.524274	-2.605760	-0.276778
C	5.317919	-1.816832	0.568666
C	3.337728	-1.458768	2.004855
H	4.974365	-3.072755	-1.154387
H	5.284107	-0.590933	2.345837
C	2.402930	-3.801415	-0.923386
H	1.338510	-3.716596	-0.679082
C	2.815258	-5.262161	-0.645991
H	2.225670	-5.958539	-1.265856
H	3.883374	-5.419772	-0.872235
H	2.649583	-5.517970	0.411833
C	2.562441	-3.451901	-2.413450
H	3.602938	-3.571456	-2.757151
H	2.254968	-2.415202	-2.609023
H	1.936834	-4.119640	-3.027743
C	2.866660	-0.848427	3.330241
H	3.499244	0.045832	3.477333
C	3.176375	-1.813960	4.498999
H	4.230458	-2.134076	4.473615
H	2.543616	-2.712695	4.435423
H	2.981918	-1.327416	5.470333
C	1.407096	-0.375598	3.406619
H	1.140217	0.239234	2.529482
H	1.258336	0.243344	4.307143
H	0.703913	-1.216349	3.452574
C	6.826295	-1.693231	0.383634
H	7.122390	-0.693813	0.741008
C	7.541066	-2.729073	1.282623
H	7.261702	-3.752580	0.981090
H	7.253847	-2.599979	2.337887
H	8.637663	-2.632053	1.203478
C	7.299381	-1.840631	-1.073030
H	7.181648	-2.876855	-1.430273
H	8.369078	-1.587090	-1.155434

H	6.735021	-1.186183	-1.755319
C	-4.885461	-2.353006	-1.302631
C	-2.436545	-2.504318	0.161478
C	-4.797435	-1.896762	0.020485
C	-3.700655	-2.797829	-1.912773
C	-2.482497	-2.874914	-1.216586
C	-3.598151	-1.948854	0.763213
H	-5.688074	-1.499896	0.513007
H	-3.742094	-3.121989	-2.955800
C	-6.215819	-2.471585	-2.038918
H	-5.981980	-2.650659	-3.103777
C	-7.098541	-1.212984	-1.958074
H	-6.580762	-0.328108	-2.358914
H	-7.390612	-0.996961	-0.918325
H	-8.026733	-1.356617	-2.535992
C	-6.985148	-3.705498	-1.514617
H	-6.365108	-4.613294	-1.584769
H	-7.913427	-3.868135	-2.088784
H	-7.257042	-3.565666	-0.454866
C	-3.688560	-1.404374	2.193909
H	-4.495142	-0.654216	2.150265
C	-2.449742	-0.657969	2.709339
H	-2.122487	0.096784	1.976793
H	-1.612821	-1.337094	2.913085
H	-2.694900	-0.125024	3.642779
C	-4.143671	-2.485414	3.199860
H	-5.028286	-3.024428	2.823375
H	-4.405510	-2.024347	4.167912
H	-3.345267	-3.219873	3.381125
C	-1.250436	-3.438435	-1.923260
H	-0.374577	-2.999094	-1.433089
C	-1.177993	-4.970436	-1.753927
H	-1.173392	-5.250949	-0.690646
H	-0.261188	-5.368640	-2.219685
H	-2.044677	-5.454668	-2.235556

C	-1.156234	-3.052672	-3.410399
H	-1.225022	-1.964411	-3.547578
H	-1.945339	-3.527428	-4.016395
H	-0.188955	-3.384584	-3.818630
C	-1.229397	-2.890868	0.966761
C	1.033910	-3.902126	2.321720
C	0.031517	-2.216056	0.841696
C	-1.328116	-4.025957	1.791023
C	-0.217954	-4.517142	2.498019
C	1.181881	-2.778930	1.491574
H	-2.288476	-4.543628	1.854823
H	-0.316045	-5.398079	3.138214
H	1.922494	-4.321239	2.801729
Ga	-0.029227	0.582741	0.119367
N	0.148692	-1.110682	0.042645

Ar*$_2$-Ga=N

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	-0.302833	-0.808995	-0.073509
N	-1.790045	-2.035424	0.038368
H	2.863963	-0.679112	-4.229975
C	1.949722	-0.262122	-3.804395
C	-0.343390	0.819684	-2.642318
C	1.688693	-0.503453	-2.433880
C	1.087391	0.487874	-4.604700
C	-0.026418	1.067283	-3.997010
C	0.456047	-0.063806	-1.838279

H	1.300804	0.648953	-5.665113
H	-0.678860	1.730653	-4.566919
C	2.860339	-1.199067	-1.778582
C	5.261944	-2.583732	-1.095020
C	2.876630	-2.614873	-1.680974
C	4.077564	-0.475813	-1.578328
C	5.244643	-1.189364	-1.245029
C	4.062160	-3.277700	-1.312861
H	6.177514	-0.640404	-1.092655
H	4.059204	-4.367514	-1.248898
C	-1.534491	1.622257	-2.183667
C	-3.844886	3.227109	-1.707030
C	-2.839758	1.081981	-2.362016
C	-1.390001	3.007082	-1.865237
C	-2.552051	3.759315	-1.595572
C	-3.964081	1.891906	-2.120301
H	-2.427348	4.811899	-1.325543
H	-4.963767	1.471582	-2.254243
C	1.691371	-3.442118	-2.160914
H	0.797771	-2.797811	-2.177481
C	1.395334	-4.638837	-1.254360
H	2.238675	-5.345645	-1.213868
H	0.526240	-5.190047	-1.635669
H	1.177207	-4.310953	-0.228017
C	1.945002	-3.911511	-3.611626
H	2.139572	-3.059460	-4.280060
H	1.072878	-4.464305	-3.998954
H	2.821487	-4.580188	-3.648572
C	4.194265	1.036443	-1.786848
H	3.182019	1.455149	-1.742608
C	5.034554	1.734691	-0.702123
H	6.100581	1.461656	-0.774026
H	4.678943	1.489617	0.303113
H	4.971820	2.826818	-0.828635
C	4.799488	1.377619	-3.168339

H	4.183684	1.006988	-3.997482
H	5.805934	0.936514	-3.265080
H	4.896891	2.471123	-3.278706
C	6.557198	-3.318627	-0.773686
H	7.316088	-2.552070	-0.535394
C	6.418929	-4.241849	0.452859
H	5.696737	-5.052755	0.262286
H	6.070433	-3.681762	1.334345
H	7.387163	-4.709730	0.697629
C	7.057677	-4.105853	-2.004458
H	7.190174	-3.438913	-2.871470
H	6.334228	-4.887785	-2.289373
H	8.022265	-4.597175	-1.791227
C	-3.037033	-0.306415	-2.964913
H	-2.114875	-0.883364	-2.802789
C	-3.255037	-0.174250	-4.490547
H	-4.167619	0.410947	-4.695108
H	-3.374367	-1.168860	-4.952194
H	-2.411626	0.332975	-4.981034
C	-4.193331	-1.091023	-2.330445
H	-4.092712	-1.138277	-1.240029
H	-4.192034	-2.123779	-2.711969
H	-5.170614	-0.647790	-2.583796
C	-5.087526	4.078836	-1.472743
H	-5.942715	3.384092	-1.395975
C	-5.343308	5.004686	-2.682633
H	-5.411782	4.423314	-3.615832
H	-4.520103	5.730028	-2.796613
H	-6.281331	5.571025	-2.552684
C	-5.024827	4.893629	-0.166515
H	-4.225022	5.650896	-0.202754
H	-4.836381	4.244474	0.701769
H	-5.975524	5.427149	-0.000235
C	-0.104212	3.846845	-1.953742
H	-0.267467	4.689016	-1.260252

C	0.013848	4.494759	-3.356149
H	0.825788	5.242195	-3.359573
H	-0.922679	4.999327	-3.641171
H	0.247705	3.742926	-4.123874
C	1.228477	3.199104	-1.558063
H	1.990943	3.985758	-1.436659
H	1.579035	2.512576	-2.336603
H	1.164700	2.646943	-0.611278
H	1.100760	0.384036	4.946365
C	0.450295	-0.142029	4.243928
C	-1.250301	-1.381729	2.440034
C	0.579184	0.146108	2.864034
C	-0.521745	-1.029230	4.723653
C	-1.419790	-1.606100	3.815288
C	-0.227345	-0.541332	1.923134
H	-0.607389	-1.227313	5.795870
H	-2.263001	-2.204528	4.167766
C	1.512426	1.259162	2.518967
C	3.287399	3.436443	2.162024
C	0.988718	2.557935	2.245887
C	2.907852	1.060531	2.654107
C	3.771399	2.157046	2.471051
C	1.894655	3.616325	2.062777
H	4.850615	2.013217	2.578621
H	1.506655	4.613514	1.852981
C	-2.287698	-1.846570	1.455536
C	-4.785171	-3.130091	0.717183
C	-2.281280	-3.243219	0.901182
C	-3.612899	-1.152423	1.635894
C	-4.758607	-1.770462	1.234768
C	-3.613038	-3.810355	0.558373
H	-5.709517	-1.241556	1.341187
H	-3.657849	-4.860668	0.258595
C	-0.523161	2.821849	2.251396
H	-1.004939	1.997091	1.703673

C	-0.940570	4.136224	1.574395
H	-0.658476	5.009837	2.185736
H	-2.033378	4.158116	1.449484
H	-0.489769	4.251427	0.583807
C	-1.084590	2.823535	3.692415
H	-0.951656	1.857549	4.192757
H	-2.162371	3.056582	3.676946
H	-0.575999	3.596585	4.292768
C	3.477298	-0.296447	3.064797
H	2.632526	-0.992210	3.167283
C	4.416602	-0.894924	2.007327
H	5.299344	-0.259289	1.832495
H	3.903031	-1.021183	1.046057
H	4.777575	-1.883937	2.333681
C	4.166586	-0.203659	4.441208
H	3.487901	0.219586	5.198621
H	5.059970	0.440846	4.396400
H	4.486217	-1.202896	4.781658
C	4.248583	4.608960	2.014916
H	5.264408	4.184661	1.924975
C	3.979566	5.454443	0.755543
H	2.992450	5.942501	0.801589
H	4.004275	4.834305	-0.153346
H	4.737583	6.249163	0.655208
C	4.214594	5.485347	3.286170
H	4.961644	6.295165	3.230303
H	4.420031	4.880356	4.183818
H	3.220057	5.945326	3.411827
C	-1.279820	-4.302513	1.407363
H	-0.292097	-3.818445	1.466949
C	-1.209174	-5.518767	0.460639
H	-2.051231	-6.205052	0.646737
H	-0.285741	-6.090867	0.638116
H	-1.242236	-5.221798	-0.594853
C	-1.642735	-4.841389	2.813172

H	-1.574412	-4.077885	3.596817
H	-0.951319	-5.659586	3.082588
H	-2.664550	-5.257813	2.822380
C	-6.128718	-3.773049	0.391938
H	-5.935852	-4.839512	0.178586
C	-6.744132	-3.142575	-0.875427
H	-6.068896	-3.254652	-1.735957
H	-6.926086	-2.065105	-0.730852
H	-7.708439	-3.619843	-1.119563
C	-7.127443	-3.704800	1.568258
H	-6.710271	-4.158456	2.481821
H	-8.056612	-4.240470	1.308658
H	-7.405617	-2.664534	1.803827
C	-3.643879	0.248905	2.237356
H	-2.640324	0.477755	2.615875
C	-4.609090	0.357327	3.431354
H	-4.361720	-0.389177	4.202616
H	-5.654351	0.192521	3.123214
H	-4.544247	1.359901	3.886138
C	-3.954877	1.290892	1.151125
H	-3.925274	2.308969	1.570054
H	-4.951214	1.127482	0.710617
H	-3.225828	1.239860	0.332629

Ga=N-Ar*$_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.932266	-2.513298	0.698902

C	4.552155	-0.461036	1.690948
C	2.331888	-1.385493	1.341759
C	4.329157	-2.549681	0.534937
C	5.161334	-1.530650	1.023143
C	3.160942	-0.376025	1.886114
H	4.779806	-3.424562	0.061869
H	5.182836	0.324297	2.116740
C	2.141848	-3.795923	0.394158
H	1.067831	-3.556671	0.418392
C	2.399767	-4.836054	1.510329
H	1.774462	-5.731375	1.355677
H	3.456988	-5.149659	1.501636
H	2.177046	-4.426612	2.504599
C	2.452790	-4.447267	-0.966636
H	3.505422	-4.764206	-1.036775
H	2.251004	-3.771600	-1.810348
H	1.828445	-5.346124	-1.099675
C	2.703199	0.715747	2.854623
H	3.367645	1.570664	2.646794
C	2.992399	0.272200	4.309905
H	4.039756	-0.044760	4.432608
H	2.345306	-0.571760	4.595914
H	2.794525	1.101059	5.011074
C	1.258674	1.217267	2.741976
H	0.978992	1.411357	1.699841
H	1.152372	2.153533	3.309370
H	0.540027	0.503005	3.158984
C	6.680858	-1.631443	0.977752
H	7.074906	-0.610876	1.114284
C	7.184972	-2.483430	2.165092
H	6.810825	-3.517852	2.083755
H	6.829233	-2.072641	3.123445
H	8.287794	-2.518083	2.186579
C	7.229433	-2.176498	-0.352064
H	6.955044	-3.234137	-0.497689

H	8.330458	-2.118745	-0.365003
H	6.840318	-1.607162	-1.208651
C	-5.388250	-2.145471	-0.664073
C	-2.809210	-1.726980	0.493949
C	-5.202383	-1.272408	0.414793
C	-4.268698	-2.860798	-1.116055
C	-2.996170	-2.688118	-0.545955
C	-3.949775	-1.074374	1.033635
H	-6.062264	-0.735729	0.820794
H	-4.406438	-3.600764	-1.908677
C	-6.767013	-2.415619	-1.255312
H	-6.613703	-2.993643	-2.184208
C	-7.531960	-1.130850	-1.622792
H	-6.954844	-0.505491	-2.321695
H	-7.749478	-0.527433	-0.727152
H	-8.496657	-1.377874	-2.096305
C	-7.596665	-3.292143	-0.290667
H	-7.062869	-4.225428	-0.049697
H	-8.573167	-3.552411	-0.733615
H	-7.782525	-2.758070	0.656045
C	-4.023365	-0.243767	2.324983
H	-4.641312	0.625348	2.055396
C	-2.743707	0.322563	2.957640
H	-2.041232	0.698648	2.208743
H	-2.221387	-0.417332	3.576885
H	-3.029091	1.164516	3.607658
C	-4.805479	-1.035639	3.403600
H	-5.790136	-1.367126	3.041167
H	-4.959257	-0.408026	4.297887
H	-4.243872	-1.930982	3.716183
C	-1.907831	-3.694831	-0.918564
H	-0.935023	-3.277507	-0.606837
C	-2.107701	-4.994740	-0.103601
H	-2.114476	-4.792672	0.977142
H	-1.302017	-5.717170	-0.318691

H	-3.070745	-5.463019	-0.370253
C	-1.832037	-4.028024	-2.419364
H	-1.773511	-3.121887	-3.040600
H	-2.709816	-4.607698	-2.747100
H	-0.938736	-4.640298	-2.624221
C	-1.501695	-1.713800	1.243372
C	0.702814	-2.238943	2.899332
C	-0.241061	-1.097983	0.898827
C	-1.605500	-2.524261	2.399341
C	-0.541468	-2.745772	3.270275
C	0.879688	-1.503795	1.709873
H	-2.576828	-2.975388	2.606143
H	-0.665564	-3.346289	4.175190
H	1.589026	-2.465617	3.494391
C	3.137932	2.420734	-0.239295
C	5.012792	0.792036	-1.522216
C	2.669798	1.386298	-1.117499
C	4.514563	2.536641	0.032390
C	5.473788	1.719399	-0.581508
C	3.649702	0.637386	-1.832158
H	4.845960	3.332925	0.700413
H	5.748086	0.205887	-2.079478
C	2.246256	3.587271	0.203974
H	1.202736	3.254004	0.190012
C	2.386155	4.741698	-0.821033
H	1.710883	5.572386	-0.557786
H	3.420491	5.124959	-0.815750
H	2.147467	4.419071	-1.841433
C	2.557199	4.167417	1.596797
H	3.520586	4.702478	1.602794
H	2.590949	3.402923	2.379388
H	1.783758	4.901644	1.871657
C	3.331342	-0.194619	-3.070365
H	2.234928	-0.264019	-3.159334
C	3.906242	-1.619864	-3.005803

H	3.696934	-2.088479	-2.036568
H	4.999787	-1.612190	-3.137073
H	3.479675	-2.247222	-3.805792
C	3.816802	0.518540	-4.352205
H	3.397866	1.532043	-4.439911
H	3.518260	-0.055562	-5.245621
H	4.915491	0.608340	-4.355833
C	6.974798	1.912620	-0.393701
H	7.448321	0.929130	-0.559380
C	7.515094	2.872251	-1.479099
H	7.064436	3.872400	-1.364241
H	7.266731	2.506392	-2.487893
H	8.611068	2.977093	-1.404881
C	7.380155	2.402616	1.006291
H	7.035149	3.433487	1.187854
H	8.477943	2.402868	1.106853
H	6.963678	1.763011	1.799515
C	-5.054182	2.658032	0.648734
C	-2.508169	1.832007	-0.352486
C	-4.944648	1.816021	-0.466073
C	-3.863963	3.093886	1.250829
C	-2.601365	2.714363	0.767422
C	-3.703290	1.413314	-0.999733
H	-5.852625	1.472429	-0.967114
H	-3.927163	3.780115	2.099042
C	-6.404545	3.155445	1.150362
H	-6.216377	3.712240	2.085630
C	-7.379734	2.008227	1.476408
H	-6.948274	1.313302	2.213652
H	-7.629615	1.431092	0.571741
H	-8.323012	2.405671	1.886876
C	-7.030994	4.138819	0.137940
H	-6.341623	4.969890	-0.080935
H	-7.972888	4.560088	0.528842
H	-7.256053	3.628941	-0.813667

C	-3.813466	0.621101	-2.312171
H	-4.608649	-0.116441	-2.118707
C	-2.597668	-0.181926	-2.794765
H	-2.129173	-0.715280	-1.959660
H	-1.844959	0.453689	-3.280496
H	-2.932450	-0.933705	-3.528280
C	-4.317318	1.532323	-3.458392
H	-5.227612	2.083100	-3.175831
H	-4.544537	0.927451	-4.352757
H	-3.548755	2.269092	-3.739882
C	-1.368493	3.427404	1.323284
H	-0.491619	2.823768	1.060018
C	-1.226580	4.802356	0.631153
H	-1.141757	4.698612	-0.459165
H	-0.332574	5.330501	0.999133
H	-2.107244	5.429032	0.849152
C	-1.355263	3.621000	2.849870
H	-1.430966	2.667290	3.386047
H	-2.177003	4.272586	3.188144
H	-0.412732	4.106097	3.149536
C	-1.185432	1.773087	-1.077756
C	1.076693	2.316786	-2.655721
C	0.003074	0.977954	-0.838878
C	-1.200387	2.725673	-2.123002
C	-0.127477	2.930285	-2.990528
C	1.205989	1.452253	-1.542324
H	-2.126286	3.284104	-2.269775
H	-0.205387	3.612063	-3.841075
H	1.985009	2.570109	-3.204384
Ga	0.496780	-1.551550	-1.875464
N	0.045733	-0.374011	-0.325673

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M062X/ Def2-TZVP

F-Ga≡N-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.356919	-0.016013	-0.000118
N	-1.315858	0.638496	0.000214
F	-2.293358	-0.364011	0.000089
F	2.087417	-0.077443	0.000152

F2-Ga=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.001715	-0.053403	0.000001
N	0.071277	-1.935250	-0.000002
F	1.454796	0.898226	-0.000001
F	-1.516142	0.790912	-0.000001

Ga=N-F2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.961357	-0.000166	0.017899
N	-0.997544	0.000071	-0.653944
F	-1.268310	-1.096602	0.223517
F	-1.267163	1.097118	0.223455

F-Ga≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.000000	-0.241824	0.000000
N	1.695850	0.370662	-0.000000
F	0.203923	1.580902	-0.000000
F	-1.522917	-1.036246	0.000000

F-Ga≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Ga	-0.902394	-0.202554	0.000002
N	0.877578	-0.419094	-0.000019
F	0.259993	1.343567	-0.000001
F	2.165693	-0.319920	0.000009

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HO-Ga≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.381877	0.188669	0.024240
N	1.259639	-0.521902	0.213046
O	2.424900	0.019424	-0.252404
H	2.941395	0.241002	0.534395
O	-2.117800	-0.198497	-0.033195
H	-2.377494	-1.003857	-0.492369

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(OH)2-Ga≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.219669	-0.253701	-0.008293

N	-1.510682	-0.678516	0.023543
O	1.881078	0.330721	-0.019148
H	2.008217	1.261347	0.186805
O	-1.430719	0.937954	0.098341
H	-1.846044	1.203588	-0.728059

Ga≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.124427	0.000000	0.000000
N	0.792107	0.000000	-0.000000
O	1.587478	-1.138331	-0.109446
H	1.956415	-1.291475	0.771744
O	1.587478	1.138331	0.109446
H	1.956415	1.291475	-0.771744

HO-Ga≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z

Ga	-0.296879	-0.229958	0.029269
N	1.431946	-0.659335	-0.108735
O	-1.922497	0.454148	0.057523
H	-2.239987	0.900394	-0.732702
O	1.810351	0.792526	-0.076536
H	2.316786	0.870263	0.738608

HO-Ga≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.758924	-0.439325	-0.008754
N	-1.434068	0.129139	0.577140
O	-2.222004	-0.092319	-0.360631
H	-3.139219	0.195166	-0.133647
O	0.891874	1.402820	-0.127452
H	0.292099	2.035923	0.269720

H-Ga≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.316923	-0.022794	-0.000005

N	1.371301	0.150235	0.000002
H	2.058992	-0.590537	0.000049
H	-1.833499	0.245517	0.000094

H2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.002564	-0.291483	0.000000
N	0.002564	1.567486	0.000000
H	-1.460090	-0.869606	0.000000
H	1.362665	-1.066819	0.000000

Ga≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.000000	0.451095	0.000000
N	-0.000000	-1.423971	0.000000
H	0.825695	-2.008074	-0.000000
H	-0.825686	-2.008089	0.000000

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H-Ga≡N-H-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.291601	0.003161	-0.000247
N	-1.541625	-0.087872	0.000294
H	0.340296	1.593341	0.002334
H	1.411451	-1.076232	0.003265

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H-Ga≡N-H-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.386689	-0.040131	-0.000222
N	1.364660	-0.005363	0.003533
H	2.354916	-0.233901	-0.015378
H	0.079831	1.515486	-0.002468

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3HC-Ga≡N-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.377367	-0.075848	-0.002518
N	1.255788	0.320341	-0.004049
C	-2.318127	0.081556	0.005563
H	-2.591470	1.135572	-0.012849
H	-2.731903	-0.374106	0.902793
H	-2.743468	-0.407505	-0.868210
C	2.632090	-0.052026	0.004883
H	2.924090	-0.580555	0.919053
H	3.256097	0.846284	-0.054164
H	2.910738	-0.687965	-0.842907

(CH3)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.151642	1.923939	-0.000431
Ga	-0.008184	0.061142	0.000311
C	-1.832709	-0.718976	0.000538
H	-1.997024	-1.260746	-0.931159
H	-2.596497	0.049310	0.097193
H	-1.934668	-1.424913	0.824518
C	1.748075	-0.872226	-0.001179
H	2.572735	-0.172826	-0.118742
H	1.780346	-1.597684	-0.813788
H	1.875138	-1.408888	0.939193

Ga≡N-(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.927101	2.092001	0.000463
C	1.563708	1.201846	0.000000
H	2.211931	1.259942	-0.884762
H	2.212943	1.259650	0.884035
N	0.762602	-0.000024	0.000092
Ga	-1.122864	-0.000030	-0.000004
C	1.563925	-1.201741	-0.000018
H	2.211556	-1.260403	0.885143
H	0.927467	-2.092000	-0.001633
H	2.213766	-1.258738	-0.883658

3HC-Ga≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.688303	1.775688	-0.004077
Ga	0.046145	0.066782	0.003147
C	-1.604143	-1.068295	-0.002540

H	-1.607480	-1.692983	-0.895830
H	-2.503923	-0.464543	0.015521
H	-1.589176	-1.721068	0.870503
C	1.956446	-0.435284	-0.000360
H	2.559859	0.310306	0.513783
H	2.307566	-0.507121	-1.030445
H	2.106954	-1.403164	0.474838

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3HC-Ga≡N-CH3-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.798519	-0.458663	-0.000576
N	-0.967056	-0.211016	0.015642
C	0.500194	1.708909	0.001179
H	1.458312	2.055304	0.377294
H	-0.316820	2.048672	0.622872
H	0.362949	1.963239	-1.043892
C	-2.367250	-0.096935	-0.009557
H	-2.855615	-0.637436	0.810904
H	-2.828766	-0.374204	-0.964607
H	-2.602417	0.968243	0.156062

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3HSi-Ga≡N-SiH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.399804	-0.005365	-0.002158
N	1.281097	-0.014822	0.008162
Si	-2.779921	0.006845	0.001295
Si	2.964643	0.007131	-0.000575
H	-3.250410	-1.279017	0.545347
H	-3.246177	0.184127	-1.385863
H	-3.233040	1.125749	0.846832
H	3.517733	0.088612	-1.377141
H	3.541123	-1.212755	0.621099
H	3.510897	1.167688	0.749392

(SiH3)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.020482	2.191833	0.000243
Ga	0.001008	0.375502	-0.000149
Si	-2.152999	-0.752852	0.000065
H	-3.296822	0.178586	0.001975
H	-2.207773	-1.611223	1.202893
H	-2.209818	-1.608843	-1.204302
Si	2.159165	-0.742842	0.000080
H	2.222160	-1.599040	-1.203853
H	3.296659	0.196705	0.000704
H	2.221387	-1.599872	1.203456

Ga≡N-(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.205406	-2.577605	0.122499
Si	1.241238	-1.517171	0.000414
H	2.185234	-1.654091	1.133250
H	1.997600	-1.760297	-1.249362
N	0.430161	-0.000048	0.000403
Ga	-1.503914	0.001411	-0.000023
Si	1.245614	1.514741	-0.000486
H	2.197134	1.643899	-1.127964
H	0.213933	2.578075	-0.132578
H	1.994959	1.760622	1.253054

3HSi-Ga≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.014844	-0.333520	-0.003150
N	0.183835	-2.139722	0.004577
Si	-2.226363	0.663937	0.001506

H	-2.419738	1.385984	1.277225
H	-3.266423	-0.374427	-0.141066
H	-2.335974	1.628013	-1.112519
Si	2.180646	0.744267	0.001052
H	2.188057	1.770609	1.067981
H	2.371955	1.408674	-1.305503
H	3.275498	-0.216537	0.243692

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3HSi-Ga≡N-SiH3-TS2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Ga	0.701974	-0.974637	0.003938
N	-0.817065	-0.120632	-0.003726
Si	1.565970	1.337900	-0.000425
H	1.330768	1.783710	-1.384275
H	3.016695	1.364710	0.298998
H	0.863404	2.146165	1.007267
Si	-2.450111	0.380559	0.001369
H	-3.247069	-0.293914	-1.056944
H	-2.477234	1.844245	-0.268521
H	-3.150327	0.154845	1.294274

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F-Ga≡N-F

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Atomic Number		Coordinates (Angstroms) X	Y	Z
Ga	0	0.359380	-0.037757	-0.000062
N	0	-1.304386	0.630879	0.000154
F	0	-2.317048	-0.326890	0.000031
F	0	2.093707	-0.033740	0.000063

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F2-Ga=N

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Atomic Number		Coordinates (Angstroms) X	Y	Z
Ga	0	-0.000948	-0.057235	-0.000005
N	0	-0.036455	-1.926174	0.000008
F	0	1.501486	0.820177	0.000006
F	0	-1.469869	0.875102	0.000006

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Ga=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	1.142032	0.000106	0.000224
N	-0.814685	0.000144	-0.002122
F	-1.649507	-1.101626	0.000440
F	-1.650515	1.101150	0.000439

F-Ga≡N-F-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.105738	0.139888	0.000063
N	1.467468	1.056253	-0.000102
F	1.037879	-1.233924	-0.000038
F	-1.815034	-0.069444	-0.000098

F-Ga≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.901940	-0.225006	-0.000024

N	0.885417	-0.368348	0.000238
F	0.224427	1.408659	0.000008
F	2.193597	-0.347146	-0.000110

HO-Ga≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.385122	0.213708	0.009455
N	1.250283	-0.523541	0.202631
O	2.427554	-0.012649	-0.226976
H	2.921634	0.229391	0.569849
O	-2.106651	-0.256322	0.006896
H	-2.302044	-1.037791	-0.520734

(OH)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.240479	-0.268121	0.000061
N	-1.489643	-0.670032	0.000194
O	1.878525	0.387561	-0.028973
H	1.911193	1.336053	0.151426

O	-1.513425	0.925186	0.105153
H	-1.859339	1.163937	-0.764094

Ga≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.123954	0.000000	0.000000
N	0.792823	0.000000	-0.000000
O	1.587063	-1.145088	-0.109947
H	1.949905	-1.299418	0.775111
O	1.587063	1.145087	0.109947
H	1.949907	1.299418	-0.775110

HO-Ga≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.059604	-0.122477	0.003623
N	1.360588	-1.281277	-0.008816
O	0.908013	1.409208	-0.038792

O	-1.824658	-0.078275	-0.006206
H	1.822891	1.300044	0.238654
H	-2.166113	0.818212	0.070718

HO-Ga≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.808695	-0.369225	-0.036579
N	-1.167720	-0.165044	0.509009
O	-2.148246	-0.178593	-0.312838
H	-2.982463	-0.000418	0.175313
O	0.453646	1.517945	0.028996
H	-0.356243	1.886873	-0.333687

H-Ga≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.314897	-0.022312	0.000006
N	1.369920	0.156096	-0.000003
H	1.993695	-0.640899	-0.000049
H	-1.821322	0.239894	-0.000100

H2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.386447	-1.004291	-0.000000
Ga	0.000326	-0.279472	-0.000000
H	1.374074	-1.027437	-0.000000
N	0.000326	1.527910	0.000000

Ga≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.000000	0.451095	0.000000
N	-0.000000	-1.423971	0.000000
H	0.825695	-2.008074	-0.000000
H	-0.825686	-2.008089	0.000000

H-Ga≡N-H-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.281755	-0.000558	-0.000989
N	-1.533424	-0.026492	0.001256
H	0.823846	1.471715	0.010203
H	1.175714	-1.268980	0.011662

H-Ga≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.386689	-0.040131	-0.000222
N	1.364660	-0.005363	0.003533
H	2.354916	-0.233901	-0.015378
H	0.079831	1.515486	-0.002468

GaC-Ga≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Ga	-0.371011	-0.080435	0.000223
N	1.245579	0.374154	0.000356
C	-2.298376	0.080656	-0.000413
H	-2.570921	1.135722	-0.049567
H	-2.709170	-0.353375	0.910556
H	-2.715169	-0.437271	-0.863518
C	2.596028	-0.070808	-0.000425
H	2.864073	-0.667973	0.882054
H	3.263396	0.802432	0.001488
H	2.864171	-0.664233	-0.885395

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(CH3)2-Ga≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.026278	1.917325	0.000453
Ga	0.000801	0.102985	-0.000302
C	-1.727410	-0.873691	0.000732
H	-1.792470	-1.456916	-0.919223
H	-2.572947	-0.192160	0.062764
H	-1.737954	-1.553903	0.853730
C	1.743850	-0.844697	-0.000171
H	2.577660	-0.149190	-0.066758
H	1.765182	-1.528714	-0.849911
H	1.821003	-1.422596	0.922209

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Ga≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.927101	2.092001	0.000463
C	1.563708	1.201846	0.000000
H	2.211931	1.259942	-0.884762
H	2.212943	1.259650	0.884035
N	0.762602	-0.000024	0.000092
Ga	-1.122864	-0.000030	-0.000004
C	1.563925	-1.201741	-0.000018
H	2.211556	-1.260403	0.885143
H	0.927467	-2.092000	-0.001633
H	2.213766	-1.258738	-0.883658

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GaC-Ga≡N-CH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.505085	1.844261	0.000703
Ga	0.023015	0.096361	-0.000697
C	-1.603306	-1.079722	0.000682
H	-1.589312	-1.678052	-0.921061
H	-2.535543	-0.507827	0.057150

H	-1.531488	-1.757339	0.862654
C	1.892439	-0.561730	-0.000678
H	2.612593	0.257174	-0.111074
H	2.041089	-1.280502	-0.818423
H	2.090001	-1.081757	0.947420

GaC-Ga≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.794074	-0.459335	-0.007095
N	-0.963336	-0.200989	0.082363
C	0.497328	1.711906	0.000332
H	1.376405	2.002573	0.570627
H	-0.412425	2.096795	0.441683
H	0.589622	1.963032	-1.052304
C	-2.353207	-0.082670	-0.042022
H	-2.832065	-0.998204	0.342332
H	-2.733491	0.112719	-1.054386
H	-2.725720	0.693986	0.645593

GaSi-Ga≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Ga	0.397734	-0.012714	0.011429
N	-1.268263	-0.157267	-0.011540
Si	2.755198	0.029545	-0.010077
H	3.193153	1.284984	-0.664859
H	3.243217	-1.145832	-0.769889
H	3.244734	-0.019643	1.387798
Si	-2.943593	0.045875	-0.005183
H	-3.571774	-0.560373	-1.216176
H	-3.350149	1.483192	0.020628
H	-3.573553	-0.603215	1.182629

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(SiH3)2-Ga≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.024837	2.170560	0.000581
Ga	0.001246	0.392208	-0.000368
Si	-2.118596	-0.765768	0.000175
H	-3.260153	0.178287	0.009340
H	-2.163660	-1.628356	1.208786
H	-2.172052	-1.615059	-1.217441
Si	2.126059	-0.753481	0.000138
H	2.181158	-1.615327	-1.208501
H	3.259964	0.199940	-0.006991
H	2.185498	-1.602364	1.217776

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Ga≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.214947	-2.566267	0.293103
Si	1.249886	-1.520228	0.007363
H	2.273262	-1.570973	1.088021
H	1.909269	-1.904004	-1.268888
N	0.448956	0.001876	-0.077221
Ga	-1.479404	-0.019708	0.004279
Si	1.191271	1.554737	0.006458
H	2.092388	1.841587	-1.142902
H	0.084686	2.561287	-0.015728
H	1.968075	1.753042	1.260822

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GaSi-Ga≡N-SiH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.022581	-0.456349	0.004160
N	0.292870	-2.198873	-0.007461
Si	-2.108702	0.748028	-0.001518
H	-2.072262	1.791088	1.054938
H	-3.248079	-0.170062	0.239313

H	-2.257390	1.400654	-1.327623
Si	2.035822	0.893283	-0.001873
H	2.058454	1.647490	1.277150
H	1.939362	1.835487	-1.145692
H	3.250157	0.055929	-0.127329

GaSi-Ga≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.709655	-0.973032	0.000446
N	-0.810839	-0.118709	-0.004163
Si	1.547058	1.344473	0.000027
H	0.978308	2.089207	-1.142428
H	3.025823	1.286917	-0.148061
H	1.219066	1.946292	1.310571
Si	-2.451826	0.370280	0.002693
H	-3.239533	-0.320541	-1.058871
H	-2.478245	1.835681	-0.279324
H	-3.162107	0.150856	1.295368

B3LYP/LANL2DZ+dp

F-Ga≡N-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.372605	-0.107485	0.000022
N	-1.252484	0.618811	0.000071
F	-2.376031	-0.218403	-0.000060
F	2.066769	0.107333	-0.000069

F2-Ga=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.000007	-0.036678	0.000001
N	0.001937	-1.905882	-0.000002
F	1.484560	0.805725	-0.000001
F	-1.486090	0.802962	-0.000001

Ga=N-F2

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Ga	1.145421	-0.000012	0.000212
N	-0.810236	-0.000018	-0.002053
F	-1.657636	-1.114073	0.000433
F	-1.657520	1.114129	0.000433

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F-Ga≡N-F-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.306760	0.207218	0.000015
N	-1.409283	0.694582	-0.000037
F	-1.821262	-0.781022	0.000004
F	1.860752	-0.472960	-0.000026

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F-Ga≡N-F-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.888793	0.265595	-0.000027
N	-0.904298	0.269861	0.000299
F	-2.225493	0.369042	-0.000132

F	-0.132561	-1.493762	-0.000007

HO-Ga≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.394164	0.227742	0.009387
N	1.227735	-0.517457	0.169148
O	2.450717	-0.027750	-0.209014
H	2.927576	0.164431	0.617954
O	-2.074033	-0.276979	-0.012914
H	-2.316093	-1.164407	-0.317575

(OH)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.195353	-0.205641	-0.004544
N	-1.481965	-0.780670	0.008008
O	1.876208	0.227136	-0.016587
H	2.116163	1.157642	0.099223
O	-1.375317	0.956952	0.105527
H	-1.805487	1.209218	-0.725931

Ga≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.124254	0.000000	0.000000
N	0.784222	0.000000	0.000000
O	1.591334	-1.159173	-0.110853
H	1.950488	-1.314310	0.782143
O	1.591334	1.159173	0.110853
H	1.950487	1.314310	-0.782143

HO-Ga≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.289177	-0.253350	0.014195
N	1.436771	-0.675644	-0.069682
O	-1.885374	0.453155	0.053805
H	-2.054848	1.214715	-0.519418
O	1.734880	0.845776	-0.080105

H	2.165880	0.977200	0.777546

HO-Ga≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.760812	-0.399138	-0.017320
N	-1.174552	0.004227	0.550107
O	-2.111087	-0.193077	-0.335309
H	-2.960533	0.133342	0.036229
O	0.562844	1.469343	-0.137043
H	-0.016822	2.000219	0.428738

H-Ga≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.314498	-0.026186	-0.000094
N	1.352654	0.150088	-0.000003
H	2.102754	-0.538026	0.001136
H	-1.821880	0.299185	0.001799

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H2-Ga≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.411405	-0.978658	-0.000000
Ga	0.000003	-0.285272	-0.000000
H	-1.411508	-0.978447	0.000000
N	0.000003	1.542932	0.000000

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Ga≡N-H2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.000001	0.449190	-0.000000
N	-0.000001	-1.414091	0.000000
H	0.827992	-2.013097	0.000000
H	-0.827944	-2.013164	0.000000

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H-Ga≡N-H-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.285185	0.000669	0.000038
N	-1.532717	-0.059391	-0.000047
H	0.573436	1.567893	-0.000367
H	1.314860	-1.172908	-0.000474

H-Ga≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
3H	-0.384654	-0.039533	0.000188
N	1.351495	-0.013198	-0.002823
H	2.355198	-0.217968	0.012212
H	0.108608	1.535885	0.001713

3HC-Ga≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.374983	-0.109705	0.000301

N	1.235945	0.325067	0.001071
C	-2.311215	0.144192	-0.000746
H	-2.532973	1.218621	-0.048866
H	-2.756159	-0.268493	0.913102
H	-2.766609	-0.350288	-0.867569
C	2.630281	-0.012459	-0.000841
H	2.941940	-0.592791	0.885984
H	3.231372	0.914733	0.001971
H	2.940876	-0.586798	-0.891929

(CH3)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.013472	1.916297	0.000085
Ga	0.000574	0.087949	-0.000068
C	-1.762178	-0.840449	0.000625
H	-1.864051	-1.416906	-0.929553
H	-2.599814	-0.138572	0.077366
H	-1.800841	-1.539714	0.847482
C	1.770071	-0.826324	-0.000593
H	2.601292	-0.118719	-0.093547
H	1.808516	-1.537543	-0.837391
H	1.884052	-1.388391	0.936959

Ga≡N-(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.920313	2.108853	0.001044
C	1.560831	1.212194	-0.000003
H	2.213779	1.274033	-0.890769
H	2.215160	1.272977	0.889802
N	0.751851	-0.000000	-0.000015
Ga	-1.119079	-0.000000	-0.000000
C	1.560832	-1.212194	-0.000002
H	2.214340	-1.273535	0.890383
H	0.920312	-2.108852	-0.000130
H	2.214602	-1.273474	-0.890189

3HC-Ga≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.505085	1.844261	0.000703
Ga	0.023015	0.096361	-0.000697
C	-1.603306	-1.079722	0.000682
H	-1.589312	-1.678052	-0.921061
H	-2.535543	-0.507827	0.057150
H	-1.531488	-1.757339	0.862654
C	1.892439	-0.561730	-0.000678

H	2.612593	0.257174	-0.111074
H	2.041089	-1.280502	-0.818423
H	2.090001	-1.081757	0.947420

3HC-Ga≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.772590	-0.483004	-0.003632
N	-0.957118	-0.155072	0.045711
C	0.575326	1.722725	-0.000280
H	1.206061	1.991903	0.852301
H	-0.413232	2.170878	0.076070
H	1.053211	1.954071	-0.956909
C	-2.369323	-0.040993	-0.018248
H	-2.795843	-1.056673	0.095141
H	-2.746833	0.356376	-0.977991
H	-2.789829	0.551689	0.815188

3HSi-Ga≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z

Ga	-0.395232	-0.002973	-0.001888
N	1.265852	0.049531	0.002682
Si	-2.781646	-0.002399	0.001601
Si	2.966053	-0.009555	0.000712
H	-3.255752	-1.322006	-0.472237
H	-3.256742	1.068408	-0.903107
H	-3.253409	0.246014	1.382062
H	3.557076	1.068188	-0.843828
H	3.487186	-1.304098	-0.526591
H	3.531177	0.156277	1.371071

(SiH3)2-Ga≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.022703	-2.174330	0.000401
Ga	-0.001278	-0.389634	-0.000249
Si	2.157170	0.763036	0.000121
H	3.298498	-0.177624	0.006943
H	2.205159	1.625872	1.206035
H	2.211542	1.616108	-1.212411
Si	-2.163750	0.752108	0.000106
H	-2.220801	1.612537	-1.207061
H	-3.298682	-0.196466	-0.003246
H	-2.222893	1.606511	1.211472

Ga≡N-(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.250347	-2.604618	0.104580
Si	1.271208	-1.516559	0.000013
H	2.214089	-1.651136	1.139922
H	2.040747	-1.737509	-1.253040
N	0.418924	0.001039	0.007004
Ga	-1.493587	-0.022491	-0.000348
Si	1.202749	1.555723	-0.000749
H	2.126713	1.726782	-1.153441
H	0.129790	2.584548	-0.108521
H	1.971652	1.823582	1.242567

3HSi-Ga≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.025311	-0.411532	-0.009651
N	-0.265415	-2.175765	0.016400
Si	2.183804	0.717911	0.004644
H	2.303530	1.470822	1.277107
H	2.236176	1.672444	-1.129247
H	3.295183	-0.253472	-0.107855
Si	-2.125524	0.838190	0.004188

H	-2.128502	1.704406	1.208314
H	-3.290087	-0.071777	0.028879
H	-2.158963	1.680014	-1.216474

3HSi-Ga≡N-SiH3-TS2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	0.718812	-0.985738	-0.001635
N	-0.796938	-0.152072	0.005202
Si	1.515801	1.381966	-0.000252
H	0.867058	2.167369	-1.067446
H	2.980946	1.357229	-0.240776
H	1.253328	1.923068	1.349027
Si	-2.442085	0.367291	0.000067
H	-3.233024	-0.230412	-1.110709
H	-2.444771	1.845983	-0.183140
H	-3.160184	0.069556	1.269894

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b97d3/LANL2DZ+dp

SiMe(SitBu3)2-In≡N-SiMe(SitBu3)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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In	-0.528612	0.083047	-0.408640
N	1.303623	-0.069554	-0.020094
Si	2.873465	0.435939	-0.530468
Si	4.061137	-1.581715	-1.364194
Si	3.567180	1.992461	1.326840
C	2.674681	1.505734	-2.114600
H	2.381062	0.847490	-2.947550
H	3.566534	2.067111	-2.429226
H	1.849299	2.218407	-1.959562
C	5.766532	-1.194402	-2.279819
C	6.297839	-2.387453	-3.112589
H	6.425865	-3.297908	-2.510827
H	7.290248	-2.122019	-3.524780
H	5.651558	-2.634085	-3.965303
C	6.879737	-0.833098	-1.273088
H	6.596399	0.002435	-0.624836
H	7.788030	-0.525801	-1.825850
H	7.160451	-1.683776	-0.636187
C	5.630344	0.015815	-3.236038
H	6.588556	0.169933	-3.767787
H	5.408667	0.942775	-2.692763
H	4.848703	-0.117406	-3.993936
C	4.355444	-2.771883	0.171842
C	4.991649	-1.969820	1.325822
H	4.438759	-1.046289	1.530204
H	6.035571	-1.699401	1.121903
H	4.982101	-2.573109	2.253126
C	5.277878	-3.986924	-0.082821
H	5.359117	-4.580579	0.848408
H	6.297880	-3.677652	-0.355873
H	4.906031	-4.659227	-0.867121
C	2.990977	-3.286124	0.692493
H	2.530605	-4.015600	0.010420

H	2.277610	-2.463394	0.843378
H	3.135700	-3.794547	1.664957
C	2.880347	-2.502352	-2.676970
C	3.273271	-3.993271	-2.847041
H	2.661180	-4.434942	-3.656875
H	3.069522	-4.575694	-1.937981
H	4.327838	-4.139000	-3.115306
C	1.390674	-2.488200	-2.265649
H	0.820557	-3.161569	-2.934562
H	0.970019	-1.478245	-2.365360
H	1.222874	-2.809372	-1.232209
C	2.920728	-1.858810	-4.085485
H	2.653431	-0.792012	-4.064864
H	2.180920	-2.368904	-4.731692
H	3.897523	-1.955056	-4.577033
C	2.445204	3.632037	1.094716
C	3.155085	1.182876	3.115168
C	5.455993	2.532061	1.145306
C	5.813293	3.817872	1.924716
H	5.573296	3.734190	2.997270
H	5.302170	4.705091	1.526473
H	6.901438	4.005089	1.844653
C	5.758096	2.772874	-0.353299
H	6.828987	3.018543	-0.481571
H	5.175907	3.593925	-0.787946
H	5.556561	1.872548	-0.947622
C	6.442780	1.436018	1.615894
H	7.443316	1.638603	1.190894
H	6.142774	0.433580	1.293617
H	6.552457	1.418799	2.706557
C	2.169401	0.006352	2.956048
H	2.587802	-0.824092	2.376374
H	1.253281	0.310005	2.436370
H	1.899706	-0.383453	3.956277
C	4.394375	0.652835	3.872152

H	4.961552	-0.097287	3.310204
H	4.053114	0.173192	4.809047
H	5.079768	1.466143	4.155233
C	2.482390	2.173960	4.092447
H	1.512095	2.530627	3.722501
H	3.115394	3.045105	4.313905
H	2.293855	1.650543	5.048869
C	0.960897	3.236167	0.948077
H	0.796211	2.675199	0.020353
H	0.332255	4.145848	0.912703
H	0.603753	2.610460	1.779557
C	2.511446	4.681163	2.244696
H	2.113661	5.639793	1.861024
H	1.891071	4.404572	3.103730
H	3.527262	4.874163	2.610290
C	2.833609	4.414497	-0.185865
H	2.912049	3.785802	-1.078513
H	3.785115	4.950532	-0.060211
H	2.059120	5.179657	-0.385869
Si	-3.000253	0.229129	0.409887
Si	-4.251176	1.600136	-1.248693
Si	-3.240861	-2.051124	1.413936
C	-2.743693	1.518527	1.826025
H	-2.516876	2.500873	1.392149
H	-1.920878	1.264341	2.504274
H	-3.653992	1.625667	2.436863
C	-2.957783	2.807231	-2.131676
C	-3.677299	3.956883	-2.886256
H	-2.922691	4.548876	-3.436601
H	-4.192696	4.646669	-2.205208
H	-4.408634	3.594065	-3.620251
C	-2.092063	2.066115	-3.177726
H	-1.593184	1.171545	-2.765909
H	-1.296167	2.741158	-3.540725
H	-2.673554	1.745051	-4.052424

C	-1.982393	3.460841	-1.129959
H	-1.291373	4.133276	-1.669533
H	-1.356189	2.717425	-0.617179
H	-2.485210	4.054399	-0.356847
C	-5.091249	0.453517	-2.589747
C	-4.096039	-0.639543	-3.040263
H	-3.251230	-0.235523	-3.611534
H	-4.613351	-1.372023	-3.686450
H	-3.688325	-1.190450	-2.184874
C	-5.565641	1.201276	-3.859498
H	-4.731293	1.638597	-4.425556
H	-6.284492	2.002331	-3.640088
H	-6.068504	0.481014	-4.531298
C	-6.318529	-0.267983	-1.987986
H	-7.135372	0.424244	-1.740597
H	-6.062118	-0.823831	-1.078467
H	-6.714832	-0.995127	-2.720940
C	-5.593799	2.693179	-0.295377
C	-6.671461	3.240794	-1.268308
H	-7.371566	3.879541	-0.697702
H	-7.267663	2.439667	-1.725657
H	-6.249857	3.855256	-2.074979
C	-6.342073	1.879932	0.784577
H	-7.076993	2.535737	1.287831
H	-5.665925	1.498817	1.562731
H	-6.899261	1.032631	0.366340
C	-4.986439	3.918323	0.434284
H	-4.525756	4.642126	-0.250398
H	-4.240891	3.635001	1.187776
H	-5.798648	4.449604	0.964102
C	-1.739860	-2.328236	2.677960
C	-4.950040	-2.094112	2.373149
C	-3.174397	-3.436660	0.027292
C	-2.931066	-4.848810	0.622337
H	-3.703879	-5.138118	1.348023

H	-1.953215	-4.945341	1.110586
H	-2.958844	-5.588334	-0.199525
C	-2.033434	-3.161018	-0.979612
H	-1.990567	-3.973618	-1.727531
H	-1.048053	-3.111206	-0.500869
H	-2.188889	-2.225792	-1.536301
C	-4.496217	-3.525641	-0.770211
H	-5.308988	-3.955901	-0.167589
H	-4.351711	-4.189668	-1.642296
H	-4.834380	-2.555363	-1.149720
C	-6.091270	-1.594037	1.464076
H	-5.846908	-0.637611	0.992840
H	-7.005999	-1.440205	2.065677
H	-6.338304	-2.310217	0.670950
C	-5.367530	-3.501612	2.865781
H	-5.528783	-4.194931	2.027720
H	-6.329442	-3.417329	3.405362
H	-4.644590	-3.958436	3.551884
C	-4.898213	-1.145038	3.594395
H	-4.628824	-0.117892	3.308481
H	-4.185423	-1.478567	4.360580
H	-5.896345	-1.104450	4.068117
C	-2.102207	-3.427704	3.710550
H	-1.210883	-3.630459	4.332066
H	-2.399339	-4.376576	3.245020
H	-2.903612	-3.112637	4.392357
C	-0.418319	-2.769748	2.004335
H	-0.491062	-3.734710	1.488179
H	0.353892	-2.878802	2.786145
H	-0.016091	-2.030595	1.297137
C	-1.389393	-1.054063	3.479546
H	-0.874297	-0.320428	2.847054
H	-2.259864	-0.568285	3.938618
H	-0.684504	-1.317216	4.288038

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[SiMe(SitBu3)2]2-In=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.206787	-0.251187	-0.642855
N	-0.891750	-1.006294	-2.493270
Si	2.542919	-0.152204	0.475809
Si	-2.574014	0.206863	0.584912
Si	3.941237	-1.691299	-1.213708
Si	3.338445	2.105956	1.370606
Si	-3.804957	1.787045	-1.241999
Si	-3.364631	-2.074085	1.394900
C	2.395962	-1.314517	2.035101
H	1.588642	-2.046952	1.889752
H	2.144400	-0.743030	2.950513
H	3.326200	-1.879536	2.245867
C	-2.428848	1.326478	2.176396
H	-3.403478	1.517453	2.672391
H	-2.001442	2.308847	1.906560
H	-1.749370	0.872252	2.929384
C	-5.562244	2.332253	-0.513012
C	-2.648501	3.355239	-1.415220
C	-3.985979	0.975641	-3.011014
C	-5.014900	1.772768	-3.873899
H	-6.022673	1.723206	-3.454500
H	-5.060107	1.311283	-4.866585
H	-4.758196	2.821896	-4.013895
C	-2.694292	0.913323	-3.855493
H	-2.378794	1.898640	-4.167607

H	-2.929508	0.341148	-4.746642
H	-1.867935	0.401742	-3.371646
C	-4.574502	-0.447596	-2.951314
H	-5.585783	-0.450845	-2.537486
H	-3.973632	-1.143594	-2.375860
H	-4.641683	-0.844941	-3.969869
C	-3.088233	4.280075	-2.587399
H	-4.125295	4.615645	-2.501646
H	-2.960951	3.811986	-3.563725
H	-2.452173	5.180857	-2.577149
C	-1.190246	2.963106	-1.726733
H	-1.080184	2.504657	-2.696678
H	-0.785166	2.313893	-0.942576
H	-0.574272	3.877990	-1.721697
C	-2.660797	4.255054	-0.159116
H	-3.636049	4.745262	-0.022730
H	-1.910307	5.058185	-0.277712
H	-2.422334	3.719662	0.770917
C	-6.171988	3.591491	-1.179380
H	-7.186707	3.750609	-0.767322
H	-6.271485	3.505382	-2.266265
H	-5.592633	4.498038	-0.956478
C	-6.581555	1.179827	-0.675203
H	-7.485457	1.396112	-0.074359
H	-6.182815	0.216579	-0.332215
H	-6.904890	1.061805	-1.716833
C	-5.458756	2.657563	0.994609
H	-6.469278	2.873979	1.395911
H	-4.827787	3.536469	1.199438
H	-5.051122	1.818226	1.576774
C	-3.825474	-3.230496	-0.093362
C	-1.770303	-2.819458	2.291170
C	-4.832756	-1.852349	2.696125
C	-5.228117	-2.863101	-0.639373
H	-5.343605	-1.799488	-0.864938

H	-6.014441	-3.142023	0.077083
H	-5.419936	-3.419913	-1.569495
C	-2.760863	-3.212424	-1.253385
H	-2.223619	-2.271454	-1.472478
H	-3.259107	-3.509275	-2.182151
H	-1.994932	-3.959969	-1.060755
C	-3.935804	-4.722107	0.334050
H	-4.677598	-4.882909	1.127007
H	-2.980750	-5.136755	0.673196
H	-4.252944	-5.313900	-0.539646
C	-5.897337	-0.902173	2.114366
H	-6.685090	-0.701122	2.869628
H	-6.393167	-1.313973	1.223096
H	-5.450042	0.065482	1.837409
C	-4.316965	-1.197228	4.001313
H	-5.179825	-0.964047	4.660489
H	-3.784812	-0.247621	3.808724
H	-3.640253	-1.854531	4.573863
C	-5.533162	-3.181157	3.064613
H	-6.307063	-2.979586	3.833153
H	-4.842854	-3.930536	3.479443
H	-6.045462	-3.627007	2.198924
C	-2.141038	-3.976516	3.252733
H	-2.732111	-3.620775	4.110740
H	-1.213792	-4.423147	3.661473
H	-2.707122	-4.780322	2.762858
C	-0.739775	-3.368158	1.282312
H	-0.443795	-2.622071	0.535854
H	-1.095897	-4.248767	0.746431
H	0.170006	-3.665294	1.830865
C	-1.043731	-1.751725	3.133483
H	-1.690757	-1.275565	3.890770
H	-0.623662	-0.947783	2.495502
H	-0.188442	-2.212011	3.671102
C	3.072964	-3.471143	-1.265724

C	1.781812	-3.461107	-2.135288
H	1.266646	-4.420911	-2.000707
H	2.014003	-3.368383	-3.199041
H	1.074758	-2.665335	-1.886296
C	4.030939	-4.544941	-1.847018
H	3.474911	-5.492745	-1.960885
H	4.873320	-4.747997	-1.168280
H	4.442696	-4.284418	-2.829320
C	2.655176	-3.983127	0.127298
H	2.284764	-5.019792	0.031727
H	1.839420	-3.390619	0.545883
H	3.475147	-3.996518	0.861913
C	3.971201	-0.952388	-3.049782
C	5.800225	-1.882332	-0.518097
C	2.562257	-0.437850	-3.454983
H	1.821025	-1.237852	-3.552717
H	2.628304	0.066674	-4.435752
H	2.143897	0.283803	-2.738014
C	4.408978	-1.998029	-4.106846
H	3.697388	-2.827220	-4.195867
H	5.403315	-2.420182	-3.898357
H	4.460580	-1.505682	-5.095470
C	4.944651	0.240352	-3.165393
H	4.702568	1.044433	-2.455724
H	4.878745	0.670754	-4.183392
H	5.996293	-0.051164	-3.006098
C	6.805888	-2.487144	-1.524276
H	6.530964	-3.502687	-1.848704
H	7.804425	-2.553068	-1.042045
H	6.921047	-1.859177	-2.422909
C	6.295580	-0.482684	-0.115871
H	5.531139	0.022658	0.500096
H	6.504009	0.166146	-0.983875
H	7.227979	-0.542856	0.487224
C	5.815147	-2.751665	0.763854

H	5.570743	-3.808912	0.566254
H	5.109564	-2.383747	1.533439
H	6.830503	-2.730473	1.216110
C	3.755842	3.318339	-0.144808
C	4.829147	1.898156	2.710257
C	1.741082	2.838861	2.310614
C	6.216719	2.275927	2.138849
H	6.485689	1.716310	1.230548
H	6.993862	2.058722	2.904629
H	6.281541	3.356335	1.911586
C	4.629863	2.779439	3.962008
H	3.715285	2.515196	4.521316
H	4.596200	3.856691	3.718357
H	5.489614	2.620561	4.648951
C	4.876166	0.429340	3.190266
H	3.961069	0.146748	3.747905
H	5.740744	0.278504	3.875426
H	4.987190	-0.278066	2.347490
C	5.176485	3.083772	-0.724169
H	5.421136	2.015529	-0.833814
H	5.965914	3.548440	-0.113083
H	5.239687	3.539257	-1.733733
C	3.679439	4.806994	0.255593
H	2.657047	5.127850	0.511950
H	4.017993	5.432472	-0.595339
H	4.339701	5.032805	1.114405
C	2.776883	3.056094	-1.320662
H	1.720089	3.164267	-1.044577
H	2.909126	2.045935	-1.738519
H	2.984430	3.772884	-2.139637
C	1.947339	4.153818	3.106940
H	0.965539	4.659372	3.222369
H	2.626204	4.865360	2.612433
H	2.333099	3.972564	4.121515
C	0.636055	3.093009	1.271424

H	-0.323675	3.303589	1.784153
H	0.503234	2.187455	0.651719
H	0.844081	3.948584	0.609819
C	1.191765	1.756235	3.267742
H	0.351969	2.167582	3.872585
H	1.952612	1.370070	3.977491
H	0.786233	0.891627	2.700399

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In=N-[SiMe(SitBu3)2]2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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In	0.357594	-1.346171	-1.537971
N	0.019862	0.011575	0.270964
Si	1.737788	0.444129	0.488289
Si	2.850786	1.988239	-1.651250
Si	3.319196	-1.766462	1.657304
C	2.179682	1.627902	1.890548
H	1.716016	2.607654	1.761153
H	3.270677	1.758807	1.861371
H	1.906332	1.238707	2.876314
C	3.973967	3.473456	-0.928313
C	4.347534	4.471125	-2.058987
H	4.832198	3.996833	-2.919808
H	5.058935	5.212225	-1.648195
H	3.477639	5.032049	-2.423276
C	5.299128	2.971990	-0.313394
H	5.127519	2.318113	0.550317
H	5.880817	3.840011	0.050130
H	5.934073	2.433897	-1.030241
C	3.281153	4.310402	0.176965

H	3.870883	5.230736	0.345963
H	3.247233	3.775526	1.131046
H	2.260530	4.617686	-0.077365
C	3.975290	0.821938	-2.788250
C	4.769777	-0.126241	-1.872983
H	4.095755	-0.666531	-1.195856
H	5.508943	0.398165	-1.254235
H	5.314945	-0.868423	-2.485434
C	4.996123	1.565300	-3.687265
H	5.548671	0.819455	-4.290353
H	5.744129	2.118529	-3.102988
H	4.521553	2.265186	-4.389138
C	3.142333	-0.087146	-3.722222
H	2.556200	0.466916	-4.467061
H	2.448593	-0.737135	-3.164400
H	3.825598	-0.758675	-4.275479
C	1.430807	2.788160	-2.772897
C	1.931045	3.207309	-4.178640
H	1.091013	3.669993	-4.731485
H	2.282102	2.356461	-4.776596
H	2.741431	3.947373	-4.137511
C	0.275938	1.783623	-2.967934
H	-0.506050	2.226864	-3.611609
H	-0.195201	1.524632	-2.008919
H	0.609385	0.857968	-3.460877
C	0.813148	4.044857	-2.122671
H	0.477547	3.849726	-1.098815
H	-0.067653	4.363604	-2.709584
H	1.509325	4.893622	-2.097562
C	1.993794	-2.470506	2.937359
C	3.975486	-3.264195	0.493138
C	4.876707	-1.028251	2.644446
C	5.791644	-2.136775	3.227956
H	6.211024	-2.795245	2.458324
H	5.273110	-2.762459	3.966977

H	6.643911	-1.654835	3.744044
C	4.477904	-0.141074	3.848447
H	5.398918	0.263056	4.309086
H	3.952317	-0.710051	4.627931
H	3.854657	0.714590	3.568298
C	5.728477	-0.163241	1.687187
H	6.463314	0.433070	2.260903
H	5.105436	0.533592	1.113183
H	6.289875	-0.772041	0.965115
C	3.008746	-3.503459	-0.687100
H	3.006519	-2.652591	-1.385269
H	1.974967	-3.685207	-0.357910
H	3.329014	-4.392768	-1.262361
C	5.377430	-3.024298	-0.127607
H	5.484271	-2.047537	-0.606071
H	5.557649	-3.791806	-0.904511
H	6.182972	-3.127677	0.612294
C	4.095995	-4.600087	1.273603
H	3.128384	-4.988232	1.616273
H	4.759964	-4.517307	2.145483
H	4.531201	-5.363179	0.600625
C	0.937056	-3.289236	2.167965
H	0.491665	-2.680837	1.368017
H	0.122396	-3.589281	2.851951
H	1.340826	-4.205446	1.718505
C	2.589605	-3.350908	4.064027
H	1.762096	-3.751604	4.680486
H	3.166566	-4.207241	3.692509
H	3.237922	-2.770073	4.736796
C	1.234862	-1.312893	3.621964
H	0.701873	-0.702613	2.885791
H	1.894708	-0.660401	4.207254
H	0.479155	-1.729498	4.312848
Si	-1.702426	-0.011659	0.740422
Si	-2.898915	2.200483	1.518265

Si	-3.352788	-1.963379	-1.100576
C	-1.955205	-1.039183	2.323336
H	-1.491626	-0.534370	3.183027
H	-1.522969	-2.043205	2.254792
H	-3.028836	-1.143794	2.539477
C	-1.438545	3.213926	2.346452
C	-1.862360	4.458574	3.161869
H	-0.951157	4.996972	3.485268
H	-2.416572	4.192929	4.072368
H	-2.472878	5.165926	2.585323
C	-0.489899	3.691913	1.232257
H	-0.159726	2.855203	0.601742
H	0.405651	4.161983	1.676142
H	-0.954462	4.447060	0.586319
C	-0.627973	2.302424	3.292533
H	0.251112	2.853013	3.670935
H	-0.259353	1.411000	2.775017
H	-1.204531	1.972788	4.162837
C	-3.636157	3.213775	-0.006407
C	-2.739627	2.993149	-1.247265
H	-1.731035	3.399272	-1.118803
H	-3.187979	3.495268	-2.125614
H	-2.637098	1.925006	-1.491684
C	-3.724530	4.737558	0.261182
H	-2.745447	5.196483	0.446934
H	-4.378364	4.975633	1.112037
H	-4.151450	5.233311	-0.630974
C	-5.055170	2.756143	-0.408009
H	-5.788257	2.845336	0.405355
H	-5.063179	1.721872	-0.760117
H	-5.413817	3.387107	-1.243011
C	-4.284495	1.952329	2.939520
C	-5.061438	3.277327	3.161906
H	-5.770114	3.132577	3.999675
H	-5.657102	3.561500	2.283810

H	-4.416015	4.124348	3.423511
C	-5.350511	0.885956	2.630235
H	-6.030594	0.795861	3.498346
H	-4.915579	-0.104843	2.452585
H	-5.965173	1.153436	1.764346
C	-3.670685	1.548719	4.302487
H	-3.052209	2.340801	4.741932
H	-3.069752	0.631349	4.238728
H	-4.493851	1.353335	5.014808
C	-2.657049	-3.866593	-0.980076
C	-5.213541	-2.030408	-0.347450
C	-3.511503	-1.380245	-3.017640
C	-4.006171	-2.520918	-3.941810
H	-4.986982	-2.914276	-3.642965
H	-3.300564	-3.362755	-3.977414
H	-4.105914	-2.133388	-4.973753
C	-2.167776	-0.885116	-3.586023
H	-2.304485	-0.520220	-4.621240
H	-1.408281	-1.680937	-3.628035
H	-1.772963	-0.040066	-3.001545
C	-4.486443	-0.189234	-3.172952
H	-5.531287	-0.472054	-2.993584
H	-4.428026	0.192046	-4.209567
H	-4.231561	0.644288	-2.504058
C	-5.732844	-0.595966	-0.158932
H	-4.975273	0.045943	0.295869
H	-6.618027	-0.597269	0.500646
H	-6.039922	-0.140588	-1.105861
C	-6.268817	-2.739814	-1.236966
H	-6.390542	-2.240015	-2.207860
H	-7.247606	-2.681075	-0.722958
H	-6.062950	-3.799244	-1.423988
C	-5.237791	-2.707968	1.044215
H	-4.514892	-2.260047	1.739621
H	-5.031953	-3.785488	0.996780

H	-6.243127	-2.587182	1.489176
C	-3.758079	-4.909263	-1.306632
H	-3.313497	-5.920660	-1.247304
H	-4.169539	-4.792212	-2.318848
H	-4.587539	-4.885825	-0.590394
C	-1.477594	-4.198436	-1.922313
H	-1.632636	-3.890650	-2.966248
H	-1.303427	-5.290331	-1.919239
H	-0.534887	-3.745326	-1.576338
C	-2.155212	-4.153330	0.453517
H	-1.298501	-3.517111	0.705048
H	-2.924893	-3.995901	1.220008
H	-1.819588	-5.205122	0.528034

SiiPrDis2-In≡N-SiiPrDis2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.313704	-0.373285	-0.002245
N	-1.453745	0.181439	-0.222950
Si	-2.985402	0.384668	0.523959
Si	2.752577	0.313422	-0.603850
C	-3.790403	-1.349981	0.736796
H	-4.883840	-1.202062	0.686285
C	-4.056894	1.609229	-0.537129
H	-4.184494	2.441773	0.187955
C	-2.722619	1.491099	2.099937
H	-2.265940	2.364146	1.591891
C	-1.678428	1.020641	3.125952

H	-1.395755	1.846144	3.805022
H	-0.754032	0.674929	2.630780
H	-2.041754	0.194875	3.753405
C	-3.988436	2.016511	2.810866
H	-3.717328	2.712009	3.626612
H	-4.588589	1.209909	3.253384
H	-4.648028	2.568143	2.123016
C	2.384749	1.418347	-2.136590
H	1.789727	2.260792	-1.750208
C	1.549923	0.739030	-3.237859
H	1.353485	1.451366	-4.057600
H	0.570174	0.392620	-2.875004
H	2.074656	-0.125200	-3.674017
C	3.684606	1.979359	-2.752484
H	3.447655	2.698153	-3.556650
H	4.289320	1.175406	-3.204766
H	4.317498	2.497668	-2.020103
C	3.104292	1.430485	0.943597
H	2.042932	1.663624	1.191141
C	3.835265	-1.133498	-1.247736
H	3.868088	-0.842522	-2.320600
Si	-3.039283	2.548358	-1.846017
Si	-5.886470	1.258004	-0.886458
Si	-3.583434	-2.250275	2.392075
Si	-3.446329	-2.529838	-0.728130
C	-4.010005	3.989245	-2.605411
H	-3.304118	4.632404	-3.161320
H	-4.502970	4.617109	-1.845792
H	-4.779809	3.655530	-3.319056
C	-1.543939	3.379249	-1.031211
H	-0.964139	3.933847	-1.790390
H	-0.890671	2.628257	-0.564451
H	-1.852948	4.103257	-0.257069
C	-2.424309	1.535232	-3.309226
H	-1.891300	2.202055	-4.010400

H	-3.247168	1.058115	-3.865845
H	-1.732305	0.748696	-2.983874
C	-6.832025	2.852760	-1.283332
H	-6.648714	3.227377	-2.300695
H	-6.585038	3.665135	-0.578779
H	-7.915132	2.656528	-1.192879
C	-6.794600	0.615452	0.652653
H	-7.881531	0.641780	0.458667
H	-6.602431	1.260255	1.525904
H	-6.544467	-0.414972	0.943393
C	-6.206135	0.069066	-2.314765
H	-5.856045	-0.952129	-2.108553
H	-5.714922	0.412244	-3.240799
H	-7.290551	0.013949	-2.515521
C	-4.414526	-3.954588	2.380876
H	-4.350823	-4.388469	3.394794
H	-3.950093	-4.669479	1.686158
H	-5.484226	-3.879811	2.121577
C	-4.470594	-1.375069	3.815860
H	-4.595672	-2.090145	4.648228
H	-5.478470	-1.044010	3.513003
H	-3.936117	-0.502163	4.211762
C	-1.767344	-2.530840	2.854583
H	-1.668443	-2.703404	3.940484
H	-1.134761	-1.669051	2.595261
H	-1.357454	-3.412910	2.339160
C	-1.993801	-3.716905	-0.436725
H	-1.071315	-3.172208	-0.176925
H	-1.794952	-4.266995	-1.373272
H	-2.175154	-4.461887	0.352575
C	-4.998105	-3.584412	-1.018556
H	-5.106609	-4.393977	-0.281160
H	-4.959512	-4.047526	-2.020092
H	-5.917988	-2.976932	-0.973831
C	-3.042324	-1.722544	-2.379464

H	-2.027626	-1.305486	-2.362223
H	-3.724230	-0.907912	-2.648461
H	-3.100503	-2.489597	-3.172817
Si	3.660077	3.271843	0.849150
Si	3.605339	0.548128	2.570559
Si	2.996736	-2.852468	-1.422542
Si	5.706410	-1.203649	-0.879782
C	2.507399	4.275298	-0.263012
H	2.623835	5.343737	-0.010313
H	1.448668	4.016129	-0.095115
H	2.713915	4.171133	-1.337637
C	3.429365	4.053257	2.557227
H	3.617329	5.137201	2.462906
H	4.124168	3.666279	3.318337
H	2.402962	3.928863	2.937479
C	5.445296	3.653194	0.374362
H	5.573266	4.747793	0.450818
H	5.720511	3.360556	-0.648429
H	6.170695	3.190517	1.061385
C	2.538055	1.159446	4.006284
H	2.871529	2.116780	4.429669
H	2.566773	0.409258	4.815843
H	1.482634	1.273020	3.706963
C	3.238555	-1.295303	2.476591
H	3.675228	-1.811897	3.348570
H	3.635985	-1.771151	1.574542
H	2.152552	-1.482878	2.503837
C	5.421392	0.785509	3.018089
H	5.688517	1.850066	3.111002
H	6.105259	0.330738	2.286918
H	5.617513	0.309779	3.994888
C	6.162976	-2.328965	0.563168
H	5.841396	-1.930275	1.535874
H	7.261224	-2.437438	0.598132
H	5.735352	-3.338618	0.456719

C	6.382383	0.519486	-0.562467
H	6.330599	1.126961	-1.479894
H	7.442558	0.468117	-0.260075
H	5.836791	1.054959	0.221154
C	6.626415	-1.802910	-2.421016
H	7.684231	-1.493141	-2.351058
H	6.213890	-1.347217	-3.338065
H	6.609530	-2.894218	-2.552314
C	4.160229	-4.105300	-2.227652
H	5.046099	-4.338373	-1.617196
H	4.508281	-3.770846	-3.217890
H	3.603161	-5.047472	-2.372644
C	1.523843	-2.768012	-2.605686
H	0.710703	-2.092782	-2.298090
H	1.081824	-3.775471	-2.691827
H	1.839217	-2.456307	-3.615002
C	2.395359	-3.662371	0.171852
H	1.645597	-3.074840	0.723511
H	3.215445	-3.892038	0.869140
H	1.915114	-4.617178	-0.104540

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[SiiPrDis2]-In=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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N	-0.363572	0.065718	-2.626117
In	0.092805	-0.385460	-0.787362
Si	2.389771	0.206219	0.426616
Si	-2.320199	-0.368895	0.526572

C	3.356982	1.287510	-0.834145
H	4.369712	1.368605	-0.390336
C	3.466347	-1.211487	1.151163
H	3.016525	-1.270575	2.159747
C	1.577921	1.111844	1.984893
H	0.530992	1.266442	1.669159
C	2.095827	2.493669	2.422700
H	1.579554	2.809009	3.348560
H	1.906385	3.265223	1.668562
H	3.171315	2.489941	2.639577
C	1.515895	0.192623	3.223175
H	0.849231	0.632362	3.983981
H	2.507365	0.084096	3.691215
H	1.138139	-0.813845	2.995047
C	-1.794646	-1.006263	2.270107
H	-1.121498	-0.230785	2.662852
C	-1.007720	-2.327216	2.242436
H	-0.690643	-2.609259	3.262103
H	-0.103014	-2.254255	1.621516
H	-1.616019	-3.159299	1.852282
C	-2.980766	-1.149865	3.247128
H	-2.612727	-1.400996	4.258535
H	-3.655933	-1.964326	2.937274
H	-3.579840	-0.233932	3.330285
C	-2.610947	1.546282	0.552873
H	-1.562856	1.877143	0.377496
C	-3.565003	-1.677839	-0.126948
H	-3.400536	-2.437046	0.668263
Si	3.288452	-3.067818	0.706674
Si	5.245611	-0.744866	1.649250
Si	2.814573	3.112364	-1.062234
Si	3.710492	0.496910	-2.548918
C	4.811754	-3.906358	-0.030376
H	4.579722	-4.981181	-0.135357
H	5.704828	-3.827877	0.607896

H	5.071265	-3.530535	-1.030019
C	2.899406	-3.967368	2.326758
H	2.709019	-5.037085	2.130808
H	1.994119	-3.554753	2.804029
H	3.720736	-3.903440	3.057018
C	1.838009	-3.494872	-0.415210
H	0.883931	-3.366192	0.113782
H	1.901513	-4.562739	-0.688077
H	1.786589	-2.925838	-1.354403
C	5.829245	-1.930923	3.003369
H	5.954940	-2.966897	2.655066
H	5.120008	-1.946149	3.848378
H	6.803100	-1.590469	3.396315
C	5.350541	0.964813	2.442666
H	6.384534	1.125278	2.795312
H	4.688516	1.058089	3.317717
H	5.112878	1.780886	1.744397
C	6.506701	-0.754003	0.249521
H	6.603269	-1.735196	-0.236835
H	7.495163	-0.493668	0.667544
H	6.275337	-0.011022	-0.528609
C	3.248044	3.891903	-2.733377
H	2.854816	4.924567	-2.710055
H	2.812677	3.394713	-3.610293
H	4.336230	3.964395	-2.881354
C	3.760319	4.231601	0.149466
H	4.196636	3.697269	1.004066
H	3.109614	5.025158	0.554878
H	4.585596	4.729373	-0.387786
C	0.946579	3.298012	-0.919446
H	0.670494	4.361206	-1.023447
H	0.523921	2.940145	0.031032
H	0.447376	2.737163	-1.726315
C	2.286187	0.660061	-3.771679
H	1.696929	1.581323	-3.665819

H	1.568308	-0.178692	-3.675538
H	2.683917	0.632808	-4.803978
C	5.275674	1.317714	-3.249779
H	5.040394	2.120453	-3.964237
H	5.880963	0.566080	-3.784723
H	5.912537	1.752044	-2.460911
C	4.125029	-1.336617	-2.486386
H	3.279506	-1.960919	-2.173033
H	4.978119	-1.545596	-1.830274
H	4.404136	-1.654666	-3.506989
Si	-2.924787	2.563169	2.161101
Si	-3.450102	2.365969	-0.979778
Si	-3.117243	-2.767835	-1.654815
Si	-5.454550	-1.434661	0.052321
C	-1.720660	2.185920	3.568106
H	-1.864775	2.962923	4.339669
H	-0.674483	2.249436	3.237240
H	-1.873470	1.213219	4.053575
C	-2.575635	4.388865	1.799651
H	-2.681673	4.946000	2.747239
H	-3.262568	4.841552	1.070104
H	-1.545628	4.545617	1.440261
C	-4.648812	2.520731	2.928781
H	-4.657669	3.278025	3.733233
H	-4.906477	1.556127	3.388240
H	-5.449847	2.783470	2.223112
C	-2.460311	3.870796	-1.563475
H	-3.142986	4.594064	-2.043414
H	-1.726488	3.553517	-2.320788
H	-1.914169	4.404135	-0.776146
C	-3.507946	1.245224	-2.473723
H	-4.038155	1.771370	-3.288138
H	-4.023901	0.296835	-2.297532
H	-2.485627	1.022172	-2.822401
C	-5.210095	2.958594	-0.618833

H	-5.242859	3.773748	0.121403
H	-5.883009	2.160072	-0.274429
H	-5.627767	3.355188	-1.561134
C	-6.314110	-0.865209	-1.527522
H	-6.144502	0.202679	-1.728619
H	-7.402203	-1.009587	-1.406493
H	-6.001436	-1.428860	-2.419734
C	-5.918650	-0.219298	1.405357
H	-5.622245	-0.587204	2.398651
H	-7.016314	-0.093283	1.414675
H	-5.470048	0.768874	1.262401
C	-6.230246	-3.071478	0.617753
H	-7.147952	-2.852308	1.190710
H	-5.557091	-3.639089	1.282639
H	-6.508312	-3.732404	-0.215242
C	-4.425054	-4.108658	-1.932398
H	-5.409182	-3.717391	-2.229766
H	-4.563074	-4.758122	-1.053601
H	-4.061017	-4.743837	-2.759193
C	-1.542204	-3.746943	-1.292262
H	-0.635769	-3.201239	-1.590440
H	-1.557534	-4.678656	-1.884751
H	-1.440158	-4.034606	-0.234334
C	-2.884841	-1.916428	-3.307139
H	-2.075144	-1.165693	-3.298361
H	-3.805407	-1.447282	-3.686365
H	-2.586414	-2.698293	-4.029248

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In=N-[SiiPrDis2]2

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Atomic	Coordinates (Angstroms)		

Number		X	Y	Z
	In	0.323833	-1.191965	-1.824126
	N	-0.033338	-0.019853	0.001772
	Si	-1.677377	-0.214407	0.621994
	Si	1.585241	0.405657	0.600576
	C	-2.709090	-1.316892	-0.629991
	H	-3.667447	-1.308018	-0.068506
	C	-2.810980	1.312658	1.137038
	H	-2.420232	1.418921	2.167876
	C	-1.447342	-1.139402	2.338669
	H	-0.391928	-1.425071	2.215568
	C	-2.223311	-2.441700	2.670938
	H	-2.904520	-2.290717	3.520067
	H	-1.535823	-3.253647	2.957970
	H	-2.837143	-2.814187	1.845932
	C	-1.505275	-0.240552	3.595770
	H	-1.084389	-0.779879	4.462381
	H	-2.543961	0.017749	3.853200
	H	-0.948503	0.699261	3.497532
	C	1.444052	1.173229	2.345087
	H	0.871773	0.391302	2.863789
	C	0.591643	2.446235	2.368501
	H	0.375642	2.755972	3.406144
	H	-0.362496	2.299018	1.856473
	H	1.099467	3.292759	1.880734
	C	2.716536	1.409799	3.172546
	H	2.451421	1.578094	4.232168
	H	3.255445	2.304501	2.832329
	H	3.419522	0.571892	3.137743
	C	2.552274	-1.317170	0.774057
	H	1.701112	-1.992120	0.542218
	C	2.356143	1.811320	-0.523742
	H	1.755286	2.621002	-0.054489

Si	-2.644443	3.174448	0.674175
Si	-4.637254	0.955270	1.625447
Si	-2.450345	-3.230810	-0.759068
Si	-3.375263	-0.617066	-2.291909
C	-4.120417	4.025201	-0.154723
H	-3.854122	5.093727	-0.253148
H	-5.042320	3.977018	0.444169
H	-4.342453	3.651294	-1.164005
C	-2.429329	4.154289	2.291233
H	-1.909450	5.104341	2.078186
H	-1.843161	3.622227	3.054509
H	-3.401554	4.407908	2.740590
C	-1.169813	3.584059	-0.428167
H	-0.756503	4.562633	-0.132568
H	-1.468280	3.658785	-1.483513
H	-0.370284	2.839734	-0.357763
C	-5.148555	2.178739	2.982529
H	-5.322130	3.199993	2.611194
H	-4.396204	2.239383	3.786123
H	-6.092835	1.831507	3.437413
C	-4.998775	-0.727461	2.408344
H	-6.078995	-0.737701	2.640058
H	-4.464832	-0.885729	3.354595
H	-4.798656	-1.588712	1.756015
C	-5.960907	1.073699	0.280388
H	-5.999533	2.039050	-0.241913
H	-6.934906	0.934604	0.783319
H	-5.874510	0.279134	-0.474143
C	-2.238606	-3.949114	-2.502450
H	-2.202806	-5.046586	-2.377560
H	-1.296352	-3.652690	-2.988858
H	-3.067806	-3.724766	-3.189226
C	-4.024784	-4.086530	-0.144363
H	-4.336791	-3.796863	0.870386
H	-3.879565	-5.180901	-0.150213

H	-4.862745	-3.862200	-0.825041
C	-0.917157	-3.884585	0.165114
H	-1.214325	-4.585313	0.961313
H	-0.319706	-3.094224	0.642274
H	-0.260267	-4.433966	-0.529837
C	-2.354264	-0.866374	-3.872288
H	-1.530334	-0.142100	-3.957590
H	-3.043884	-0.642162	-4.707359
H	-1.952978	-1.871395	-4.046317
C	-5.048036	-1.437403	-2.637618
H	-4.942577	-2.490016	-2.945053
H	-5.555374	-0.905752	-3.461542
H	-5.720094	-1.415513	-1.765018
C	-3.626706	1.242702	-2.277194
H	-2.688472	1.775324	-2.071707
H	-4.369179	1.566154	-1.544281
H	-3.976434	1.559041	-3.276092
Si	2.982525	-2.117772	2.481679
Si	3.861884	-1.970286	-0.483491
Si	1.921588	2.306491	-2.334778
Si	4.114829	2.484646	-0.104189
C	1.683515	-1.971569	3.845617
H	2.060800	-2.566289	4.697138
H	0.716524	-2.405455	3.554185
H	1.511441	-0.951360	4.211438
C	3.072791	-3.996482	2.223721
H	3.078298	-4.479102	3.217100
H	3.980861	-4.328130	1.698343
H	2.201168	-4.385120	1.672022
C	4.625702	-1.603898	3.291419
H	5.227527	-2.507082	3.489970
H	4.438443	-1.117037	4.262194
H	5.247725	-0.925667	2.695281
C	3.304061	-3.651976	-1.163554
H	3.522844	-4.483598	-0.477682

H	3.833921	-3.853298	-2.111060
H	2.223595	-3.678671	-1.383672
C	4.086875	-0.878755	-1.993626
H	4.871993	-1.318823	-2.633346
H	4.391912	0.143693	-1.745240
H	3.175562	-0.818584	-2.605740
C	5.616584	-2.225183	0.178180
H	5.681571	-2.947194	1.004617
H	6.094824	-1.291007	0.505386
H	6.220565	-2.625326	-0.656032
C	5.281192	2.822727	-1.562661
H	5.639102	1.902682	-2.050189
H	6.169208	3.319368	-1.130702
H	4.879961	3.488468	-2.338982
C	5.151040	1.355422	1.007042
H	5.337223	1.815829	1.988989
H	6.130899	1.161580	0.539958
H	4.668351	0.389206	1.185594
C	3.916425	4.167855	0.740833
H	4.904842	4.556794	1.042682
H	3.287358	4.123252	1.643478
H	3.463859	4.906689	0.060091
C	2.005197	4.200672	-2.395058
H	3.020658	4.605676	-2.270180
H	1.364913	4.652923	-1.620617
H	1.632391	4.544954	-3.375675
C	0.161905	1.889236	-2.924947
H	-0.502775	1.533483	-2.129680
H	0.195387	1.137305	-3.730507
H	-0.298988	2.792696	-3.357031
C	2.979650	1.666075	-3.768216
H	2.681913	0.649510	-4.068375
H	4.063885	1.663958	-3.607618
H	2.772133	2.327209	-4.629551

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Tbt2-In=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.179339	1.265086	-0.807299
N	0.351783	2.089650	-2.705549
C	-2.719108	1.238039	0.370505
C	-3.266424	-1.368998	-0.691974
C	-3.934811	0.566213	0.645203
C	-1.784779	0.552960	-0.465454
C	-2.062640	-0.722550	-1.058388
C	-4.220758	-0.722820	0.133143
H	-4.718266	1.056098	1.243676
H	-3.507103	-2.351290	-1.113397
C	-2.529952	2.687151	0.792266
H	-1.449487	2.930610	0.699332
C	-5.564982	-1.349305	0.458915
H	-6.176954	-0.542565	0.924231
C	-1.166071	-1.242859	-2.181088
H	-0.305755	-0.554571	-2.303537
Si	-0.341335	-2.957472	-1.975281
Si	-2.070449	-1.003588	-3.866027
Si	-6.582011	-1.828447	-1.080010
Si	-5.404489	-2.608831	1.882195
Si	-3.416126	3.852294	-0.461667
Si	-2.923739	3.124667	2.606860
C	-3.204799	-2.467384	-4.220096
H	-2.638346	-3.400887	-4.363043
H	-3.782437	-2.284295	-5.142134

H	-3.927399	-2.634702	-3.407240
C	-3.034378	0.607046	-3.801289
H	-3.443290	0.804996	-2.794640
H	-3.865875	0.621915	-4.526151
H	-2.353786	1.437769	-4.048102
C	-0.819562	-0.808821	-5.257573
H	-0.199972	0.075264	-5.084096
H	-1.362850	-0.650323	-6.202801
H	-0.162221	-1.672214	-5.393766
C	1.151763	-2.804684	-0.852857
H	1.935735	-2.200806	-1.327945
H	1.577451	-3.802833	-0.662647
H	0.935123	-2.338301	0.113403
C	0.377810	-3.610628	-3.594783
H	0.880964	-4.566662	-3.368766
H	1.138873	-2.934671	-4.005327
H	-0.368174	-3.809771	-4.375925
C	-1.527797	-4.271191	-1.335263
H	-2.428622	-4.361755	-1.963206
H	-1.850757	-4.078402	-0.302508
H	-1.018491	-5.250845	-1.346034
C	-6.174868	-0.632810	-2.476803
H	-5.142376	-0.767344	-2.831367
H	-6.269333	0.417351	-2.144399
H	-6.853219	-0.778442	-3.337168
C	-6.253550	-3.598758	-1.653751
H	-6.720434	-3.781222	-2.638527
H	-6.667466	-4.339574	-0.946897
H	-5.174563	-3.806482	-1.754757
C	-8.412118	-1.634931	-0.652535
H	-9.041823	-1.777500	-1.549627
H	-8.615442	-0.618913	-0.265055
H	-8.748076	-2.355926	0.111695
C	-7.126402	-3.137386	2.454693
H	-7.775448	-2.264473	2.651693

H	-7.063374	-3.723109	3.390348
H	-7.634487	-3.768648	1.704257
C	-4.405432	-4.130027	1.401731
H	-4.197970	-4.748576	2.294717
H	-3.434537	-3.836301	0.973110
H	-4.924322	-4.765644	0.665496
C	-4.511086	-1.732138	3.291693
H	-4.360062	-2.394656	4.163237
H	-5.063746	-0.839188	3.639843
H	-3.517336	-1.394592	2.950326
C	-3.397046	5.644331	0.145706
H	-3.795335	6.291435	-0.654685
H	-2.369163	5.979018	0.354953
H	-4.002243	5.823777	1.047291
C	-2.515915	3.869579	-2.108528
H	-1.623204	4.501323	-2.061247
H	-3.175753	4.277348	-2.894206
H	-2.190453	2.865713	-2.420059
C	-5.196019	3.284769	-0.717713
H	-5.223128	2.289872	-1.195938
H	-5.725326	3.995097	-1.378326
H	-5.764324	3.216594	0.225793
C	-1.943769	4.679316	3.070080
H	-1.678550	4.663409	4.141625
H	-2.528342	5.594081	2.888932
H	-1.005377	4.768661	2.502034
C	-2.412713	1.676406	3.684679
H	-3.092428	0.821016	3.534082
H	-2.417361	1.934645	4.758091
H	-1.401549	1.340896	3.414389
C	-4.748708	3.470301	2.958217
H	-5.388448	2.591842	2.760871
H	-5.148987	4.316837	2.376648
H	-4.862634	3.723613	4.028919
C	3.038566	0.758680	-0.507416

C	3.015359	-1.086210	1.614707
C	1.869801	0.666241	0.325570
C	4.110610	-0.141005	-0.301831
C	4.133273	-1.059118	0.762056
C	1.894777	-0.249317	1.440809
H	4.985783	-0.057618	-0.947891
H	3.055138	-1.738403	2.486251
C	3.350731	1.913078	-1.485426
H	4.457840	1.991405	-1.383678
C	0.845061	-0.200090	2.543456
H	-0.061298	0.285122	2.112234
C	5.361984	-1.890524	1.055824
H	5.286039	-2.230774	2.107362
Si	6.976520	-0.869334	1.007982
Si	5.329215	-3.524292	0.069607
Si	0.158135	-1.827441	3.289326
Si	1.566591	1.071863	3.814784
Si	3.007562	3.670595	-0.828404
Si	3.340719	1.527635	-3.395640
C	4.001135	-4.608393	0.856073
H	4.332525	-4.964619	1.846744
H	3.780339	-5.496064	0.239379
H	3.061746	-4.052648	0.995558
C	6.970551	-4.444379	0.205807
H	7.249383	-4.617317	1.258039
H	7.800000	-3.905910	-0.278558
H	6.887363	-5.431319	-0.281026
C	4.943760	-3.217949	-1.744988
H	4.865032	-4.175357	-2.286422
H	5.726987	-2.618784	-2.234547
H	3.991168	-2.686444	-1.865576
C	7.707863	-0.731938	-0.728181
H	7.903935	-1.720193	-1.172557
H	8.666316	-0.185704	-0.691476
H	7.048020	-0.183233	-1.418872

C	8.235272	-1.692178	2.145753
H	8.627342	-2.634838	1.734703
H	7.788153	-1.913602	3.130050
H	9.092548	-1.018745	2.317465
C	6.642583	0.866097	1.661825
H	6.309571	0.837400	2.712036
H	5.857884	1.373239	1.081315
H	7.556082	1.483584	1.614921
C	-1.050863	-1.518727	4.713181
H	-1.765440	-0.703103	4.533835
H	-0.538247	-1.316518	5.665594
H	-1.641602	-2.443328	4.849083
C	-0.828371	-2.797390	2.004876
H	-1.600854	-3.399126	2.515880
H	-0.208296	-3.490703	1.418535
H	-1.345471	-2.120036	1.300868
C	1.489391	-2.949367	4.036022
H	2.172151	-2.391641	4.701077
H	2.097121	-3.472428	3.280866
H	0.995238	-3.722299	4.652709
C	1.198387	2.794989	3.147041
H	1.924506	3.536178	3.517888
H	0.196585	3.121026	3.458260
H	1.237433	2.809539	2.048650
C	0.878975	0.987162	5.569810
H	1.175216	0.060590	6.088632
H	-0.215974	1.075964	5.618547
H	1.311837	1.832397	6.135755
C	3.429757	0.850108	3.995649
H	3.966168	1.032047	3.054846
H	3.692737	-0.165792	4.335801
H	3.806409	1.562889	4.750277
C	3.788212	3.735790	0.887488
H	3.501352	2.862314	1.489061
H	3.497207	4.642369	1.440344

H	4.887809	3.732225	0.801696
C	3.946034	4.887683	-1.923831
H	3.522729	4.960607	-2.934742
H	5.007652	4.605590	-2.022272
H	3.911135	5.893282	-1.474960
C	1.225643	4.286496	-0.789294
H	1.241506	5.356164	-0.540082
H	0.591331	3.810464	-0.036272
H	0.764680	4.169542	-1.770154
C	5.187271	1.561651	-3.844343
H	5.600147	2.578595	-3.703636
H	5.345202	1.289531	-4.903175
H	5.787733	0.871084	-3.226420
C	2.537538	2.720871	-4.630504
H	2.435215	3.745263	-4.247187
H	1.534995	2.389770	-4.917220
H	3.170377	2.763768	-5.535304
C	2.709524	-0.218937	-3.712647
H	3.271460	-0.954146	-3.121825
H	2.850546	-0.459605	-4.776125
H	1.649112	-0.334025	-3.492757

In=N-Tbt2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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C	-2.280434	0.991932	0.734469
C	-2.856217	-1.184384	-0.961963
C	-3.535406	0.341780	0.738791

C	-1.196117	0.419452	-0.037231
C	-1.574624	-0.581897	-1.023549
C	-3.855028	-0.769547	-0.058295
H	-4.319233	0.753784	1.375289
H	-3.098980	-1.947094	-1.700958
C	-2.220002	2.323170	1.486700
H	-1.177991	2.684358	1.495636
C	-5.246841	-1.379439	0.040999
H	-5.826831	-0.698060	0.696901
C	-0.759475	-0.823425	-2.295952
H	0.185807	-0.257621	-2.217072
Si	-0.129525	-2.594550	-2.655485
Si	-1.699986	-0.126107	-3.833378
Si	-6.313260	-1.412566	-1.540348
Si	-5.253392	-2.994570	1.058063
Si	-3.293610	3.715764	0.672976
Si	-2.715345	2.256275	3.352480
C	-2.847653	-1.397167	-4.633289
H	-2.306038	-2.260033	-5.048516
H	-3.382847	-0.910142	-5.467123
H	-3.609001	-1.780834	-3.939511
C	-2.759511	1.377254	-3.400732
H	-3.209383	1.313760	-2.399817
H	-3.575933	1.482552	-4.135086
H	-2.161704	2.300786	-3.457838
C	-0.500388	0.479574	-5.161464
H	0.129902	1.302087	-4.787442
H	-1.085170	0.877252	-6.009943
H	0.163911	-0.302926	-5.552071
C	1.273401	-2.987165	-1.498295
H	2.121142	-2.312061	-1.674434
H	1.619267	-4.018898	-1.662826
H	1.002825	-2.868689	-0.446082
C	0.624109	-2.723879	-4.386618
H	1.082837	-3.725360	-4.472485

H	1.428368	-1.986686	-4.540329
H	-0.097012	-2.624395	-5.211492
C	-1.451593	-3.931198	-2.517418
H	-2.331567	-3.746955	-3.151001
H	-1.796497	-4.059543	-1.482885
H	-1.011904	-4.892263	-2.837719
C	-5.950563	0.076055	-2.629523
H	-4.977553	-0.011590	-3.126755
H	-5.949097	1.015368	-2.053253
H	-6.722877	0.163504	-3.413568
C	-6.076298	-2.980727	-2.564422
H	-6.565458	-2.870338	-3.547678
H	-6.524611	-3.857409	-2.069326
H	-5.014329	-3.209077	-2.744459
C	-8.131177	-1.293041	-1.035580
H	-8.753616	-1.085884	-1.923678
H	-8.294324	-0.467809	-0.320900
H	-8.512029	-2.215239	-0.572206
C	-7.020011	-3.560934	1.415119
H	-7.649029	-2.742052	1.801959
H	-7.000697	-4.355049	2.182148
H	-7.518901	-3.978269	0.525733
C	-4.343890	-4.402013	0.206859
H	-4.237806	-5.254834	0.899848
H	-3.334345	-4.099480	-0.098687
H	-4.876217	-4.761515	-0.686175
C	-4.427348	-2.596176	2.696659
H	-4.366277	-3.480518	3.352090
H	-4.985098	-1.813697	3.239029
H	-3.406844	-2.225539	2.533056
C	-3.222302	5.276914	1.740251
H	-3.682368	6.106308	1.175478
H	-2.180593	5.565773	1.957190
H	-3.753719	5.196544	2.698347
C	-2.782495	4.359129	-1.028333

H	-1.803778	4.864486	-1.039139
H	-3.536556	5.120956	-1.300326
H	-2.801052	3.601931	-1.823501
C	-5.086090	3.188468	0.397610
H	-5.141464	2.403698	-0.372676
H	-5.650032	4.061124	0.023203
H	-5.601006	2.818177	1.293073
C	-1.773029	3.608533	4.286428
H	-1.562630	3.279420	5.318393
H	-2.360048	4.536894	4.353147
H	-0.810672	3.855787	3.814140
C	-2.364971	0.566534	4.078440
H	-2.997795	-0.193042	3.598367
H	-2.595814	0.567956	5.157283
H	-1.323573	0.260202	3.956589
C	-4.551375	2.520015	3.739484
H	-5.193221	1.732769	3.312822
H	-4.952409	3.494587	3.426707
H	-4.659012	2.459894	4.837556
C	2.590571	0.810357	-0.293838
C	2.630399	-1.553639	1.184079
C	1.324914	0.343650	0.260273
C	3.732648	-0.021087	-0.228000
C	3.793182	-1.236148	0.468437
C	1.447580	-0.780690	1.181299
H	4.643485	0.348397	-0.703307
H	2.676724	-2.395382	1.871226
C	2.946049	2.222162	-0.839766
H	4.045933	2.200786	-0.677232
C	0.507846	-1.037998	2.369462
H	-0.436773	-0.491874	2.218191
C	5.069898	-2.062978	0.601312
H	4.968475	-2.653679	1.534668
Si	6.678357	-1.077138	0.888725
Si	5.194714	-3.405970	-0.750286

Si	-0.039115	-2.837019	2.739880
Si	1.389602	-0.207546	3.884105
Si	2.854846	3.703602	0.378858
Si	3.213728	2.461427	-2.750992
C	3.959249	-4.764864	-0.315414
H	4.376138	-5.396399	0.488564
H	3.746310	-5.421187	-1.176624
H	3.005603	-4.351952	0.039287
C	6.881436	-4.260799	-0.800634
H	7.146635	-4.696523	0.176493
H	7.702637	-3.595514	-1.109605
H	6.838944	-5.090587	-1.528631
C	4.896548	-2.656769	-2.454085
H	4.876274	-3.442743	-3.228579
H	5.705118	-1.953879	-2.714359
H	3.947967	-2.105461	-2.507090
C	7.453925	-0.447037	-0.717125
H	7.735562	-1.268847	-1.394448
H	8.371310	0.124829	-0.491756
H	6.778874	0.222926	-1.273204
C	7.935104	-2.179423	1.773188
H	8.425833	-2.897032	1.099833
H	7.461006	-2.753466	2.587995
H	8.723700	-1.554343	2.227237
C	6.376739	0.407706	2.005248
H	6.055238	0.092303	3.010486
H	5.600529	1.070591	1.600890
H	7.306248	0.993144	2.117291
C	-1.229372	-2.913548	4.211150
H	-1.905497	-2.054327	4.295458
H	-0.687746	-3.006439	5.163606
H	-1.855033	-3.815448	4.101529
C	-0.933871	-3.592464	1.264675
H	-1.660398	-4.341323	1.617547
H	-0.245351	-4.102640	0.577604

H	-1.480276	-2.829104	0.691641
C	1.369430	-4.003497	3.237177
H	2.006963	-3.574379	4.027689
H	2.017222	-4.299398	2.397932
H	0.924179	-4.927792	3.646832
C	1.143793	1.658201	3.771314
H	2.001362	2.195343	4.207289
H	0.250189	1.958683	4.332190
H	1.024630	1.990109	2.730836
C	0.783320	-0.739841	5.599232
H	1.086777	-1.770500	5.843628
H	-0.302080	-0.661392	5.746700
H	1.269764	-0.076351	6.337298
C	3.243566	-0.547819	3.947097
H	3.775890	-0.119520	3.089626
H	3.480422	-1.622554	3.984042
H	3.643486	-0.088059	4.869102
C	3.750425	3.155865	1.941913
H	3.446888	2.152483	2.267574
H	3.562647	3.856461	2.772547
H	4.838173	3.135890	1.764987
C	3.874609	5.122124	-0.344432
H	3.470429	5.534948	-1.281615
H	4.915831	4.812164	-0.531903
H	3.908304	5.945232	0.390948
C	1.191950	4.446785	0.884675
H	1.393031	5.211431	1.656703
H	0.512716	3.706191	1.328796
H	0.666143	4.958336	0.061091
C	5.059333	2.810221	-2.978614
H	5.340798	3.801080	-2.587234
H	5.313147	2.798225	-4.053017
H	5.691113	2.056907	-2.479273
C	2.341829	3.907244	-3.625937
H	2.122291	4.744816	-2.944500

H	1.392919	3.619530	-4.103053
H	3.010943	4.292450	-4.416652
C	2.839070	0.831147	-3.611433
H	3.570813	0.067409	-3.305960
H	2.896981	0.945291	-4.707073
H	1.841400	0.440249	-3.366434
In	-0.000670	2.618419	-1.528255
N	0.119375	1.031686	-0.041875

Tbt2-In≡N-Tbt2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.030948	1.291197	-0.073561
C	-3.789352	-1.439291	-0.269406
C	-4.207694	0.811525	0.536811
C	-2.230082	0.351352	-0.778930
C	-2.611992	-1.011968	-0.920509
C	-4.582950	-0.546479	0.483091
H	-4.848305	1.502283	1.086988
H	-4.087822	-2.485231	-0.341318
C	-2.659088	2.768553	-0.016157
H	-1.558232	2.866958	-0.154167
C	-5.821490	-1.009170	1.218661
H	-6.261975	-0.113727	1.702272
C	-1.789094	-1.985028	-1.754379
H	-0.842873	-1.471669	-2.044814
Si	-1.151790	-3.535885	-0.831817
Si	-2.594077	-2.264538	-3.462624

Si	-7.190626	-1.572280	0.018564
Si	-5.383149	-2.111041	2.712460
Si	-3.392559	3.672646	-1.539724
Si	-2.917818	3.652543	1.661760
C	-4.293421	-3.059287	-3.327393
H	-4.254058	-4.052559	-2.855388
H	-4.727872	-3.183935	-4.334309
H	-4.984174	-2.433831	-2.743613
C	-2.777511	-0.577644	-4.278202
H	-3.452430	0.065597	-3.691978
H	-3.191873	-0.668641	-5.296545
H	-1.806437	-0.060189	-4.357846
C	-1.481360	-3.345017	-4.534740
H	-0.445664	-2.969307	-4.557552
H	-1.855893	-3.353444	-5.573022
H	-1.451927	-4.389927	-4.186031
C	0.458772	-4.134691	-1.604998
H	0.350680	-4.440616	-2.655789
H	0.829602	-5.006222	-1.038298
H	1.242598	-3.363730	-1.559311
C	-2.382291	-4.965096	-0.851545
H	-2.004126	-5.784417	-0.215675
H	-2.512066	-5.372509	-1.867593
H	-3.375947	-4.685998	-0.470252
C	-0.761088	-3.012728	0.924432
H	-1.644830	-2.632280	1.457664
H	-0.006469	-2.208830	0.919590
H	-0.339798	-3.848876	1.505867
C	-7.091593	-0.474871	-1.511292
H	-6.105857	-0.543598	-1.996571
H	-7.250632	0.582701	-1.241785
H	-7.859594	-0.753789	-2.252637
C	-7.033051	-3.385032	-0.475322
H	-7.728910	-3.619773	-1.299101
H	-7.281041	-4.049525	0.368688

H	-6.019735	-3.641541	-0.818758
C	-8.868963	-1.304879	0.837011
H	-9.682621	-1.436695	0.102890
H	-8.953502	-0.282811	1.244795
H	-9.047678	-2.009760	1.664382
C	-6.941530	-2.410638	3.732472
H	-7.483146	-1.471590	3.935839
H	-6.685366	-2.865206	4.705035
H	-7.639726	-3.094494	3.222501
C	-4.633142	-3.773601	2.240214
H	-4.411628	-4.348240	3.156706
H	-3.685410	-3.651406	1.696494
H	-5.306328	-4.383992	1.619600
C	-4.116696	-1.175554	3.748656
H	-3.840763	-1.745531	4.652608
H	-4.502120	-0.195348	4.076166
H	-3.195055	-0.993421	3.172720
C	-3.208282	5.544317	-1.410149
H	-3.535515	6.005912	-2.358127
H	-2.159137	5.837621	-1.244316
H	-3.812298	5.983600	-0.601422
C	-2.433321	3.139300	-3.072862
H	-1.373593	3.443318	-3.003441
H	-2.846926	3.616361	-3.978412
H	-2.471835	2.051228	-3.226686
C	-5.205180	3.206471	-1.722711
H	-5.316931	2.126612	-1.904932
H	-5.664152	3.745835	-2.568710
H	-5.780579	3.450709	-0.815292
C	-1.859276	5.219637	1.701683
H	-1.471012	5.385913	2.720539
H	-2.438415	6.111302	1.415614
H	-0.987985	5.161274	1.032059
C	-2.348288	2.499243	3.028684
H	-2.968695	1.593651	3.093838

H	-2.380099	3.004525	4.008839
H	-1.309978	2.177469	2.855764
C	-4.709856	4.169831	1.964737
H	-5.412565	3.322135	1.989053
H	-5.064569	4.876966	1.197337
H	-4.779789	4.682913	2.940084
C	3.507456	0.566080	-0.860136
C	3.624098	-0.483041	1.748780
C	2.439808	0.845502	0.062034
C	4.502084	-0.357234	-0.490072
C	4.565225	-0.924710	0.799252
C	2.562038	0.380112	1.430874
H	5.265501	-0.619431	-1.227323
H	3.726043	-0.848980	2.771972
C	3.625757	1.247309	-2.221624
H	4.690966	1.094023	-2.495509
C	1.614194	0.887662	2.515058
H	0.621183	1.051470	2.050962
C	5.629448	-1.932397	1.185969
H	5.542697	-2.098438	2.279111
Si	7.386316	-1.230504	0.980978
Si	5.227714	-3.642550	0.457677
Si	1.338288	-0.218582	4.050233
Si	2.198584	2.655071	3.010061
Si	3.604040	3.158836	-2.202452
Si	2.813083	0.426624	-3.740370
C	3.541646	-4.177873	1.117658
H	3.537304	-4.236030	2.219167
H	3.260765	-5.171893	0.728010
H	2.756702	-3.464902	0.819474
C	6.525481	-4.904704	0.996807
H	6.667416	-4.898738	2.090769
H	7.505424	-4.706361	0.531841
H	6.220102	-5.924708	0.705237
C	5.128457	-3.632926	-1.423980

H	4.935723	-4.653830	-1.798047
H	6.054410	-3.269165	-1.894944
H	4.301856	-2.991279	-1.764061
C	8.102877	-1.517888	-0.742920
H	8.221199	-2.592133	-0.961149
H	9.099609	-1.050214	-0.823094
H	7.469845	-1.081404	-1.532308
C	8.517912	-2.052664	2.249360
H	8.661582	-3.125728	2.044861
H	8.099214	-1.959709	3.266479
H	9.513288	-1.575505	2.255401
C	7.325533	0.621263	1.324307
H	6.878495	0.823585	2.312034
H	6.708409	1.143994	0.576913
H	8.336235	1.064129	1.309682
C	-0.271109	0.249478	4.923354
H	-1.138805	0.110247	4.259611
H	-0.298482	1.281810	5.298202
H	-0.412347	-0.423047	5.788156
C	1.140871	-2.049899	3.647943
H	1.242472	-2.637196	4.577736
H	1.874941	-2.429020	2.923988
H	0.136564	-2.247018	3.247396
C	2.741718	-0.085230	5.313958
H	2.868292	0.934166	5.708675
H	3.713189	-0.401907	4.902589
H	2.516035	-0.744850	6.170616
C	1.744703	3.915065	1.688561
H	2.343392	3.799497	0.778942
H	1.886962	4.939775	2.075229
H	0.691591	3.798695	1.396617
C	1.379826	3.312988	4.587311
H	1.572449	2.711159	5.487636
H	0.288225	3.406251	4.468848
H	1.773581	4.327607	4.777175

C	4.066090	2.641610	3.255078
H	4.582218	2.319623	2.338347
H	4.369834	1.956240	4.061303
H	4.428531	3.651225	3.515186
C	4.659743	3.691242	-0.734213
H	4.340929	3.194788	0.192751
H	4.620872	4.781523	-0.571462
H	5.713509	3.413177	-0.908992
C	4.505147	3.719499	-3.774596
H	3.925604	3.516582	-4.690653
H	5.487994	3.231010	-3.885481
H	4.678773	4.809386	-3.736942
C	1.952658	4.073454	-2.218217
H	1.396397	3.922281	-1.284849
H	1.319205	3.739331	-3.054794
H	2.138730	5.154242	-2.356115
C	4.168127	0.210149	-5.041707
H	4.569066	1.181362	-5.374999
H	3.789984	-0.319848	-5.933193
H	5.012107	-0.375411	-4.637279
C	1.413373	1.379278	-4.590612
H	1.744071	2.364664	-4.955655
H	0.535247	1.548262	-3.944346
H	1.068096	0.802243	-5.467245
C	2.162245	-1.289157	-3.313045
H	2.978461	-1.952866	-2.990418
H	1.675504	-1.753155	-4.188579
H	1.425676	-1.263234	-2.492670
In	-0.215184	0.846172	-1.143684
N	1.337473	1.584816	-0.330550

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Ar*2-In=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.133668	-0.664092	-0.156751
N	-1.973340	-2.191737	-0.129949
H	3.014833	-0.447633	-4.451495
C	2.123719	-0.003698	-4.001778
C	-0.149591	1.129054	-2.802426
C	1.832538	-0.296499	-2.648258
C	1.299559	0.833276	-4.760348
C	0.192068	1.422529	-4.142287
C	0.633472	0.199723	-2.045880
H	1.529577	1.041666	-5.809398
H	-0.433441	2.124606	-4.697270
C	2.901978	-1.108834	-1.960654
C	5.128378	-2.677618	-1.115839
C	2.804042	-2.525772	-1.905093
C	4.129175	-0.478385	-1.595925
C	5.213333	-1.278912	-1.190630
C	3.907001	-3.279234	-1.460342
H	6.159744	-0.799679	-0.925764
H	3.821920	-4.367054	-1.429769
C	-1.331653	1.907446	-2.280923
C	-3.606159	3.505566	-1.622275
C	-2.652628	1.406805	-2.484686
C	-1.159086	3.241449	-1.800683
C	-2.302195	3.992591	-1.456485
C	-3.754064	2.215703	-2.151497
H	-2.151810	5.006763	-1.076045
H	-4.763045	1.826248	-2.300290
C	1.589507	-3.250498	-2.476503
H	0.741988	-2.546557	-2.495590

C	1.165613	-4.467941	-1.645911
H	1.937845	-5.253979	-1.640986
H	0.253351	-4.909209	-2.071357
H	0.954930	-4.187888	-0.603637
C	1.872556	-3.664734	-3.938263
H	2.136619	-2.794142	-4.556949
H	0.986653	-4.149526	-4.381123
H	2.712233	-4.378989	-3.977354
C	4.329953	1.032526	-1.708132
H	3.334963	1.490719	-1.758701
C	5.053925	1.638287	-0.492559
H	6.101348	1.298356	-0.428043
H	4.548976	1.382913	0.446316
H	5.074859	2.736004	-0.579969
C	5.087978	1.403706	-3.001723
H	4.554018	1.060059	-3.898391
H	6.093028	0.948719	-3.006437
H	5.207737	2.498127	-3.072901
C	6.351730	-3.509301	-0.749002
H	7.131960	-2.805475	-0.408028
C	6.080662	-4.501734	0.398016
H	5.328780	-5.254011	0.108426
H	5.709226	-3.982236	1.294652
H	7.003698	-5.041882	0.667736
C	6.896040	-4.241562	-1.995645
H	7.109827	-3.529150	-2.808501
H	6.159617	-4.970690	-2.372565
H	7.824164	-4.788093	-1.756868
C	-2.912126	0.060222	-3.161151
H	-2.053110	-0.597682	-2.956615
C	-3.015043	0.244004	-4.694104
H	-3.842181	0.931916	-4.938903
H	-3.219401	-0.724650	-5.180648
H	-2.091170	0.654411	-5.124020
C	-4.181306	-0.647714	-2.650493

H	-4.219306	-0.691542	-1.554299
H	-4.200130	-1.682998	-3.023044
H	-5.093521	-0.149173	-3.021223
C	-4.832946	4.360741	-1.327859
H	-5.700965	3.678253	-1.301676
C	-5.062134	5.368088	-2.476633
H	-5.139747	4.848468	-3.444898
H	-4.220081	6.077616	-2.541464
H	-5.986540	5.947934	-2.314084
C	-4.763012	5.085556	0.029131
H	-3.941665	5.819758	0.052532
H	-4.605913	4.375713	0.855130
H	-5.700186	5.634472	0.219416
C	0.153204	4.040014	-1.769801
H	-0.020457	4.841299	-1.031172
C	0.369276	4.759441	-3.123337
H	1.204823	5.475651	-3.043780
H	-0.534435	5.310811	-3.427309
H	0.617646	4.039349	-3.916723
C	1.438785	3.319349	-1.343660
H	2.220656	4.066895	-1.134912
H	1.805278	2.664979	-2.141601
H	1.303400	2.715396	-0.435479
H	0.861336	0.019470	5.145083
C	0.236428	-0.420245	4.362629
C	-1.403118	-1.469181	2.335379
C	0.461146	-0.045855	3.018832
C	-0.804653	-1.298632	4.698316
C	-1.652946	-1.778380	3.689434
C	-0.319869	-0.627084	1.987962
H	-0.980797	-1.566781	5.744849
H	-2.534150	-2.366199	3.953146
C	1.455133	1.042999	2.768816
C	3.328446	3.156530	2.511944
C	0.993893	2.372375	2.530506

C	2.840361	0.779397	2.897532
C	3.753141	1.844584	2.768194
C	1.945849	3.397947	2.400226
H	4.824768	1.647346	2.867204
H	1.602455	4.416591	2.217855
C	-2.442645	-1.872980	1.293227
C	-4.995146	-3.103252	0.650146
C	-2.481740	-3.293410	0.801889
C	-3.751787	-1.167167	1.551137
C	-4.928893	-1.756921	1.194822
C	-3.844373	-3.828565	0.514652
H	-5.864784	-1.208125	1.336100
H	-3.922574	-4.866318	0.176635
C	-0.504874	2.694091	2.495437
H	-1.000331	1.887346	1.933409
C	-0.848745	4.018835	1.798797
H	-0.546059	4.886776	2.408291
H	-1.935547	4.086507	1.642980
H	-0.365990	4.101099	0.819253
C	-1.108770	2.705919	3.917867
H	-0.998157	1.737413	4.420621
H	-2.183894	2.946285	3.869582
H	-0.612290	3.474964	4.533281
C	3.352610	-0.625768	3.203812
H	2.478331	-1.289217	3.272317
C	4.245393	-1.170971	2.076814
H	5.157253	-0.566100	1.948792
H	3.718022	-1.177090	1.112852
H	4.557878	-2.203869	2.299026
C	4.072412	-0.670698	4.566666
H	3.419626	-0.296362	5.371503
H	4.983457	-0.049635	4.558925
H	4.369774	-1.703601	4.814094
C	4.340505	4.292565	2.423384
H	5.337109	3.829366	2.312792

C	4.112781	5.212482	1.208800
H	3.148176	5.740774	1.278747
H	4.113895	4.640269	0.269284
H	4.905158	5.977229	1.151377
C	4.341809	5.107755	3.735379
H	5.120753	5.888715	3.714623
H	4.523187	4.454459	4.603693
H	3.366663	5.601331	3.883544
C	-1.506190	-4.376607	1.335965
H	-0.526792	-3.889955	1.467284
C	-1.370374	-5.524184	0.315590
H	-2.223546	-6.218866	0.387124
H	-0.458604	-6.112328	0.506762
H	-1.332341	-5.135894	-0.709103
C	-1.915706	-5.003504	2.697113
H	-1.856973	-4.295669	3.533323
H	-1.242668	-5.847638	2.936450
H	-2.941405	-5.406968	2.658993
C	-6.344363	-3.658780	0.208333
H	-6.189691	-4.718712	-0.060549
C	-6.821666	-2.916350	-1.060518
H	-6.070829	-2.991720	-1.861402
H	-6.980616	-1.845000	-0.853665
H	-7.774390	-3.335100	-1.427312
C	-7.422408	-3.605228	1.311780
H	-7.088491	-4.126279	2.223389
H	-8.354316	-4.081944	0.961987
H	-7.669626	-2.566575	1.586738
C	-3.734468	0.233938	2.159188
H	-2.734055	0.409593	2.573902
C	-4.730647	0.409838	3.319584
H	-4.559914	-0.344999	4.103344
H	-5.774745	0.316550	2.979872
H	-4.614397	1.409473	3.771938
C	-3.950928	1.291547	1.064052

H	-3.864603	2.306507	1.482983
H	-4.947327	1.191617	0.604323
H	-3.210308	1.194976	0.258958

In=N-Ar*2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.944478	-2.435422	0.841322
C	4.529848	-0.334302	1.783634
C	2.322926	-1.294662	1.440412
C	4.344035	-2.463045	0.697089
C	5.159261	-1.419734	1.162202
C	3.135382	-0.257406	1.958144
H	4.810866	-3.348371	0.260466
H	5.146363	0.471896	2.190444
C	2.171321	-3.735559	0.567204
H	1.094807	-3.502516	0.550479
C	2.402472	-4.729883	1.730234
H	1.794045	-5.638836	1.588254
H	3.463389	-5.028707	1.767676
H	2.141078	-4.287187	2.699926
C	2.530375	-4.444528	-0.753010
H	3.582147	-4.771219	-0.766125
H	2.371466	-3.807415	-1.635639
H	1.905294	-5.344511	-0.874100
C	2.656899	0.862899	2.883903
H	3.312505	1.718179	2.650634
C	2.940253	0.473237	4.355676

H	3.990712	0.174900	4.497352
H	2.302084	-0.369252	4.665010
H	2.725556	1.322733	5.026495
C	1.207588	1.343005	2.744748
H	0.934742	1.504123	1.695347
H	1.085112	2.293113	3.285264
H	0.494845	0.631207	3.175331
C	6.680385	-1.506321	1.142389
H	7.062304	-0.478065	1.253520
C	7.175058	-2.316401	2.362618
H	6.813343	-3.356967	2.307356
H	6.800047	-1.880627	3.302388
H	8.277717	-2.338122	2.402064
C	7.254644	-2.085690	-0.161752
H	6.990282	-3.149224	-0.281075
H	8.355310	-2.019825	-0.158505
H	6.875902	-1.544206	-1.040728
C	-5.430920	-2.108530	-0.479232
C	-2.829598	-1.671175	0.624553
C	-5.216510	-1.180856	0.547478
C	-4.328657	-2.865645	-0.905253
C	-3.046774	-2.684294	-0.358934
C	-3.952962	-0.971202	1.140245
H	-6.062694	-0.610514	0.935875
H	-4.488841	-3.645896	-1.653791
C	-6.822481	-2.389941	-1.034517
H	-6.692877	-3.035755	-1.921444
C	-7.564793	-1.118297	-1.484636
H	-6.983418	-0.556557	-2.232277
H	-7.758634	-0.448260	-0.632072
H	-8.540300	-1.377237	-1.928815
C	-7.659138	-3.177217	-0.001332
H	-7.140575	-4.100306	0.303667
H	-8.644357	-3.450557	-0.416254
H	-7.826916	-2.571477	0.904720

C	-3.997477	-0.082540	2.393095
H	-4.608376	0.782409	2.095439
C	-2.701655	0.491415	2.983893
H	-2.008950	0.837572	2.211785
H	-2.174867	-0.233005	3.617391
H	-2.968975	1.355375	3.612327
C	-4.772902	-0.818523	3.515464
H	-5.767149	-1.151743	3.181813
H	-4.904673	-0.152763	4.385299
H	-4.217202	-1.707322	3.855671
C	-1.980786	-3.730760	-0.686346
H	-0.996041	-3.312905	-0.412967
C	-2.190046	-4.977321	0.206063
H	-2.164423	-4.714364	1.272748
H	-1.407966	-5.731543	0.013713
H	-3.170483	-5.434643	-0.010426
C	-1.939856	-4.158037	-2.165055
H	-1.897110	-3.294796	-2.846527
H	-2.826843	-4.753425	-2.433903
H	-1.054370	-4.787316	-2.353004
C	-1.512241	-1.641572	1.357397
C	0.698395	-2.115201	3.019001
C	-0.252625	-1.033446	0.982888
C	-1.611122	-2.413461	2.540187
C	-0.544420	-2.608278	3.414060
C	0.870243	-1.418125	1.806691
H	-2.583891	-2.851028	2.769537
H	-0.665616	-3.175271	4.340648
H	1.586629	-2.317348	3.620099
C	3.101529	2.476537	-0.245596
C	5.018578	0.830856	-1.437065
C	2.657928	1.405225	-1.092350
C	4.471711	2.620805	0.044617
C	5.452312	1.795256	-0.521401
C	3.662785	0.648006	-1.764378

H	4.780848	3.446614	0.686941
H	5.770732	0.235823	-1.961374
C	2.192831	3.651128	0.134175
H	1.152822	3.308980	0.111925
C	2.345478	4.761773	-0.936306
H	1.660526	5.598616	-0.722796
H	3.377306	5.151905	-0.928707
H	2.127908	4.391928	-1.945698
C	2.472944	4.286605	1.509059
H	3.435502	4.823136	1.515482
H	2.489986	3.552410	2.320978
H	1.693609	5.029868	1.738449
C	3.384468	-0.224064	-2.984235
H	2.290389	-0.308994	-3.097307
C	3.979221	-1.638152	-2.870435
H	3.766087	-2.083970	-1.890835
H	5.074274	-1.615253	-2.985204
H	3.577162	-2.294441	-3.660082
C	3.887591	0.459778	-4.275421
H	3.463232	1.467271	-4.396594
H	3.611550	-0.139281	-5.159629
H	4.985289	0.558584	-4.259575
C	6.946919	2.015573	-0.313293
H	7.437479	1.035230	-0.444791
C	7.492734	2.954753	-1.413618
H	7.025236	3.950587	-1.333650
H	7.268694	2.558805	-2.416724
H	8.585442	3.078554	-1.322240
C	7.320445	2.547816	1.080203
H	6.956262	3.577255	1.229329
H	8.416246	2.568491	1.199011
H	6.900749	1.922121	1.882668
C	-5.071575	2.746437	0.585277
C	-2.526963	1.867596	-0.383459
C	-4.965894	1.855092	-0.490558

C	-3.878703	3.204942	1.163997
C	-2.618372	2.801160	0.694742
C	-3.726436	1.423892	-1.006827
H	-5.875757	1.492168	-0.974469
H	-3.937844	3.929368	1.980046
C	-6.419478	3.265748	1.070585
H	-6.223008	3.887436	1.962270
C	-7.375742	2.133498	1.490935
H	-6.923570	1.495539	2.266188
H	-7.632443	1.493186	0.631800
H	-8.317171	2.547475	1.889224
C	-7.072342	4.171650	0.004236
H	-6.395990	4.993485	-0.280420
H	-8.012912	4.608371	0.381161
H	-7.306488	3.598030	-0.908033
C	-3.846974	0.569867	-2.278915
H	-4.647883	-0.150653	-2.047765
C	-2.639161	-0.267723	-2.720180
H	-2.184001	-0.766658	-1.855560
H	-1.878307	0.339674	-3.229450
H	-2.978936	-1.048305	-3.421124
C	-4.344586	1.426816	-3.468909
H	-5.245153	2.004339	-3.209604
H	-4.586621	0.779819	-4.329399
H	-3.568118	2.137296	-3.792944
C	-1.385686	3.540871	1.213025
H	-0.509975	2.921620	0.985776
C	-1.243785	4.874932	0.444842
H	-1.148618	4.709765	-0.637006
H	-0.356705	5.429194	0.789958
H	-2.130153	5.507067	0.619388
C	-1.374926	3.820138	2.726199
H	-1.466555	2.899396	3.314907
H	-2.188033	4.501990	3.023232
H	-0.426628	4.307690	3.002020

C	-1.202102	1.765098	-1.103172
C	1.069672	2.236671	-2.694062
C	-0.013016	0.975034	-0.818776
C	-1.214329	2.656162	-2.201247
C	-0.136499	2.822095	-3.072023
C	1.196120	1.430245	-1.536987
H	-2.141360	3.202190	-2.384129
H	-0.211709	3.458422	-3.957266
H	1.981015	2.473605	-3.245412
In	0.495859	-1.641304	-1.920767
N	0.030818	-0.332294	-0.239387

Ar*-In≡N-Ar*

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.887103	3.168093	0.035716
C	-4.398647	1.408590	1.592539
C	-2.283641	2.535541	1.164501
C	-4.244005	2.937602	-0.250139
C	-5.030337	2.082581	0.535055
C	-3.049434	1.619913	1.942730
H	-4.699557	3.460479	-1.093158
H	-4.983892	0.704926	2.193339
C	-2.126712	4.161002	-0.843219
H	-1.067454	4.129069	-0.559233
C	-2.613370	5.602591	-0.589644
H	-2.024696	6.321642	-1.183914
H	-3.674503	5.719253	-0.865111

H	-2.508369	5.865947	0.474626
C	-2.213406	3.792749	-2.336762
H	-3.248980	3.835631	-2.710692
H	-1.837889	2.773178	-2.519525
H	-1.613422	4.493189	-2.939601
C	-2.577294	0.891789	3.206417
H	-3.260284	0.029936	3.306923
C	-2.798425	1.784925	4.449166
H	-3.832638	2.164094	4.483941
H	-2.115273	2.649017	4.437364
H	-2.606355	1.212256	5.372249
C	-1.153041	0.318494	3.195697
H	-0.974826	-0.320452	2.316737
H	-1.004908	-0.309992	4.088985
H	-0.392856	1.108792	3.221064
C	-6.535518	1.961376	0.341656
H	-6.836512	0.978468	0.735844
C	-7.246256	3.038114	1.195161
H	-6.968325	4.047903	0.848769
H	-6.958568	2.955700	2.255302
H	-8.342655	2.938009	1.121897
C	-6.989507	2.049252	-1.125223
H	-6.845994	3.063928	-1.532092
H	-8.063767	1.815448	-1.206579
H	-6.432143	1.345865	-1.762146
C	5.094607	1.986287	-1.315720
C	2.714085	2.484138	0.183813
C	4.918952	1.459012	-0.028043
C	4.021240	2.698878	-1.874194
C	2.839027	2.955697	-1.158795
C	3.756998	1.688911	0.738250
H	5.709985	0.857187	0.420690
H	4.127603	3.096269	-2.887636
C	6.420463	1.915928	-2.066848
H	6.186360	1.954925	-3.146247

C	7.242314	0.643323	-1.805958
H	6.670568	-0.266884	-2.040595
H	7.565990	0.583165	-0.754761
H	8.152546	0.645941	-2.427419
C	7.255749	3.172471	-1.723643
H	6.694117	4.094188	-1.943267
H	8.197136	3.189866	-2.298520
H	7.507982	3.179945	-0.649756
C	3.774856	1.076658	2.141736
H	4.431803	0.197365	2.049760
C	2.440474	0.547717	2.679532
H	1.944281	-0.105613	1.946752
H	1.756359	1.358643	2.957464
H	2.627995	-0.056069	3.581327
C	4.440564	2.033782	3.155667
H	5.416358	2.388092	2.786124
H	4.600875	1.519561	4.118426
H	3.805903	2.913405	3.345368
C	1.760868	3.810605	-1.824077
H	0.850543	3.742801	-1.215274
C	2.179116	5.295605	-1.841305
H	2.384792	5.653271	-0.820115
H	1.379604	5.920859	-2.273373
H	3.091835	5.441387	-2.442769
C	1.407893	3.308273	-3.237290
H	1.100855	2.249668	-3.220894
H	2.262188	3.393731	-3.927940
H	0.580989	3.900469	-3.658758
C	1.537290	2.957408	0.993713
C	-0.676650	4.029483	2.402061
C	0.240386	2.408656	0.834389
C	1.705487	4.042742	1.880457
C	0.611280	4.556341	2.597134
C	-0.880424	2.960052	1.504821
H	2.696441	4.488416	1.996404

H	0.757314	5.393003	3.286593
H	-1.535652	4.465539	2.918435
C	-3.227568	-2.902333	0.091123
C	-4.761794	-1.367891	-1.664091
C	-2.637591	-2.434923	-1.118000
C	-4.575498	-2.620611	0.370940
C	-5.374585	-1.872586	-0.505520
C	-3.416784	-1.636304	-1.998435
H	-5.015346	-3.027743	1.283046
H	-5.359886	-0.770212	-2.361525
C	-2.466941	-3.812152	1.052247
H	-1.410202	-3.796714	0.764904
C	-2.952195	-5.269334	0.905451
H	-2.368947	-5.942109	1.556584
H	-4.016520	-5.362239	1.180335
H	-2.838492	-5.611566	-0.135082
C	-2.554913	-3.333903	2.511841
H	-3.589458	-3.354125	2.891706
H	-2.174432	-2.307671	2.607473
H	-1.953184	-3.988135	3.163150
C	-2.964141	-1.111367	-3.366425
H	-3.627068	-0.253115	-3.579076
C	-3.236918	-2.165100	-4.465599
H	-4.273553	-2.533429	-4.402705
H	-2.559604	-3.025390	-4.357469
H	-3.080841	-1.731721	-5.468549
C	-1.523423	-0.589050	-3.471378
H	-1.310630	0.148025	-2.675914
H	-1.374628	-0.082451	-4.439913
H	-0.784651	-1.396463	-3.392606
C	-6.876157	-1.705498	-0.296963
H	-7.160818	-0.726564	-0.716780
C	-7.631521	-2.786775	-1.104659
H	-7.366385	-3.792256	-0.736626
H	-7.365179	-2.739514	-2.172146

H	-8.723936	-2.661034	-1.009773
C	-7.318498	-1.740576	1.176475
H	-7.206095	-2.749760	1.605385
H	-8.382853	-1.466567	1.262779
H	-6.731329	-1.046452	1.797634
C	4.847210	-2.460068	1.301896
C	2.380693	-2.625879	-0.138387
C	4.750949	-2.036570	-0.031413
C	3.662183	-2.871811	1.933304
C	2.436365	-2.953070	1.250655
C	3.545236	-2.098224	-0.763243
H	5.641417	-1.662818	-0.542562
H	3.708980	-3.170375	2.983705
C	6.183283	-2.581137	2.027185
H	5.958241	-2.726464	3.099061
C	7.086407	-1.340983	1.900771
H	6.587508	-0.436304	2.280741
H	7.371077	-1.160532	0.852335
H	8.017937	-1.483856	2.473523
C	6.925824	-3.842591	1.529919
H	6.291666	-4.737513	1.632063
H	7.857348	-4.004900	2.098948
H	7.188951	-3.737293	0.463972
C	3.634467	-1.594568	-2.209160
H	4.479674	-0.885940	-2.201967
C	2.423016	-0.794874	-2.710462
H	2.196885	0.029277	-2.012784
H	1.531019	-1.425015	-2.821926
H	2.648063	-0.342608	-3.690665
C	4.012707	-2.719134	-3.199859
H	4.865804	-3.303776	-2.818131
H	4.296740	-2.291774	-4.177054
H	3.170334	-3.406851	-3.363418
C	1.208524	-3.481905	1.990617
H	0.329089	-3.066476	1.487082

C	1.138497	-5.020417	1.897244
H	1.133940	-5.353052	0.848915
H	0.222599	-5.397047	2.382441
H	2.006544	-5.478919	2.401282
C	1.127529	-3.022731	3.457673
H	1.181686	-1.928034	3.537046
H	1.931676	-3.453717	4.076524
H	0.171250	-3.347141	3.896368
C	1.163616	-3.031965	-0.922591
C	-1.116499	-4.083071	-2.226649
C	-0.100783	-2.351860	-0.797678
C	1.252714	-4.192399	-1.711702
C	0.134316	-4.705507	-2.390944
C	-1.257160	-2.933878	-1.432963
H	2.210877	-4.715129	-1.768501
H	0.225699	-5.608055	-3.001436
H	-2.008249	-4.520356	-2.684061
In	-0.024029	0.604387	-0.244270
N	-0.215267	-1.246528	-0.005078

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M062X/Def2-TZVP

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F-In≡N-F

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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In	0.287136	-0.019627	-0.000002
N	-1.603652	0.658373	0.000122
F	-2.542670	-0.367793	-0.000040
F	2.226660	-0.037416	-0.000046

F2-In=N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.066754	0.000171	-0.000000
N	-2.140759	0.005878	-0.000001
F	1.009421	-1.605151	0.000000
F	1.019050	1.599648	0.000000

In=N-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.773362	0.013194	-0.004739
N	-1.435454	-0.009690	0.681327
F	-1.622681	1.064001	-0.256955
F	-1.471384	-1.128300	-0.247165

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F-In≡N-F-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.117497	-0.151276	0.029658
N	1.744062	-0.909540	-0.087890
F	-1.981601	0.246258	-0.078846
F	1.264812	1.284774	-0.014268

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F-In≡N-F-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.677601	-0.275521	-0.018403
N	-1.861363	-0.104382	0.667452
F	-2.563343	-0.123492	-0.405178
F	0.321910	1.704737	-0.013758

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HO-In≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.313790	-0.176079	-0.010855
N	1.582282	0.635680	-0.215476
O	2.685971	0.038781	0.246712
H	3.173543	-0.305331	-0.516882
O	-2.234115	0.379677	0.005263
H	-2.488669	1.135755	0.541324

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(OH)2-In≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.066874	0.037413	0.001597
N	-2.094799	0.676068	-0.003774
O	1.484873	1.260318	-0.003237
H	2.333756	0.808504	-0.001947
O	0.492763	-1.867448	-0.002167
H	-0.214407	-2.517175	-0.006660

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In≡N-(OH)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.928636	0.000000	0.000000
N	-1.204731	0.000000	0.000000
O	-2.016151	1.136572	-0.107065
H	-2.405819	1.266150	0.768861
O	-2.016151	-1.136572	0.107065
H	-2.405819	-1.266150	-0.768861

HO-In≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.163789	-0.169995	0.017114
N	-1.772868	-1.044506	-0.053469
O	-1.531882	1.343723	-0.093402
H	-2.093681	1.277313	0.688778
O	2.031161	0.395851	-0.139334
H	2.483884	0.447412	0.708810

HO-In≡N-OH-TS2

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
In	-0.726231	-0.189487	0.017038
N	1.268253	-0.369195	-0.231310
O	2.507312	-0.469577	-0.010656
H	2.689875	-0.493855	0.950753
O	0.356866	1.759139	-0.067875
H	1.104230	2.046580	0.461807

H-In≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.240264	0.012850	-0.000001
N	1.645868	-0.159921	0.000038
H	2.163146	0.719099	-0.000094
H	-1.911308	-0.229280	-0.000112

H2-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-0.000103	-0.225148	-0.000000
N	-0.000103	1.848159	0.000000
H	-1.559812	-0.960198	-0.000000
H	1.565597	-0.944660	-0.000000

In≡N-H

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

In	0.000000	-0.344806	0.000000
N	0.000000	1.745441	-0.000000
H	-0.820055	2.338691	-0.000000
H	0.820052	2.338694	-0.000000

H-In≡N-H-TS1

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

In	0.225413	0.003791	0.000000
N	-1.797669	-0.131090	0.000000
H	-0.051793	1.738886	-0.000000
H	1.590221	-1.007037	-0.000000

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H-In≡N-H-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.299408	-0.027115	0.001245
N	1.677469	-0.011452	-0.036066
H	2.638887	-0.285919	0.164440
H	0.289832	1.694696	0.027014

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3HC-In≡N-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.289205	-0.067272	0.004161
N	1.511744	0.517717	0.004307
C	-2.415420	0.110029	-0.013097
H	-2.683432	1.163302	-0.083022
H	-2.831410	-0.305463	0.902323
H	-2.825830	-0.421732	-0.868998
C	2.806061	-0.108732	-0.010520
H	3.013332	-0.740359	0.862836
H	3.566353	0.683688	-0.002064
H	3.005960	-0.714901	-0.903384

(CH3)-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.026881	2.220128	0.006884
In	0.000986	0.030554	-0.003177
C	-1.953098	-0.912587	0.005249
H	-2.516207	-0.591370	-0.871277
H	-2.503207	-0.586032	0.888388
H	-1.886364	-1.998257	0.008493
C	1.970483	-0.879901	0.009090
H	2.702683	-0.176496	0.400738
H	2.256595	-1.140311	-1.010931
H	1.982056	-1.790640	0.606043

In≡N-(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.925690	0.000000	0.000000
N	1.177522	0.000000	-0.000010
C	1.986407	1.193386	0.000002

H	1.359693	2.091588	-0.000020
H	2.639986	1.251435	-0.883635
H	2.639944	1.251443	0.883670
C	1.986408	-1.193386	0.000001
H	2.639983	-1.251416	0.883643
H	1.359692	-2.091587	0.000041
H	2.639947	-1.251462	-0.883663

3HC-In≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.695102	-0.307292	0.000934
N	1.317234	-0.197917	-0.018106
C	-0.110848	1.983709	-0.000198
H	0.635074	2.153087	-0.765117
H	0.256467	2.215285	0.993521
H	-1.047553	2.488051	-0.219113
C	2.715663	-0.272533	0.009390
H	3.143281	-0.645428	0.949880
H	3.066093	0.772306	-0.090162
H	3.157109	-0.807640	-0.843204

3HC-In≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.679157	-0.322721	-0.004217
N	1.325389	-0.134820	0.084530
C	-0.196279	1.991524	-0.002546
H	0.387412	2.242369	-0.878947
H	0.303267	2.256036	0.920852
H	-1.203661	2.394766	-0.052581
C	2.721151	-0.207200	-0.030690
H	2.988937	-1.277658	-0.050201
H	3.254433	0.210995	0.834410
H	3.121329	0.224630	-0.959214

3HSi-In≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.308016	0.035134	-0.005477
N	1.514418	0.469310	0.008974
Si	-2.833958	-0.100867	0.007299
H	-3.384964	1.223912	0.349456
H	-3.230764	-1.097542	1.019420
H	-3.290913	-0.519072	-1.330711
Si	3.085719	-0.153970	0.004058
H	3.343583	-1.155350	1.077123
H	4.074367	0.937271	0.203177
H	3.455901	-0.828232	-1.271914

(SiH3)-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.020998	2.377357	-0.001182
In	-0.000739	0.336091	0.000464
Si	2.281488	-0.928759	-0.000332
H	3.471449	-0.053764	-0.014926
H	2.316931	-1.805939	-1.192636
H	2.332886	-1.788222	1.204159
Si	-2.287660	-0.917950	-0.000406
H	-2.334303	-1.788064	1.196678
H	-3.472667	-0.036175	0.002830
H	-2.338647	-1.783833	-1.200239

In≡N-(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.292757	-0.000075	-0.000019
N	-0.877641	0.000001	0.000598
Si	-1.645480	1.523213	0.000236

H	-0.577666	2.563669	0.085321
H	-2.558780	1.730545	1.150443
H	-2.424011	1.798115	-1.232423
Si	-1.645873	-1.523020	-0.000333
H	-2.561497	-1.727588	-1.149230
H	-0.578570	-2.563686	-0.089277
H	-2.422114	-1.800088	1.233276

3HSi-In≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.480722	-1.616390	-0.002469
In	-0.154290	-0.394111	0.001032
Si	-2.513146	0.672776	-0.003763
H	-3.498120	-0.429881	0.101365
H	-2.743451	1.443570	-1.247753
H	-2.654710	1.567416	1.169934
Si	2.383843	1.025534	0.001155
H	2.425518	1.579098	1.375052
H	3.716526	0.651114	-0.500895
H	1.759643	2.038502	-0.894450

3HSi-In≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.670907	-0.780203	0.000085
N	-1.090800	0.061614	-0.001477
Si	1.360132	1.784301	0.000056
H	0.841608	2.407351	-1.236461
H	2.845134	1.848076	0.003191
H	0.836387	2.409731	1.233107
Si	-2.775863	0.338653	0.000275
H	-3.484263	-0.207745	-1.196529
H	-2.976243	1.820591	-0.003794
H	-3.481233	-0.200708	1.202040

B3PW91/DeF2-TZVP

F-In≡N-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.287136	-0.019627	-0.000002
N	-1.603652	0.658373	0.000122
F	-2.542670	-0.367793	-0.000040
F	2.226660	-0.037416	-0.000046

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F2-In=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.070579	0.010629	-0.000448
N	-2.118120	0.185371	0.001087
F	0.853876	-1.689972	0.000786
F	1.177813	1.487924	0.000805

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In=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.797932	0.060183	-0.009429
N	-1.428104	0.000221	0.667007
F	-1.991081	0.893029	-0.268563
F	-1.242470	-1.220862	-0.198884

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F-In≡N-F-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.000000	0.162884	0.000000
N	2.015122	-0.029054	0.000000
F	-1.745473	0.948336	-0.000000
F	0.178156	-1.812549	-0.000000

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F-In≡N-F-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.694880	-0.211061	-0.034646
N	-1.617059	-0.567780	0.516060
F	-2.486750	-0.059667	-0.315314
F	-0.038772	1.650381	0.102564

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HO-In≡N-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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In	-0.318983	-0.200858	0.003576
N	1.555575	0.656590	-0.117011
O	2.708899	0.060953	0.166044
H	3.134073	-0.161523	-0.679582
O	-2.202287	0.476937	-0.077243
H	-2.445835	1.104309	0.613035

(OH)2-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.073940	0.038026	0.001347
N	-2.114425	0.572684	-0.003260
O	1.440961	1.310082	-0.002597
H	2.281865	0.840102	-0.002900
O	0.591814	-1.838335	-0.001609
H	-0.120050	-2.486128	-0.006657

In≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.924191	0.000000	0.000000

N	-1.200033	0.000000	-0.000000
O	-2.006905	1.143697	-0.108103
H	-2.387324	1.280019	0.772721
O	-2.006905	-1.143698	0.108103
H	-2.387324	-1.280019	-0.772721

HO-In≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.058531	0.112006	-0.015061
N	1.541519	1.354027	0.045470
O	1.068915	-1.556889	0.060064
H	1.957261	-1.435914	-0.291200
O	-1.991649	-0.210382	0.024195
H	-2.498012	0.607575	0.036835

HO-In≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.722930	-0.194826	0.017766
N	1.270914	-0.340476	-0.256652

O	2.517664	-0.462290	-0.001500
H	2.669621	-0.507230	0.966450
O	0.327810	1.771558	-0.064274
H	1.093774	1.962877	0.485766

H-In≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.239236	0.013264	0.000005
N	1.639724	-0.162278	-0.000021
H	2.142790	0.727704	-0.000018
H	-1.898308	-0.241696	-0.000081

H2-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.001667	-0.214743	0.000000
N	0.001667	1.800824	0.000000
H	-1.542830	-0.962459	0.000000
H	1.449506	-1.120920	0.000000

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In≡N-H2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000000	-0.343041	-0.000000
N	0.000000	1.736419	-0.000000
H	-0.822054	2.327025	0.000000
H	0.822052	2.327029	-0.000000

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H-In≡N-H-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.215595	-0.001442	0.000000
N	-1.786416	-0.069118	-0.000000
H	0.486945	1.711943	-0.000000
H	1.453820	-1.157435	-0.000000

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H-In≡N-H-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.297986	-0.027236	0.001349
N	1.671632	-0.007227	-0.040298
H	2.624363	-0.295774	0.183803
H	0.275505	1.680928	0.032200

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3HC-In≡N-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.287593	-0.070367	-0.000154
N	1.503586	0.525288	-0.000138
C	-2.403610	0.118214	0.000549
H	-2.663892	1.176964	-0.031283
H	-2.811437	-0.329492	0.905849
H	-2.816462	-0.384029	-0.873282
C	2.789893	-0.107112	0.000400
H	2.996985	-0.724373	0.886146
H	3.546883	0.690835	-0.000105
H	2.997164	-0.725525	-0.884519

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(CH3)2-In≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.038664	2.215226	-0.004945
In	0.001286	0.028379	0.002549
C	-1.943971	-0.912903	-0.004411
H	-2.482805	-0.614836	-0.905797
H	-2.509673	-0.549875	0.855806
H	-1.876380	-1.999198	0.036824
C	1.968081	-0.867269	-0.000291
H	2.682624	-0.192535	0.474233
H	2.280869	-1.028678	-1.036738
H	1.968329	-1.831021	0.513598

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In≡N-(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.921071	0.000004	-0.000001
N	1.175025	0.000006	0.000020
C	1.975016	1.195937	-0.000003
H	1.342726	2.091582	0.000023
H	2.630510	1.263161	-0.884514
H	2.630573	1.263153	0.884461
C	1.974963	-1.195961	-0.000004
H	2.630506	-1.263216	0.884468

H	1.342631	-2.091578	0.000010
H	2.630463	-1.263209	-0.884509

3HC-In≡N-CH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.702186	-0.297513	0.000144
N	1.302785	-0.216765	-0.005779
C	-0.035988	1.989522	-0.000062
H	0.630334	2.195011	-0.828169
H	0.398252	2.202868	0.969630
H	-1.017180	2.439639	-0.130345
C	2.694156	-0.310032	0.002722
H	3.123993	-0.752477	0.916542
H	3.074760	0.729886	-0.023708
H	3.128449	-0.796359	-0.886521

3HC-In≡N-CH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.027092	-0.113269	0.002173

N	-1.056925	-1.800076	-0.005862
C	2.112632	0.399100	-0.005372
H	2.294044	1.139256	-0.784471
H	2.727010	-0.481720	-0.182426
H	2.367568	0.833507	0.961739
C	-1.480370	1.498688	-0.003490
H	-1.397193	2.027120	0.945723
H	-2.475376	1.079587	-0.122969
H	-1.238656	2.166265	-0.829854

3HSi-In≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.296471	0.066068	-0.012717
N	1.513752	0.551340	0.026674
Si	-2.811976	-0.158225	0.017726
H	-3.395513	1.147066	0.414019
H	-3.198408	-1.203501	0.995688
H	-3.278168	-0.513735	-1.344462
Si	3.035271	-0.212735	0.004588
H	3.214477	-1.232559	1.087458
H	4.097333	0.806278	0.251797
H	3.364954	-0.906846	-1.280479

(SiH3)2-In≡N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.051711	2.381495	0.004560
In	-0.000811	0.415567	-0.001533
Si	2.128576	-1.052326	0.001120
H	3.366903	-0.236607	-0.027570
H	2.083376	-1.933349	-1.194213
H	2.108897	-1.888067	1.229276
Si	-2.146502	-1.021127	0.001271
H	-2.116508	-1.899802	1.198847
H	-3.372221	-0.186089	0.027565
H	-2.141711	-1.860994	-1.224172

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In≡N-(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.283691	-0.000176	-0.000023
N	-0.880764	0.000013	0.000734
Si	-1.632660	1.533907	0.000069
H	-0.543708	2.565849	0.037586
H	-2.509805	1.777823	1.181542
H	-2.448872	1.806130	-1.218336
Si	-1.633554	-1.533434	-0.000200
H	-2.512209	-1.774676	-1.181084

H	-0.545358	-2.565988	-0.040535
H	-2.448558	-1.807210	1.218646

3HSi-In≡N-SiH3-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.505901	-2.311312	0.017266
In	-0.020663	-0.411874	-0.005845
Si	-2.231301	0.882567	0.005270
H	-3.397996	-0.033419	0.058569
H	-2.308914	1.707079	-1.228249
H	-2.256106	1.779196	1.189633
Si	2.090723	1.154392	0.003717
H	2.031628	1.990702	1.230332
H	3.350010	0.373665	-0.013339
H	2.020636	2.026369	-1.197201

3HSi-In≡N-SiH3-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.670907	-0.780203	0.000085

N	-1.090800	0.061614	-0.001477
Si	1.360132	1.784301	0.000056
H	0.841608	2.407351	-1.236461
H	2.845134	1.848076	0.003191
H	0.836387	2.409731	1.233107
Si	-2.775863	0.338653	0.000275
H	-3.484263	-0.207745	-1.196529
H	-2.976243	1.820591	-0.003794
H	-3.481233	-0.200708	1.202040

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B3LYP/LANL2DZ+dp

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F-In≡N-F

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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In	0.296704	-0.037620	0.000082
N	-1.545238	0.661486	-0.000010
F	-2.562717	-0.322867	-0.000193
F	2.149183	0.013196	-0.000246

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F2-In=N

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.036967	0.001019	-0.000000
N	-2.092501	0.050744	-0.000001
F	0.875250	-1.606267	0.000000
F	0.953515	1.561251	0.000000

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In=N-F2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.757361	0.013571	-0.005229
N	-1.399220	-0.008658	0.694979
F	-1.591614	1.095979	-0.261403
F	-1.443513	-1.163131	-0.250667

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F-In≡N-F-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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In	-0.112636	-0.111430	-0.001057
N	1.657923	-1.014896	0.002740
F	-1.922148	0.157494	0.002746
F	1.245895	1.238546	0.000879

F-In≡N-F-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.675791	-0.234507	-0.016498
N	-1.558026	-0.054309	0.599018
F	-2.478814	-0.314080	-0.317592
F	0.011306	1.633078	-0.058485

HO-In≡N-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.326845	-0.215978	-0.002884
N	1.502203	0.607149	-0.224199
O	2.685997	0.119597	0.233580
H	3.207596	-0.149364	-0.550302
O	-2.108682	0.528136	-0.017231

H	-2.326120	1.300375	0.530202

(OH)2-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.005772	0.051546	-0.000117
N	-0.956526	1.876913	0.000342
O	1.895233	-0.090775	-0.000102
H	2.277726	-0.979166	0.003539
O	-1.055061	-1.555699	-0.000389
H	-2.020616	-1.513169	0.003734

In≡N-(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.915270	0.000000	0.000000
N	-1.173349	0.000000	0.000000
O	-1.992861	1.157980	-0.108615
H	-2.374515	1.292145	0.778699
O	-1.992861	-1.157980	0.108615
H	-2.374515	-1.292145	-0.778699

HO-In≡N-OH-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.087251	0.089025	0.007418
N	1.498189	1.313612	-0.023277
O	1.278400	-1.307813	0.097944
H	1.767960	-1.550431	-0.700658
O	-1.954085	-0.253017	-0.043683
H	-2.574526	0.479562	0.066037

HO-In≡N-OH-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.702993	-0.203486	0.014119
N	1.272274	-0.280198	-0.391307
O	2.465692	-0.467989	0.082278
H	2.424418	-0.656078	1.050806
O	0.323002	1.774681	0.122010

H	0.806738	2.134722	-0.637789

H-In≡N-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.236498	0.019447	-0.000001
N	1.601086	-0.167294	0.000019
H	2.275745	0.602709	-0.000012
H	-1.894955	-0.384551	-0.000057

H2-In≡N

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.001887	-0.216812	0.000000
N	0.001887	1.801567	0.000000
H	-1.591187	-0.894193	0.000000
H	1.485528	-1.092988	0.000000

In≡N-H2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000000	-0.337887	0.000000
N	0.000000	1.704749	0.000000
H	-0.822937	2.311619	-0.000000
H	0.822933	2.311625	0.000000

H-In≡N-H-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.217150	0.000805	-0.000000
N	-1.771050	-0.102865	0.000000
H	0.213293	1.754680	0.000000
H	1.543718	-1.074083	0.000000

H-In≡N-H-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-0.291748	-0.027003	0.000068
N	1.626618	-0.014024	-0.001805
H	2.620793	-0.272887	0.008076
H	0.288533	1.694217	0.001249

3HC-In≡N-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.291126	-0.111322	0.002314
N	1.460896	0.477442	0.011498
C	-2.384755	0.246348	-0.008915
H	-2.564826	1.302515	-0.249316
H	-2.815473	0.026057	0.975308
H	-2.880541	-0.378955	-0.760706
C	2.821350	-0.000178	-0.009878
H	3.101359	-0.612242	0.867263
H	3.493270	0.878846	-0.000716
H	3.085534	-0.580568	-0.912924

(CH3)2-In≡N

Atomic	Coordinates (Angstroms)

Number		X	Y	Z
	N	0.168821	2.077817	0.001568
	In	-0.005489	0.064970	-0.000682
	C	-1.966017	-0.836146	0.001760
	H	-2.115998	-1.391520	-0.933921
	H	-2.749596	-0.075359	0.093330
	H	-2.049712	-1.540700	0.839935
	C	1.870791	-1.012994	0.000463
	H	2.719135	-0.327197	-0.102425
	H	1.883476	-1.730566	-0.830702
	H	1.971278	-1.568082	0.942898

In≡N-(CH3)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
In	-0.912190	-0.000010	0.000002
N	1.142889	-0.000014	-0.000061
C	1.962304	1.203893	0.000010
H	1.333390	2.109682	0.000119
H	2.620340	1.262868	-0.889387
H	2.620408	1.262720	0.889367
C	1.962422	-1.203837	0.000015
H	2.620201	-1.262842	0.889602
H	1.333598	-2.109687	-0.000386
H	2.620799	-1.262498	-0.889151

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3HC-In≡N-CH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.704092	-0.283997	-0.000085
N	1.249121	-0.259841	-0.001019
C	0.046576	1.983849	-0.000217
H	0.725321	2.172144	-0.831926
H	0.493853	2.189365	0.973196
H	-0.916604	2.487354	-0.130318
C	2.659051	-0.346097	0.001597
H	3.091709	-0.781487	0.923214
H	3.043913	0.696825	-0.046469
H	3.084723	-0.855975	-0.884670

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3HC-In≡N-CH3-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.046317	-0.089279	-0.000597
N	-1.031815	-1.768973	0.001250
C	2.130047	0.405644	0.000164
H	2.342117	1.133237	-0.794065

H	2.749845	-0.484865	-0.156705
H	2.400989	0.859508	0.962805
C	-1.614946	1.341881	0.000563
H	-1.557579	1.929109	0.926211
H	-2.581364	0.832211	-0.055184
H	-1.491444	2.003134	-0.866917

3HSi-In≡N-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.308016	0.035134	-0.005477
N	1.514418	0.469310	0.008974
Si	-2.833958	-0.100867	0.007299
H	-3.384964	1.223912	0.349456
H	-3.230764	-1.097542	1.019420
H	-3.290913	-0.519072	-1.330711
Si	3.085719	-0.153970	0.004058
H	3.343583	-1.155350	1.077123
H	4.074367	0.937271	0.203177
H	3.455901	-0.828232	-1.271914

(SiH3)2-In≡N

Atomic	Coordinates (Angstroms)

Number		X	Y	Z
	N	0.020998	2.377357	-0.001182
	In	-0.000739	0.336091	0.000464
	Si	2.281488	-0.928759	-0.000332
	H	3.471449	-0.053764	-0.014926
	H	2.316931	-1.805939	-1.192636
	H	2.332886	-1.788222	1.204159
	Si	-2.287660	-0.917950	-0.000406
	H	-2.334303	-1.788064	1.196678
	H	-3.472667	-0.036175	0.002830
	H	-2.338647	-1.783833	-1.200239

In≡N-(SiH3)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
In	1.292757	-0.000075	-0.000019
N	-0.877641	0.000001	0.000598
Si	-1.645480	1.523213	0.000236
H	-0.577666	2.563669	0.085321
H	-2.558780	1.730545	1.150443
H	-2.424011	1.798115	-1.232423
Si	-1.645873	-1.523020	-0.000333
H	-2.561497	-1.727588	-1.149230
H	-0.578570	-2.563686	-0.089277
H	-2.422114	-1.800088	1.233276

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3HSi-In≡N-SiH3-TS1

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Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.480722	-1.616390	-0.002469
In	-0.154290	-0.394111	0.001032
Si	-2.513146	0.672776	-0.003763
H	-3.498120	-0.429881	0.101365
H	-2.743451	1.443570	-1.247753
H	-2.654710	1.567416	1.169934
Si	2.383843	1.025534	0.001155
H	2.425518	1.579098	1.375052
H	3.716526	0.651114	-0.500895
H	1.759643	2.038502	-0.894450

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3HSi-In≡N-SiH3-TS2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.670907	-0.780203	0.000085
N	-1.090800	0.061614	-0.001477
Si	1.360132	1.784301	0.000056
H	0.841608	2.407351	-1.236461

H	2.845134	1.848076	0.003191
H	0.836387	2.409731	1.233107
Si	-2.775863	0.338653	0.000275
H	-3.484263	-0.207745	-1.196529
H	-2.976243	1.820591	-0.003794
H	-3.481233	-0.200708	1.202040

M06-2x/Def2-tzvp

F2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.753332	-0.004042	0.000016
Sb	-1.925425	-0.001827	-0.000008
F	2.036569	1.568983	-0.000046
F	2.094184	-1.522254	-0.000048

F2Tl-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.772600	-0.073952	-0.000009
Sb	1.904582	-0.051761	0.000005
F	-1.270320	1.931086	0.000017

F	-2.568908	-0.972209	0.000039

F-Tl-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.982115	-0.030128	-0.000007
Sb	1.764941	-0.277858	0.000005
F	1.828804	1.666687	-0.000001
F	-2.991103	0.178997	0.000037

Tl-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.680733	-0.136414	0.000001
Sb	-2.037305	0.119960	-0.000283
F	0.152038	1.413911	0.000692
F	-3.733901	-0.865962	0.000907

Tl-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-1.756578	0.002794	-0.227821
Tl	1.293669	-0.000249	-0.061189
F	-0.851708	-1.347944	0.914882
F	-0.837373	1.334351	0.926803

(OH)2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.752998	-0.000119	0.000002
Sb	-1.954605	-0.000023	-0.000005
O	2.046639	1.633205	-0.000013
H	2.966985	1.353543	0.000085
O	2.047992	-1.632130	0.000023
H	2.967983	-1.351381	-0.000031

(OH)2Tl-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.783162	-0.095833	-0.011322
Sb	1.896988	-0.077124	0.007173
O	-0.838039	2.019467	-0.000561
H	-1.720372	2.384066	0.114009
O	-2.752123	-0.654460	0.050851
H	-2.868580	-1.608327	0.034927

HO-Tl-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.975751	-0.046472	0.001725
Sb	1.750491	-0.285960	-0.000216
O	1.902634	1.697467	-0.110823
H	2.006550	2.097951	0.755502
O	-3.002572	0.285291	0.094343
H	-3.446305	0.388202	-0.752311

Tl-Sb(OH)2 (TS2)

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
Tl	1.460265	-0.174813	0.000058
Sb	-1.787203	0.206515	0.000950
O	-3.132264	-1.283892	-0.002316
H	-2.768472	-2.172923	-0.008753
O	0.066957	1.679524	-0.002115
H	0.156784	2.635412	-0.008943

Tl-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-1.667220	0.018217	-0.343603
Tl	1.376473	-0.012725	-0.012436
O	-1.264747	1.526024	0.991978
H	-2.085478	1.867317	1.380789
O	-1.489912	-1.529626	0.978367
H	-2.343392	-1.736856	1.387530

H2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	1.010032	-0.000001	0.000014
H	1.884555	-1.496094	0.000027
Sb	-1.678070	-0.000001	-0.000023
H	1.884401	1.496196	0.000027

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H2Tl-Sb (TS1)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.997890	-0.004468	0.000046
H	2.398845	-0.969967	0.000111
Sb	-1.653526	-0.008684	-0.000077
H	1.101877	1.774804	0.000061

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H-Tl-Sb-H

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.005703	-0.003699	0.000000
H	-2.733075	0.085645	0.000002
Sb	1.623887	-0.028720	0.000000

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H	1.376781	1.678720	0.000000

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Tl-SbH2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.133921	-0.021285	0.004203
Sb	-1.792612	-0.014014	-0.023895
H	-1.358567	0.699791	1.479010
H	0.934121	1.739027	-0.600813

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Tl-SbH2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.191397	0.000003	-0.002780
Sb	-1.832079	-0.000080	-0.040305
H	-1.532840	-1.220781	1.142251
H	-1.534326	1.224667	1.138492

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(CH3)2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.761734	-0.000362	0.000176
Sb	1.933125	-0.000796	-0.000087
C	-1.975349	1.861444	-0.002894
H	-2.198419	2.120888	1.030776
H	-1.438264	2.679461	-0.474645
H	-2.904083	1.666730	-0.534618
C	-1.986348	-1.854004	0.001945
H	-2.920776	-1.650161	0.519937
H	-2.197231	-2.120365	-1.032468
H	-1.459976	-2.671271	0.486872

(CH3)2Tl-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.771889	-0.046411	-0.000188
Sb	1.886772	-0.124266	0.000089
C	-0.970438	2.225393	0.000185
H	-1.595872	2.486310	-0.851103
H	-1.468981	2.500907	0.927360
H	-0.019799	2.747225	-0.072353
C	-2.649927	-1.164059	0.000943

H	-3.196523	-0.918947	-0.907523
H	-2.464232	-2.232869	0.043141
H	-3.234728	-0.853760	0.864450

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H3C-Tl-Sb-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	1.686121	-0.364528	-0.001478
Tl	-0.942619	-0.006746	0.002163
C	2.137441	1.791783	0.000105
H	1.737781	2.302327	-0.873051
H	3.226892	1.845245	-0.044283
H	1.810133	2.281905	0.913244
C	-3.130675	0.206338	-0.008049
H	-3.563478	-0.660394	-0.512437
H	-3.395567	1.115747	-0.552287
H	-3.496417	0.263768	1.016655

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Tl-Sb(CH3)2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	-1.192259	-0.233862	0.078274
Sb	1.803440	-0.177647	-0.272960
C	1.604902	0.932576	1.579465
H	2.094061	0.379130	2.381530
H	2.149938	1.870322	1.450378
H	0.575095	1.157695	1.864457
C	-1.085630	2.000653	-0.804785
H	-2.108818	2.344902	-0.669963
H	-0.821491	2.018873	-1.859481
H	-0.406928	2.632540	-0.234204

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Tl-Sb(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.331181	0.000257	-0.021106
Sb	1.623626	-0.000503	-0.395873
C	1.399192	1.573194	1.125842
H	0.459667	1.522222	1.688362
H	2.210689	1.477869	1.846119
H	1.464146	2.553325	0.655319
C	1.395153	-1.572724	1.126830
H	2.206752	-1.478873	1.847230
H	0.455565	-1.519240	1.689154
H	1.457830	-2.553293	0.656861

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(SiH3)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	1.866238	-2.207489	0.000750
H	2.740909	-2.247416	-1.191701
H	2.713662	-2.257479	1.212500
H	0.990973	-3.398742	-0.014414
Si	1.837582	2.224832	0.000760
H	2.682541	2.286809	1.213643
H	2.713335	2.273878	-1.190588
H	0.947463	3.405108	-0.017208
Tl	0.541014	-0.000396	-0.000596
Sb	-2.126756	-0.005351	0.000292

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(SiH3)2Tl-Sb (TS1)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-3.209305	-0.131694	0.000029
H	-3.671855	0.469011	1.265713
H	-3.678566	0.669993	-1.144940
H	-3.716778	-1.510465	-0.112653
Si	0.728450	2.168111	-0.000053
H	0.867578	3.000330	-1.215037
H	0.862272	3.006991	1.210300

H	2.192271	1.601027	0.006698
Tl	-0.696584	-0.144623	-0.000158
Sb	1.927458	-0.471221	0.000060

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H3Si-Tl-Sb-SiH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.786167	-0.202851	0.000959
Sb	-1.848002	-0.524868	-0.000815
Si	-1.600125	2.056299	0.000236
H	-2.197830	2.691283	-1.195494
H	-2.196988	2.690106	1.197213
H	-0.159359	2.473108	-0.000169
Si	3.299892	0.369177	-0.002049
H	3.657912	1.072327	1.245995
H	4.048695	-0.901938	-0.090120
H	3.619405	1.217703	-1.168154

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Tl-Sb(SiH3)2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	-1.026456	-0.567653	0.056679
Sb	1.656209	0.051464	-0.666949
Si	-1.676426	2.081803	-0.218770
H	-1.721212	2.377702	-1.667824
H	-3.049771	2.214169	0.319199
H	-0.822590	3.071668	0.473811
Si	1.634492	0.372482	1.869192
H	0.236908	0.391510	2.409624
H	2.351578	-0.726286	2.559702
H	2.268428	1.666440	2.222980

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Tl-Sb(SiH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.482469	-0.000019	-0.053596
Sb	-1.544044	0.000192	-0.720770
Si	-1.236398	-1.717843	1.135415
H	0.165394	-1.680563	1.692678
H	-2.106227	-1.494033	2.310514
H	-1.418269	-3.102126	0.646629
Si	-1.236211	1.717355	1.135954
H	-2.108894	1.495700	2.309305
H	0.164586	1.677578	1.695760
H	-1.413828	3.102040	0.646522

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B3PW91/Def2-TZVP

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F2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.759055	-0.002373	-0.000003
Sb	1.928791	-0.001299	0.000001
F	-2.031108	1.588315	0.000008
F	-2.067209	-1.559603	0.000009

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F2Tl-Sb (TS1)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.779389	-0.073616	-0.000024
Sb	1.901869	-0.062488	0.000013
F	-1.171660	1.966472	0.000042
F	-2.591096	-0.949830	0.000099

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F-Tl-Sb-F

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	-0.973678	-0.026999	-0.000001
Sb	1.741289	-0.283252	-0.000006
F	1.883762	1.658623	-0.000006
F	-2.987965	0.189463	0.000051

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Tl-SbF2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	1.407623	-0.158369	0.000004
Sb	-1.710796	0.194757	0.000087
F	-0.092580	1.728742	-0.000269
F	-2.881518	-1.407047	-0.000266

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Tl-SbF2

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Atomic Number	Coordinates (Angstroms) X	Y	Z

-

Sb	1.708819	-0.001418	-0.250714
Tl	-1.284342	0.000064	-0.054764
F	0.940608	1.377573	0.953479
F	0.935163	-1.370119	0.960113

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(OH)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.742993	-0.000025	0.000005
Sb	1.935158	0.000034	-0.000012
O	-2.038630	-1.635661	0.000020
H	-2.944974	-1.308590	-0.000016
O	-2.038906	1.635672	0.000003
H	-2.945344	1.308783	0.000051

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(OH)2Tl-Sb (TS1)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.779650	-0.086437	-0.018823
Sb	1.898932	-0.076204	0.012544

O	-0.926359	2.036437	-0.028831
H	-1.736984	2.287309	0.429751
O	-2.726004	-0.747549	0.074883
H	-2.738028	-1.710590	0.086804

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HO-Tl-Sb-OH

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.974884	-0.042769	-0.010909
Sb	1.734304	-0.291871	0.009554
O	1.986290	1.686250	-0.117471
H	2.047281	2.057868	0.767651
O	-3.000490	0.301552	0.159253
H	-3.417627	0.389482	-0.705560

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Tl-Sb(OH)2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.417601	-0.173618	0.000027
Sb	-1.729612	0.210264	0.000897
O	-3.018973	-1.346838	-0.002907

H	-2.582442	-2.204846	-0.002484
O	0.007277	1.706440	-0.001712
H	0.060533	2.667659	-0.008500

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Tl-Sb(OH)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-1.663841	0.004838	-0.341979
Tl	1.380050	-0.003453	-0.010131
O	-1.370552	1.534822	0.975515
H	-2.217182	1.831613	1.338358
O	-1.432773	-1.537069	0.969953
H	-2.284370	-1.780678	1.359406

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H2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.998425	0.000000	0.000014
H	1.923802	-1.473605	0.000027
Sb	-1.661176	0.000000	-0.000023
H	1.923761	1.473634	0.000027

H2Tl-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.990251	-0.005423	0.000047
H	2.397661	-0.979045	0.000109
Sb	-1.644622	-0.006627	-0.000077
H	1.267722	1.756309	0.000064

H-Tl-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.002151	-0.003267	0.000000
H	-2.733968	0.063838	0.000001
Sb	1.618378	-0.028992	0.000000
H	1.370894	1.679382	0.000000

Tl-SbH2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.110983	-0.020430	0.004517
Sb	-1.753837	-0.014288	-0.025363
H	-1.417190	0.664012	1.521597
H	0.873257	1.719507	-0.593987

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Tl-SbH2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.188415	0.000001	-0.002330
Sb	1.825564	-0.000010	-0.041529
H	1.579035	1.216176	1.153155
H	1.578818	-1.215719	1.153605

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(CH3)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	-0.737099	-0.000058	-0.000179
Sb	1.918777	-0.000088	0.000091
C	-2.048595	1.810695	-0.001560
H	-2.369640	1.981147	1.026751
H	-1.497518	2.672210	-0.372490
H	-2.910811	1.599805	-0.633367
C	-2.049655	-1.809989	0.002360
H	-2.882051	-1.618019	0.678798
H	-2.417652	-1.946290	-1.015240
H	-1.485427	-2.683854	0.320650

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(CH3)2Tl-Sb (TS1)

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Tl	0.747513	-0.067613	-0.000037
Sb	-1.882775	-0.094044	0.000020
C	1.131758	2.205133	0.000131
H	1.729117	2.388510	0.891722
H	1.706763	2.392573	-0.905193
H	0.223767	2.800458	0.012718
C	2.675611	-1.118405	-0.000152
H	3.206679	-0.852148	0.913063
H	2.517077	-2.193204	-0.044096
H	3.245328	-0.783620	-0.866153

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H3C-Tl-Sb-CH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.939453	-0.006443	0.000443
Sb	1.678391	-0.365511	-0.000308
C	2.150352	1.791822	-0.000088
H	1.785012	2.288759	0.895345
H	3.240849	1.823362	0.001470
H	1.787807	2.289151	-0.896480
C	-3.129112	0.214069	-0.001735
H	-3.428567	0.808147	-0.864338
H	-3.571026	-0.780878	-0.066840
H	-3.443772	0.699083	0.921573

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Tl-Sb(CH3)2 (TS2)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.179978	-0.236773	0.045213
Sb	1.720085	-0.078946	-0.358209
C	1.898890	0.298234	1.794929
H	2.393004	-0.571125	2.251101
H	2.556534	1.164842	1.943718
H	0.941677	0.472649	2.304377

C	-1.033851	2.150102	-0.283072
H	-2.066069	2.398697	-0.016544
H	-0.830633	2.391433	-1.330948
H	-0.330835	2.658339	0.383603

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Tl-Sb(CH3)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.384070	-0.000126	0.010443
Sb	1.591084	0.000168	-0.424815
C	1.706218	1.604320	1.073302
H	0.967341	1.503613	1.872307
H	2.701362	1.583837	1.520850
H	1.566877	2.566572	0.577668
C	1.708150	-1.604122	1.073115
H	2.700337	-1.578029	1.525844
H	0.964836	-1.508934	1.868186
H	1.577442	-2.566608	0.576307

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(SiH3)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Si	-1.989640	-2.126567	-0.001469
H	-2.796057	-2.149758	1.248502
H	-2.914149	-2.069879	-1.167321
H	-1.190135	-3.377948	-0.083456
Si	-1.957500	2.147715	-0.001433
H	-2.853284	2.120722	-1.189084
H	-2.793683	2.165333	1.228269
H	-1.139779	3.388181	-0.045070
Tl	-0.492390	-0.001491	0.000974
Sb	2.133934	-0.004941	-0.000591

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(SiH3)2Tl-Sb (TS1)

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Si	3.226498	-0.110439	0.003298
H	3.705658	0.630034	-1.189724
H	3.697221	0.565336	1.238021
H	3.750923	-1.496925	-0.031349
Si	-0.727062	2.149234	0.000316
H	-0.881267	2.988581	1.218987
H	-0.884295	2.986573	-1.219598
H	-2.209508	1.584990	0.002771
Tl	0.694506	-0.151766	-0.001549
Sb	-1.929918	-0.460954	0.001094

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H3Si-Tl-Sb-SiH3

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.777897	-0.199280	0.000230
Sb	-1.831268	-0.527124	-0.000192
Si	-1.618683	2.042374	0.000036
H	-2.231166	2.667090	-1.203667
H	-2.233503	2.666774	1.202725
H	-0.184041	2.493527	0.001587
Si	3.308311	0.372151	-0.000476
H	3.665461	1.130878	1.224760
H	4.059603	-0.909593	-0.026147
H	3.653869	1.172996	-1.201959

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Tl-Sb(SiH3)2 (TS2) ----------

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.038564	-0.565121	-0.117680
Sb	1.571774	0.379885	-0.642324
Si	-1.694014	2.001981	0.637773
H	-1.855540	2.769024	-0.625067
H	-3.028460	1.866859	1.281831
H	-0.808996	2.737028	1.574619
Si	1.946566	-0.496066	1.743508

H	0.679808	-0.796576	2.488847
H	2.730437	-1.761335	1.690200
H	2.710231	0.502907	2.542239

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Tl-Sb(SiH3)2 ---

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
Tl	-1.458973	0.000011	-0.062287
Sb	1.544486	-0.000140	-0.691482
Si	1.181573	1.769580	1.115731
H	-0.248849	1.781720	1.618900
H	2.004007	1.590066	2.341764
H	1.408243	3.135081	0.571191
Si	1.181423	-1.769229	1.116099
H	2.003945	-1.589673	2.342071
H	-0.248966	-1.780942	1.619379
H	1.407726	-3.134922	0.571884

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B3LYP/LANL2DZ+dp

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F2Tl-Sb

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Atomic	Coordinates (Angstroms)

Number	X	Y	Z
Tl	-0.799547	-0.000012	-0.000001
Sb	1.936842	-0.000020	0.000001
F	-1.889574	1.528202	0.000004
F	-1.889939	-1.527979	0.000004

F2Tl-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.819718	-0.067876	-0.000001
Sb	-1.881331	-0.093441	0.000000
F	0.725787	1.862647	0.000001
F	2.557625	-0.722269	0.000003

F-Tl-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.993642	-0.033108	-0.000004
Sb	-1.752133	-0.284439	0.000003

F	-1.859302	1.692382	-0.000001
F	2.845282	0.217411	0.000023

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Tl-SbF2 (TS2)

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Tl	1.462847	-0.160721	0.000003
Sb	-1.780532	0.191574	0.000068
F	0.140306	1.552089	-0.000205
F	-3.216242	-1.191187	-0.000209

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Tl-SbF2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Sb	1.771857	-0.000377	-0.198098
Tl	-1.268265	0.000101	-0.069211
F	0.688445	1.357186	0.872199
F	0.685421	-1.355964	0.873250

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(OH)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.790302	-0.000024	0.000005
Sb	-1.943018	-0.000017	-0.000011
O	1.842104	1.653878	0.000006
H	2.801072	1.519536	0.000032
O	1.842517	-1.653629	0.000016
H	2.801476	-1.518717	0.000002

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(OH)2Tl-Sb (TS1)

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.816553	-0.057958	-0.014846
Sb	1.902049	-0.102907	0.009372
O	-0.722194	1.923490	-0.029529
H	-1.435810	2.427701	0.389246
O	-2.620094	-0.767499	0.062066
H	-2.689640	-1.732740	0.075032

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HO-Tl-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.996869	-0.036661	-0.004807
Sb	1.750246	-0.299711	0.004367
O	2.009152	1.694751	-0.114445
H	2.103713	2.078369	0.770245
O	-2.910058	0.277606	0.125796
H	-3.412596	0.397590	-0.694429

Tl-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.449278	-0.178778	0.000001
Sb	-1.773645	0.212522	0.000028
O	-3.226997	-1.198074	-0.000109
H	-2.897352	-2.110813	0.000108
O	0.179719	1.597954	-0.000120
H	0.339940	2.554187	0.000167

Tl-Sb(OH)2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-1.669205	0.004194	-0.349646
Tl	1.393411	-0.003264	-0.007334
O	-1.415329	1.545304	0.986849
H	-2.275916	1.846527	1.321739
O	-1.475001	-1.546653	0.981526
H	-2.338254	-1.785243	1.357232

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H2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.014406	-0.000001	0.000014
H	1.875087	-1.492028	0.000026
Sb	-1.684644	-0.000001	-0.000023
H	1.874879	1.492159	0.000026

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H2Tl-Sb (TS1)

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Atomic	Coordinates (Angstroms)

Number	X	Y	Z
Tl	0.995776	-0.004614	0.000047
H	2.428159	-0.914120	0.000110
Sb	-1.649069	-0.009436	-0.000078
H	1.016467	1.769118	0.000057

H-Tl-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-1.002171	-0.003233	0.000000
H	-2.727977	0.061592	0.000001
Sb	1.618295	-0.029223	-0.000001
H	1.370754	1.690659	0.000000

Tl-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.112282	-0.019670	0.005200
Sb	-1.754765	-0.015767	-0.025010

H	-1.432274	0.720274	1.509753
H	0.830418	1.677107	-0.655452

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Tl-SbH2

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.194555	0.000000	-0.002236
Sb	-1.834570	-0.000004	-0.041914
H	-1.597881	-1.229029	1.159475
H	-1.597992	1.229228	1.159279

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(CH3)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.776364	0.000125	-0.001534
Sb	-1.937798	-0.000264	0.000698
C	1.925358	1.857056	0.004722
H	2.524091	1.896426	-0.914765
H	1.283659	2.742595	0.059120
H	2.603678	1.842910	0.867791
C	1.931342	-1.853854	0.002486

H	2.961821	-1.636520	-0.304477
H	1.937316	-2.271073	1.017907
H	1.491437	-2.590209	-0.680214

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(CH3)2Tl-Sb (TS1)

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Tl	0.776556	-0.052902	-0.000224
Sb	-1.865002	-0.143089	0.000120
C	0.745471	2.212785	0.000365
H	1.314583	2.510393	0.890091
H	1.275548	2.513335	-0.912146
H	-0.237716	2.695272	0.022859
C	2.708783	-0.995301	0.000504
H	3.241320	-0.717932	0.918749
H	2.611772	-2.084650	-0.049204
H	3.283028	-0.638731	-0.863511

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H3C-Tl-Sb-CH3

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Tl	0.943719	-0.004202	0.000040
Sb	-1.679978	-0.370914	-0.000030
C	-2.155603	1.805403	-0.000023
H	-1.793239	2.311821	-0.900296
H	-3.252860	1.846526	0.002039
H	-1.789754	2.312383	0.898541
C	3.101414	0.207809	-0.000190
H	3.423567	0.741742	0.902197
H	3.553481	-0.793021	-0.009785
H	3.421601	0.758254	-0.893150

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Tl-Sb(CH3)2 (TS2)

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

-

Tl	-1.179978	-0.236773	0.045213
Sb	1.720085	-0.078946	-0.358209
C	1.898890	0.298234	1.794929
H	2.393004	-0.571125	2.251101
H	2.556534	1.164842	1.943718
H	0.941677	0.472649	2.304377
C	-1.033851	2.150102	-0.283072
H	-2.066069	2.398697	-0.016544
H	-0.830633	2.391433	-1.330948
H	-0.330835	2.658339	0.383603

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Tl-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.384500	-0.000379	0.007264
Sb	-1.601879	0.000244	-0.426927
C	-1.683698	-1.610103	1.090703
H	-0.911353	-1.518875	1.868764
H	-2.663806	-1.580747	1.583833
H	-1.575001	-2.586347	0.600279
C	-1.677782	1.611992	1.089704
H	-2.658388	1.586809	1.582519
H	-0.906147	1.518483	1.868521
H	-1.565122	2.587627	0.598597

(SiH3)2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-1.903346	-2.205362	0.001072
H	-2.771723	-2.243049	1.205674
H	-2.768507	-2.249192	-1.205591
H	-1.036984	-3.409868	0.005310
Si	-1.869422	2.226236	0.001027
H	-2.738963	2.281260	-1.202094
H	-2.732060	2.279462	1.209269

H	-0.985033	3.417624	-0.000622
Tl	-0.530674	-0.000684	-0.000760
Sb	2.134051	-0.006139	0.000396

(SiH3)2Tl-Sb (TS1)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Si	3.211570	-0.292935	0.001083
H	3.755502	0.366759	-1.209506
H	3.753384	0.369378	1.211128
H	3.606457	-1.720343	0.003005
Si	-0.699517	2.201025	0.000244
H	-0.730413	3.038561	1.225255
H	-0.731616	3.037557	-1.225430
H	-2.162967	1.685021	0.001545
Tl	0.681429	-0.085490	-0.000504
Sb	-1.918723	-0.520891	0.000318

H3Si-Tl-Sb-SiH3

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	-0.794512	-0.172714	-0.001076
Sb	1.802805	-0.572421	0.000904
Si	1.793928	2.031510	-0.000088
H	2.467784	2.587280	1.202353
H	2.472308	2.585144	-1.201028
H	0.410932	2.604262	-0.003633
Si	-3.329590	0.393649	0.002407
H	-3.686148	1.162044	-1.214271

H	-4.076629	-0.888261	0.015145
H	-3.676535	1.180631	1.209979

Tl-Sb(SiH3)2 (TS2)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	-1.072836	-0.575437	-0.071497
Sb	1.530092	0.365450	-0.687343
Si	-1.676865	2.034901	0.629171
H	-1.889859	2.760720	-0.649767
H	-2.985679	1.918356	1.326118
H	-0.766256	2.812203	1.504816
Si	2.205556	-0.440089	1.672377
H	1.056196	-0.688104	2.593146
H	2.951357	-1.720134	1.535091
H	3.097566	0.561992	2.314642

Tl-Sb(SiH3)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	-1.494017	-0.000544	-0.024256
Sb	1.484998	0.000585	-0.729405
Si	1.340715	1.830630	1.084388
H	-0.037029	1.931894	1.684687
H	2.258550	1.613182	2.231294
H	1.614050	3.162691	0.485995
Si	1.344593	-1.829765	1.084261
H	2.269380	-1.615736	2.226219
H	-0.030070	-1.927874	1.691819

H	1.611275	-3.162077	0.483312

B97D3/LANL2DZ+dp

(SiMe(SitBu3)2)2Tl-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.020571	0.548831	1.045916
Sb	-1.086238	0.081658	3.430207
Si	2.071210	0.121353	-3.647309
Si	-1.902481	1.991217	-2.020199
Si	4.042701	-1.630809	3.608028
Si	3.632936	3.100870	3.248951
C	1.382447	-0.228607	-5.457710
C	3.281111	1.683604	-3.657397
C	3.098023	-1.469228	-3.058187
C	-3.062541	1.448305	-3.521655
C	-1.320041	3.855443	-2.197326
C	3.861541	-1.448307	5.550973
C	2.713171	-2.965601	2.961224
C	5.854667	-2.287876	3.132389
C	1.878491	3.617047	3.995748
C	3.987126	4.260150	1.682389
C	5.069240	3.305129	4.571854
C	-2.936555	1.830134	-0.335946
C	0.207041	-1.239506	-5.427832
H	0.552380	-2.259492	-5.209513
H	-0.287025	-1.263110	-6.418157
H	-0.563167	-0.991836	-4.686026
C	0.905889	1.100975	-6.093316
H	1.759017	1.711576	-6.427921

H	0.305539	1.716357	-5.411457
H	0.281926	0.893155	-6.983754
C	2.443770	-0.821791	-6.418877
H	3.342729	-0.194997	-6.500895
H	2.000655	-0.897478	-7.431305
H	2.756553	-1.835164	-6.127876
C	2.389412	-2.803692	-3.401669
H	2.944449	-3.634860	-2.926002
H	2.377148	-3.006608	-4.481732
H	1.355758	-2.846930	-3.033112
C	4.503283	-1.532417	-3.712281
H	5.164539	-0.721721	-3.374213
H	4.464979	-1.505455	-4.810255
H	4.987961	-2.485868	-3.424449
C	3.301849	-1.473224	-1.532253
H	3.778898	-0.561774	-1.152760
H	3.947563	-2.325033	-1.249296
H	2.349759	-1.598913	-1.000939
C	4.084545	1.725173	-2.342504
H	3.415874	1.646279	-1.471537
H	4.624465	2.688139	-2.260508
H	4.835035	0.925350	-2.272363
C	4.279875	1.698047	-4.839738
H	4.970890	2.554985	-4.715484
H	3.771854	1.835064	-5.806699
H	4.893637	0.788883	-4.901903
C	2.490866	3.005995	-3.714979
H	3.195299	3.859086	-3.658416
H	1.799628	3.097480	-2.866998
H	1.916312	3.119503	-4.644343
C	-4.391138	2.350668	-0.477539
H	-4.448891	3.383720	-0.850100
H	-4.870625	2.331505	0.522409
H	-5.000862	1.711573	-1.135358
C	-3.045576	0.354722	0.118095

H	-2.059908	-0.075177	0.374939
H	-3.527913	-0.299372	-0.627668
H	-3.652589	0.292399	1.055087
C	-2.293750	2.621256	0.831033
H	-2.809632	2.366642	1.773900
H	-2.381334	3.704907	0.693037
H	-1.238217	2.380078	0.972124
C	-3.707429	0.070652	-3.233395
H	-2.957725	-0.695698	-2.976352
H	-4.238799	-0.281039	-4.139806
H	-4.447341	0.111011	-2.418877
C	-4.185163	2.457136	-3.854946
H	-3.777655	3.428722	-4.174472
H	-4.876290	2.634449	-3.019932
H	-4.782522	2.061756	-4.700423
C	-2.211310	1.281216	-4.791338
H	-1.317558	0.683825	-4.582160
H	-1.881010	2.242546	-5.208261
H	-2.788391	0.759669	-5.579938
C	-0.831903	4.113974	-3.640461
H	-0.135426	3.341247	-3.989814
H	-0.302222	5.084525	-3.691487
H	-1.672621	4.160589	-4.349442
C	-0.143367	4.154501	-1.232336
H	0.674633	3.425857	-1.324151
H	-0.458236	4.165512	-0.183170
H	0.277708	5.152737	-1.456777
C	-2.435104	4.889434	-1.906621
H	-2.050558	5.904876	-2.120441
H	-2.758266	4.881181	-0.857155
H	-3.323608	4.735249	-2.535616
C	3.725514	5.760065	1.986719
H	4.313026	6.130795	2.837326
H	2.667828	5.977685	2.182090
H	4.017911	6.357406	1.102127

C	5.456690	4.172035	1.202805
H	6.161379	4.564794	1.950213
H	5.574079	4.790863	0.292246
H	5.769343	3.152022	0.946890
C	3.082713	3.883583	0.485921
H	3.377779	4.473442	-0.402481
H	2.027496	4.100349	0.673142
H	3.170051	2.825622	0.206854
C	1.280870	2.543001	4.918530
H	1.911230	2.318676	5.793723
H	1.098384	1.593562	4.380302
H	0.304609	2.884340	5.293632
C	0.799380	3.904678	2.918643
H	-0.156030	4.080192	3.420760
H	0.641992	3.069318	2.235890
H	1.023392	4.793561	2.322638
C	1.998735	4.908484	4.852415
H	2.616670	4.753550	5.746643
H	0.993077	5.199677	5.202099
H	2.411893	5.757797	4.295503
C	6.272260	2.453275	4.104304
H	7.077413	2.480038	4.864662
H	6.700117	2.810238	3.154594
H	5.984654	1.399683	3.960421
C	5.557603	4.756077	4.780510
H	6.317832	4.767577	5.585752
H	4.745238	5.432912	5.083320
H	6.034248	5.171432	3.880770
C	4.618876	2.763699	5.948178
H	5.500564	2.640775	6.607281
H	4.126148	1.784995	5.874436
H	3.924291	3.448726	6.457544
C	3.653825	-2.769981	6.321016
H	4.466766	-3.490906	6.152582
H	2.702251	-3.255093	6.063007

H	3.623302	-2.550410	7.406491
C	2.651971	-0.531677	5.821411
H	2.593368	-0.253231	6.895978
H	1.680976	-0.993824	5.547856
H	2.723912	0.399456	5.233503
C	5.116288	-0.754714	6.136273
H	5.984129	-1.430907	6.168643
H	4.914930	-0.428834	7.176524
H	5.409595	0.138115	5.565970
C	6.308640	-3.435143	4.072227
H	7.287732	-3.815808	3.722603
H	5.615458	-4.285418	4.088270
H	6.447947	-3.091143	5.106976
C	6.930075	-1.181285	3.243182
H	7.922530	-1.618289	3.016452
H	6.990274	-0.744756	4.249929
H	6.764765	-0.365833	2.527659
C	5.914886	-2.834930	1.684169
H	6.966140	-3.065296	1.425174
H	5.546295	-2.115456	0.939226
H	5.344530	-3.765968	1.564321
C	3.131699	-4.421734	3.308064
H	4.020795	-4.752548	2.756183
H	2.309590	-5.102871	3.027643
H	3.320882	-4.568286	4.378336
C	2.518626	-2.910119	1.435793
H	3.440770	-3.070281	0.869595
H	2.109844	-1.941378	1.122802
H	1.795889	-3.681144	1.122835
C	1.313329	-2.752730	3.581472
H	1.293338	-2.936880	4.660134
H	0.600630	-3.439865	3.115924
H	0.936627	-1.734729	3.416584
Si	0.171772	0.467183	-1.921697
C	-0.536472	-1.335173	-1.770203

H	0.222007	-2.024216	-1.366324
H	-0.854450	-1.740877	-2.745504
H	-1.403075	-1.371290	-1.094668
Si	3.679329	0.676845	2.419781
C	5.003549	0.715280	1.019468
H	5.996658	1.018278	1.395486
H	4.717388	1.431915	0.235809
H	5.109660	-0.268780	0.539229

(SiMe(SitBu3)2)-Tl-(Sb-SiMe(SitBu3)2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	0.892187	-0.117760	-0.967152
Sb	-1.343855	-0.074734	0.963312
Si	-4.310218	2.338140	0.583730
Si	-4.449237	-2.193536	-0.565977
Si	4.462606	2.251038	-0.474190
Si	4.315721	-2.281544	0.691882
C	4.738399	-2.975142	-1.092612
C	2.806417	-3.307305	1.472471
C	5.854735	-2.413797	1.901729
C	4.194087	2.372659	-2.429848
C	6.363150	2.338013	-0.005648
C	3.463356	3.722384	0.384585
C	-4.873453	2.067979	2.439779
C	-2.822894	3.668489	0.542800
C	-5.795604	3.019065	-0.516951
C	-4.520182	-3.058261	1.207114
C	-3.220326	-3.233193	-1.730338
C	-6.230648	-2.189987	-1.399995
C	3.760856	5.078298	-0.310155
H	3.245420	5.883348	0.246452

H	3.390642	5.112447	-1.343136
H	4.831028	5.325467	-0.324867
C	1.927661	3.521145	0.338520
H	1.590637	2.596974	0.827452
H	1.528727	3.517606	-0.682645
H	1.439167	4.360451	0.867523
C	3.864567	3.895122	1.869612
H	3.749827	2.975077	2.455970
H	3.218011	4.665716	2.328916
H	4.902136	4.241914	1.974395
C	2.750159	2.767322	-2.819916
H	1.995395	2.085002	-2.396111
H	2.647076	2.716875	-3.919406
H	2.483406	3.787062	-2.516163
C	5.134158	3.425517	-3.072640
H	5.014334	4.427940	-2.639950
H	4.906452	3.502058	-4.152339
H	6.191875	3.142418	-2.985481
C	4.468786	1.026655	-3.131883
H	3.796939	0.234053	-2.767748
H	5.503029	0.685631	-3.001506
H	4.293691	1.135939	-4.218721
C	7.003047	3.741676	-0.113384
H	6.573239	4.448897	0.610236
H	6.909831	4.179336	-1.116539
H	8.083034	3.663519	0.113760
C	6.547535	1.856311	1.452207
H	6.098998	2.539562	2.184442
H	7.624994	1.774351	1.686120
H	6.100768	0.865655	1.605969
C	7.169010	1.376722	-0.908941
H	6.743654	0.365330	-0.920186
H	8.204841	1.295123	-0.530820
H	7.227437	1.727634	-1.948987
C	7.139649	-1.912480	1.207286

H	7.959008	-1.853389	1.947422
H	7.015065	-0.913173	0.773065
H	7.466930	-2.594700	0.410325
C	6.119829	-3.868031	2.364575
H	5.313398	-4.261765	2.997181
H	7.046224	-3.887589	2.968660
H	6.260310	-4.560719	1.523244
C	5.647605	-1.546188	3.166143
H	5.562166	-0.479480	2.922545
H	6.522516	-1.661537	3.832679
H	4.755829	-1.828896	3.738211
C	5.449164	-4.350360	-1.096993
H	4.858153	-5.144252	-0.623273
H	6.427090	-4.307344	-0.595651
H	5.634234	-4.654382	-2.144284
C	5.665263	-1.983715	-1.825046
H	6.683378	-1.981660	-1.416528
H	5.276421	-0.962840	-1.768757
H	5.736442	-2.253574	-2.895157
C	3.453994	-3.097389	-1.946902
H	2.749031	-3.844698	-1.557596
H	3.723772	-3.402865	-2.974663
H	2.922784	-2.134500	-2.023734
C	2.956206	-4.824013	1.183176
H	2.147215	-5.365614	1.708152
H	3.910568	-5.238381	1.535848
H	2.856486	-5.056696	0.114232
C	1.446113	-2.872735	0.894637
H	0.643458	-3.529014	1.277198
H	1.401163	-2.925707	-0.202370
H	1.178606	-1.854312	1.215871
C	2.677572	-3.158049	3.009246
H	1.768516	-3.693413	3.340361
H	2.572304	-2.112707	3.329284
H	3.525381	-3.597816	3.550476

C	-5.104999	-2.088759	2.254133
H	-6.148474	-1.819350	2.047713
H	-4.519983	-1.165521	2.316951
H	-5.077992	-2.563221	3.253122
C	-3.114750	-3.454038	1.721364
H	-2.434511	-2.590371	1.764027
H	-2.637877	-4.233749	1.111703
H	-3.211102	-3.856692	2.747799
C	-5.398791	-4.333049	1.236132
H	-6.459662	-4.113867	1.048820
H	-5.334683	-4.780676	2.246152
H	-5.074400	-5.099477	0.520153
C	-1.737828	-2.929303	-1.431963
H	-1.471977	-1.916825	-1.762708
H	-1.092571	-3.637026	-1.988822
H	-1.476907	-2.998549	-0.368875
C	-3.419282	-4.760819	-1.549842
H	-4.455776	-5.081302	-1.721713
H	-3.114112	-5.110216	-0.554984
H	-2.783855	-5.288261	-2.286858
C	-3.424944	-2.941420	-3.237227
H	-4.377697	-3.337543	-3.613874
H	-2.620510	-3.440944	-3.810120
H	-3.382576	-1.869989	-3.472519
C	-6.263721	-1.282000	-2.654403
H	-7.308825	-1.171136	-2.998877
H	-5.687030	-1.700539	-3.488029
H	-5.876889	-0.274180	-2.461966
C	-7.272299	-1.643074	-0.395117
H	-8.235969	-1.476929	-0.911944
H	-6.967042	-0.685665	0.045134
H	-7.460119	-2.349710	0.425582
C	-6.722616	-3.587466	-1.854665
H	-7.752609	-3.493797	-2.248844
H	-6.750852	-4.318870	-1.036598

H	-6.105991	-4.005133	-2.662656
C	-6.825401	1.911361	-0.816050
H	-7.590585	2.298901	-1.514712
H	-7.349641	1.564295	0.082456
H	-6.360248	1.041654	-1.290924
C	-6.582220	4.181457	0.137171
H	-7.348004	4.541455	-0.576244
H	-5.956668	5.041105	0.406928
H	-7.115809	3.851124	1.040249
C	-5.264834	3.498095	-1.889971
H	-6.118129	3.798548	-2.526499
H	-4.722331	2.702180	-2.419439
H	-4.598001	4.365774	-1.808571
C	-6.198551	1.272243	2.456381
H	-6.421009	0.932671	3.484712
H	-6.156153	0.382219	1.817249
H	-7.044431	1.891381	2.124734
C	-5.120972	3.386799	3.215503
H	-5.487150	3.141903	4.230577
H	-5.876616	4.026306	2.739671
H	-4.203960	3.978861	3.338099
C	-3.817903	1.274541	3.247634
H	-4.242150	0.981214	4.225886
H	-2.914598	1.866005	3.442208
H	-3.497515	0.345478	2.750357
C	-1.959895	3.562610	-0.736500
H	-2.545634	3.663348	-1.660767
H	-1.416417	2.606473	-0.759522
H	-1.206303	4.372387	-0.730867
C	-3.367973	5.118821	0.618996
H	-3.995039	5.288461	1.505620
H	-3.940907	5.411712	-0.270475
H	-2.507363	5.810431	0.690355
C	-1.847192	3.531163	1.734751
H	-2.321361	3.757530	2.698722

H	-1.019849	4.252115	1.599584
H	-1.391853	2.529801	1.786430
Si	3.582774	0.107999	0.432489
C	2.857451	0.505197	2.180780
H	2.244957	-0.329848	2.549794
H	2.214228	1.394307	2.180030
H	3.660407	0.674452	2.917962
Si	-3.529076	0.148204	-0.382767
C	-3.058995	0.569097	-2.208908
H	-3.940238	0.584345	-2.869810
H	-2.364542	-0.188281	-2.604346
H	-2.559562	1.543677	-2.283531

Tl-Sb(SiMe(SitBu3)2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.103897	0.395162	1.717147
Tl	1.264012	1.743872	4.135349
Si	0.005735	-3.986238	1.683960
Si	-2.836051	-1.760618	4.685248
Si	-2.366531	3.346087	-1.030834
Si	2.287199	2.586393	-1.106135
C	-4.300535	-3.119820	4.775577
C	-3.682108	0.042846	4.775028
C	-1.640482	-1.968587	6.258012
C	-5.029106	-3.283395	3.419595
H	-4.377872	-3.712577	2.649240
H	-5.432162	-2.340088	3.029623
H	-5.882026	-3.976777	3.549094
C	-5.378108	-2.746451	5.825768
H	-4.959723	-2.597442	6.829884
H	-6.105751	-3.577974	5.894127

H	-5.945560	-1.847802	5.553782
C	-3.777696	-4.518374	5.176709
H	-3.462024	-4.559813	6.229279
H	-2.942667	-4.853954	4.554603
H	-4.591722	-5.258652	5.056945
C	-2.386095	-2.061446	7.613533
H	-3.017800	-2.959347	7.666941
H	-3.013211	-1.190413	7.835811
C	-0.648838	-0.784351	6.334512
H	0.095298	-0.972650	7.131875
H	-1.145235	0.167239	6.567387
H	-0.095612	-0.670435	5.385846
C	-4.169378	0.427152	6.195578
H	-4.836355	-0.312525	6.655584
H	-4.729638	1.379579	6.128191
H	-3.327409	0.606821	6.879755
C	-4.895478	0.145674	3.822085
H	-4.631268	-0.113399	2.788907
H	-5.263537	1.188643	3.811877
H	-5.737579	-0.486374	4.132867
C	-2.699125	1.145212	4.344408
H	-1.778994	1.150143	4.945157
H	-3.172618	2.137434	4.464593
H	-2.394232	1.042131	3.298174
C	0.006125	-4.121993	-0.300731
C	1.844340	-3.641533	2.337920
C	-0.681450	-5.717222	2.370031
C	-0.017373	-6.945100	1.696513
H	-0.243684	-7.018157	0.625466
H	-0.407331	-7.865382	2.173232
H	1.074252	-6.956724	1.818121
C	-0.431549	-5.865879	3.883442
H	-0.906941	-5.067696	4.456570
H	0.638306	-5.875492	4.134757
H	-0.859880	-6.823639	4.236126

C	1.846365	-3.138244	3.797898
H	2.878257	-2.859789	4.086962
H	1.511209	-3.904166	4.509342
H	1.218748	-2.242516	3.924835
C	-2.208454	-5.831677	2.137622
H	-2.609738	-6.692182	2.705711
H	-2.459663	-5.994670	1.082607
H	-2.749124	-4.938215	2.474410
C	2.758525	-4.890877	2.289479
H	2.836112	-5.320441	1.282072
H	2.428085	-5.682854	2.977078
H	3.780332	-4.598438	2.599453
C	2.527423	-2.537167	1.504568
H	2.703849	-2.836383	0.464652
H	3.515260	-2.305205	1.947168
H	1.947358	-1.603273	1.501494
C	1.214899	-4.934186	-0.833928
H	1.110718	-5.049807	-1.930140
H	1.281240	-5.943989	-0.407606
H	2.172289	-4.425756	-0.657053
C	-1.270938	-4.789441	-0.867789
H	-1.267956	-4.684047	-1.969422
H	-2.192665	-4.319630	-0.499179
H	-1.320966	-5.865203	-0.653162
C	0.074110	-2.723973	-0.939272
H	0.204794	-2.818076	-2.034670
H	0.902265	-2.122866	-0.556149
H	-0.850698	-2.161710	-0.769119
C	-0.786100	-3.244074	6.151736
H	-0.279167	-3.307379	5.186980
H	-1.379995	-4.154480	6.294514
H	-1.640604	-2.146875	8.427807
H	-0.006994	-3.240613	6.937958
C	2.842817	4.155853	-0.032263
C	3.494858	1.070126	-0.687240

C	2.439617	3.001392	-3.040768
C	-3.763875	2.700794	0.198864
C	-3.038896	3.117684	-2.906404
C	-2.023989	5.256561	-0.647456
C	-4.120316	4.174858	-3.249723
H	-3.706880	5.192623	-3.284778
H	-4.968963	4.171735	-2.555561
H	-4.521876	3.956627	-4.258377
C	-3.679078	1.723447	-3.120271
H	-3.972103	1.621729	-4.182859
H	-4.588216	1.580749	-2.522030
H	-2.987450	0.901037	-2.895748
C	-1.948765	3.268834	-3.989257
H	-1.154673	2.517309	-3.901767
H	-1.483336	4.261930	-3.981740
H	-2.410893	3.134458	-4.986126
C	-5.193407	3.171736	-0.169975
H	-5.273892	4.261679	-0.277228
H	-5.884975	2.871171	0.640542
H	-5.566715	2.707527	-1.093361
C	-3.778100	1.158401	0.247504
H	-2.881670	0.773381	0.752323
H	-3.843550	0.687524	-0.740881
H	-4.655687	0.819261	0.826721
C	-3.486500	3.188903	1.638697
H	-2.466182	2.946546	1.969099
H	-4.185710	2.689477	2.330323
H	-3.647248	4.269716	1.752100
C	-1.177759	5.401379	0.640898
H	-0.289915	4.758063	0.629306
H	-1.750372	5.155608	1.544053
H	-0.829630	6.446726	0.745685
C	-1.248430	5.925835	-1.805349
H	-0.341204	5.379623	-2.079536
H	-0.943382	6.946476	-1.505232

H	-1.864703	6.026922	-2.710344
C	-3.310297	6.096975	-0.445536
H	-3.026178	7.157340	-0.301188
H	-3.879500	5.793816	0.442840
H	-3.983325	6.056780	-1.312516
C	2.259037	5.474030	-0.589973
H	2.489321	6.303051	0.105998
H	1.172890	5.442983	-0.710895
H	2.704725	5.737900	-1.559034
C	2.369063	4.017236	1.435749
H	2.581581	4.952792	1.987515
H	2.903112	3.205944	1.952404
H	1.287698	3.824955	1.510550
C	4.381844	4.347867	-0.005147
H	4.620384	5.277489	0.546889
H	4.808407	4.454816	-1.012229
H	4.907741	3.527328	0.500116
C	3.785373	3.651290	-3.446399
H	3.783421	3.816645	-4.541433
H	4.657925	3.029225	-3.213789
H	3.928920	4.634960	-2.976824
C	2.265556	1.723673	-3.897175
H	2.240927	2.005480	-4.966976
H	1.330896	1.190384	-3.679186
H	3.097488	1.018184	-3.769544
C	1.330567	3.983216	-3.463206
H	1.535732	5.009222	-3.133083
H	0.357372	3.686387	-3.064679
H	1.242276	4.008907	-4.565554
C	4.876600	1.189870	-1.378679
H	5.387750	2.139560	-1.172326
H	4.808654	1.065491	-2.468514
H	5.530097	0.378444	-1.005173
C	2.871143	-0.265539	-1.141396
H	3.584493	-1.087948	-0.949640

H	2.626439	-0.288488	-2.210820
H	1.961493	-0.476117	-0.567421
C	3.750960	0.929763	0.830919
H	4.316050	1.773874	1.249594
H	4.347835	0.017501	1.015189
H	2.806986	0.812298	1.384610
Si	-1.489867	-1.950703	2.321999
C	-2.939203	-2.058088	1.063023
H	-2.626665	-1.694717	0.074030
H	-3.797180	-1.451034	1.378497
H	-3.285402	-3.094663	0.944171
Si	-0.224845	1.825780	-0.618914
C	-0.542176	0.460908	-1.921827
H	0.281923	-0.259722	-1.960401
H	-0.683945	0.872839	-2.930075
H	-1.457025	-0.090205	-1.656990

(SiiPrDis2)2Tl-Sb

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	-0.137100	-0.568744	1.492383
Si	2.454770	0.174341	0.578372
Si	-2.739075	-0.062636	0.485613
C	3.283338	0.024967	2.335020
H	2.873643	-0.993125	2.580230
C	4.812394	-0.132741	2.430730
H	5.177473	-0.926883	1.758476
H	5.101457	-0.419470	3.465497
H	5.354802	0.797669	2.187232
C	2.754956	0.949929	3.450336
H	3.228285	1.942491	3.411585
H	2.981299	0.513253	4.437943

H	1.667859	1.092262	3.403266
C	-3.993091	-0.168124	1.989798
H	-4.224156	0.907235	2.125473
C	-5.326363	-0.872490	1.670565
H	-5.210108	-1.967586	1.685799
H	-5.733154	-0.591329	0.684095
H	-6.092027	-0.617812	2.429915
C	-3.443481	-0.646258	3.345541
H	-2.564322	-0.066559	3.674940
H	-3.122543	-1.705365	3.331842
H	-4.215046	-0.549675	4.137047
C	-3.045867	1.741957	-0.160049
H	-2.351416	1.878070	-1.009570
Si	-2.485183	3.116806	1.060530
Si	-4.763974	2.130023	-0.905452
C	-1.494270	4.411529	0.108198
H	-0.514201	4.019580	-0.203983
H	-1.308781	5.294263	0.745312
H	-2.017336	4.756714	-0.798838
C	-3.871637	4.040068	1.954783
H	-4.511876	3.381767	2.563679
H	-4.522280	4.615425	1.277471
H	-3.395352	4.761224	2.642638
C	-1.370990	2.518308	2.469333
H	-1.873308	1.801438	3.132000
H	-1.090926	3.391325	3.079455
H	-0.425987	2.079816	2.116134
C	-4.604472	3.744625	-1.885259
H	-3.782972	3.688867	-2.622253
H	-4.407514	4.612739	-1.233007
H	-5.537806	3.951156	-2.440199
C	-6.149379	2.336381	0.377541
H	-7.080549	1.890337	-0.014290
H	-6.353287	3.398768	0.586682
H	-5.934885	1.847759	1.339412

C	-5.451113	0.853754	-2.125940
H	-5.741698	-0.091959	-1.637295
H	-4.780252	0.613108	-2.963289
H	-6.373204	1.286700	-2.557772
C	-3.077201	-1.419100	-0.875164
H	-4.129816	-1.205666	-1.153886
Si	-3.247160	-3.258524	-0.333163
Si	-2.243076	-1.247278	-2.588548
C	-2.775314	-3.646886	1.452765
H	-2.667249	-4.736059	1.542911
H	-3.537956	-3.327637	2.176517
H	-1.823694	-3.201038	1.758400
C	-5.049943	-3.738956	-0.639123
H	-5.242669	-4.772048	-0.303862
H	-5.273723	-3.692180	-1.718893
H	-5.762557	-3.076869	-0.123561
C	-2.260593	-4.533232	-1.327355
H	-1.174653	-4.448793	-1.209387
H	-2.493706	-4.528090	-2.401788
H	-2.554781	-5.520127	-0.934435
C	-3.434276	-1.974478	-3.870568
H	-3.574739	-3.060034	-3.742203
H	-3.044187	-1.810608	-4.891228
H	-4.430566	-1.503540	-3.815914
C	-0.589164	-2.146406	-2.806412
H	-0.720285	-3.221966	-2.979717
H	0.099527	-2.025018	-1.957435
H	-0.080033	-1.731327	-3.692407
C	-1.887436	0.530196	-3.132159
H	-1.148477	1.020319	-2.479146
H	-2.779888	1.172027	-3.177484
H	-1.446652	0.501390	-4.145307
Sb	0.230219	-2.090497	4.176670
C	2.224804	1.970708	-0.231223
H	1.134247	2.104262	-0.040950

C	3.230018	-1.226774	-0.507458
H	2.609275	-1.201506	-1.423673
Si	2.170158	2.130925	-2.144423
Si	2.893505	3.557511	0.621257
C	3.777952	2.728603	-2.950911
H	4.373225	3.407254	-2.318835
H	3.529342	3.276391	-3.878523
H	4.429315	1.885159	-3.231850
C	1.673864	0.529522	-3.013806
H	0.916144	-0.022810	-2.439919
H	2.516228	-0.150852	-3.202533
H	1.220446	0.771218	-3.991847
C	0.789351	3.334319	-2.633730
H	0.648958	3.279933	-3.729345
H	0.994506	4.384231	-2.377647
H	-0.175070	3.058999	-2.174128
C	4.717007	3.483630	1.092224
H	4.981736	4.423173	1.610871
H	5.374837	3.394320	0.211283
H	4.954032	2.650363	1.771568
C	1.868797	4.023569	2.148961
H	0.945711	4.538400	1.836622
H	2.448332	4.736773	2.762210
H	1.582048	3.190196	2.796967
C	2.706625	5.122796	-0.439035
H	3.216570	5.097307	-1.414471
H	3.143122	5.958611	0.139612
H	1.646986	5.372968	-0.611080
Si	5.011970	-0.993909	-1.195750
Si	2.929445	-3.038042	0.041751
C	3.894271	-3.589209	1.565062
H	4.985032	-3.455919	1.492992
H	3.698137	-4.662447	1.734021
H	3.539854	-3.054384	2.470626
C	1.135392	-3.464810	0.482153

H	1.008270	-4.545592	0.361364
H	0.370707	-2.988340	-0.140845
H	0.938764	-3.239316	1.531442
C	3.343172	-4.160009	-1.426847
H	4.392034	-4.104428	-1.754233
H	2.707560	-3.911044	-2.293017
H	3.134010	-5.207100	-1.154267
C	6.320371	-2.180935	-0.506180
H	6.516233	-2.023323	0.568435
H	7.267100	-1.968488	-1.038646
H	6.092292	-3.247625	-0.656007
C	5.726370	0.724415	-0.883317
H	6.176075	0.802642	0.120455
H	4.972542	1.517189	-0.973553
H	6.522056	0.937335	-1.621478
C	4.974124	-1.281296	-3.070363
H	4.579901	-0.407906	-3.617428
H	4.359682	-2.153771	-3.348308
H	5.999321	-1.461286	-3.442427

(SiiPrDis2)-Tl-Sb-(SiiPrDis2)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	0.680411	0.029575	0.640271
Si	3.298112	0.192338	-0.347537
C	4.323618	-1.417997	-0.349811
H	4.696000	-1.438795	0.692535
Si	5.964718	-1.299636	-1.321393
Si	3.501400	-3.145630	-0.478563
C	2.949790	0.722847	-2.185355
C	4.155790	1.424977	0.838835
H	5.239136	1.259999	0.693959

Si	3.908761	0.995473	2.685703
Si	3.955912	3.277579	0.478746
C	2.464741	1.928110	3.483649
H	2.670875	3.006154	3.570729
H	2.302794	1.539335	4.503913
H	1.507804	1.826982	2.943447
C	5.488654	1.434112	3.621411
H	5.470882	0.993704	4.632899
H	5.630172	2.519168	3.727967
H	6.372158	1.029623	3.098604
C	3.627193	-0.840777	3.067773
H	3.420678	-0.933718	4.148628
H	4.526999	-1.440987	2.858518
H	2.786050	-1.308916	2.533948
C	4.886981	4.334247	1.740180
H	4.439991	4.309803	2.746035
H	4.881175	5.384766	1.400540
H	5.940196	4.020055	1.825132
C	4.782453	3.704299	-1.167209
H	5.877991	3.631539	-1.059256
H	4.548401	4.746336	-1.445267
H	4.486313	3.060815	-2.006006
C	2.156452	3.852066	0.520136
H	1.458344	3.191075	-0.011420
H	2.073695	4.849284	0.054064
H	1.796089	3.948762	1.555512
C	6.915332	0.285040	-0.925675
H	7.884156	0.253297	-1.453904
H	7.132493	0.387326	0.150436
H	6.388283	1.191679	-1.258738
C	7.096737	-2.716199	-0.785988
H	8.103186	-2.564009	-1.212418
H	6.738415	-3.702015	-1.119816
H	7.200706	-2.749312	0.311471
C	5.806386	-1.341833	-3.200171

H	6.823585	-1.384128	-3.627546
H	5.322238	-0.436998	-3.598016
H	5.254046	-2.213211	-3.577784
C	4.254178	-4.228591	0.875561
H	5.339667	-4.365018	0.759633
H	3.785199	-5.227561	0.858925
H	4.070820	-3.794250	1.872575
C	1.642930	-3.199942	-0.172606
H	1.313532	-4.250721	-0.257947
H	1.043965	-2.620168	-0.892454
H	1.365034	-2.872314	0.843691
C	3.755696	-4.031750	-2.127860
H	4.815831	-4.195126	-2.374344
H	3.283507	-3.507219	-2.972740
H	3.276926	-5.023915	-2.056065
H	3.953635	1.000985	-2.562088
C	2.454179	-0.474742	-3.024878
H	3.113466	-1.347625	-2.957531
H	2.390084	-0.183789	-4.088499
H	1.441809	-0.785521	-2.720233
C	2.001596	1.912976	-2.441825
H	2.334250	2.848187	-1.979193
H	0.980912	1.696468	-2.085403
H	1.919951	2.092234	-3.528571
Sb	-1.204122	-0.300556	-1.376461
Si	-3.658446	-0.313180	-0.729468
C	-4.386812	-1.090570	-2.355108
H	-4.077163	-2.143866	-2.219175
C	-3.753505	-0.661531	-3.693368
H	-3.908027	0.396717	-3.937875
H	-4.167614	-1.259045	-4.525667
H	-2.661907	-0.836273	-3.688703
C	-5.931691	-1.080334	-2.393841
H	-6.357834	-1.764821	-1.641628
H	-6.302577	-1.409640	-3.382146

H	-6.352789	-0.083464	-2.202077
C	-4.243276	-1.685859	0.525242
H	-4.899347	-2.249850	-0.169332
C	-4.160239	1.515830	-0.376906
H	-5.212579	1.507817	-0.036116
Si	-3.003700	-3.091001	0.920835
Si	-5.508983	-1.400310	1.917131
Si	-3.212677	2.363903	1.060121
Si	-4.216476	2.707125	-1.878504
C	-1.717198	-2.643285	2.235270
H	-2.157809	-2.668068	3.244519
H	-1.283043	-1.644277	2.082969
H	-0.890447	-3.373389	2.209803
C	-2.167526	-3.801363	-0.615948
H	-1.510980	-3.082449	-1.123494
H	-2.920453	-4.148666	-1.344485
H	-1.561401	-4.675958	-0.319785
C	-3.914635	-4.608648	1.603809
H	-4.356471	-4.460160	2.600352
H	-3.189608	-5.438526	1.680554
H	-4.711870	-4.937893	0.916683
C	-6.853577	-2.724736	1.741085
H	-7.276049	-2.728318	0.721305
H	-7.681898	-2.518974	2.441327
H	-6.481084	-3.737551	1.952240
C	-4.809890	-1.554729	3.668933
H	-4.627308	-2.608787	3.932950
H	-5.541861	-1.156775	4.393070
H	-3.867971	-1.008301	3.813281
C	-6.468858	0.224154	1.817079
H	-6.895272	0.381223	0.812612
H	-5.880932	1.112551	2.085395
H	-7.314425	0.161269	2.524539
C	-4.301539	3.676437	1.894316
H	-5.368279	3.399912	1.892559

H	-4.212958	4.657810	1.406311
H	-3.991631	3.799519	2.946723
C	-2.745306	1.191537	2.469050
H	-2.333615	0.229169	2.137523
H	-3.617369	0.985659	3.106595
H	-1.990482	1.687129	3.106504
C	-1.622582	3.236131	0.517088
H	-1.057257	2.631733	-0.206749
H	-0.978104	3.403366	1.397997
H	-1.813797	4.220707	0.062534
C	-4.540493	4.497008	-1.341696
H	-3.691551	4.964229	-0.821372
H	-5.430054	4.588269	-0.698661
H	-4.729068	5.087813	-2.255561
C	-2.642423	2.776913	-2.915549
H	-2.254219	1.788960	-3.198322
H	-1.832483	3.286477	-2.371447
H	-2.843737	3.349120	-3.838914
C	-5.703020	2.358015	-2.995161
H	-5.616664	1.451129	-3.605217
H	-5.827145	3.212093	-3.683397
H	-6.628867	2.278741	-2.400291

Tl-Sb(SiiPrDis2)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Sb	0.835025	0.314887	0.832623
Tl	-1.991810	1.100312	1.884369
Si	0.750545	0.124308	-1.780343
Si	1.495285	-1.922183	2.060177
C	0.189977	-1.762226	-1.791272
H	0.620437	-2.065960	-0.825610

C	0.719145	-2.790532	-2.795699
H	1.815616	-2.838196	-2.773268
H	0.403861	-2.588754	-3.824618
H	0.339585	-3.794392	-2.532411
C	-1.333712	-1.915494	-1.627278
H	-1.863871	-1.789385	-2.581908
H	-1.749374	-1.190152	-0.909110
H	-1.574731	-2.924507	-1.248482
C	0.001243	-3.136947	1.730523
H	0.111131	-3.337818	0.651518
C	-0.073017	-4.502054	2.440277
H	0.894206	-5.000641	2.557226
H	-0.734425	-5.184178	1.876269
H	-0.515218	-4.386416	3.436944
C	-1.378725	-2.475952	1.921151
H	-1.514272	-2.119937	2.959655
H	-2.187408	-3.200331	1.718786
H	-1.502916	-1.625362	1.237615
C	2.545114	0.462669	-2.454127
H	3.104378	-0.287396	-1.852949
C	-0.709310	1.249484	-2.399834
H	-1.481993	0.849067	-1.709016
C	3.094584	-2.594571	1.158652
H	2.814232	-2.298058	0.122648
C	1.508683	-1.446183	3.963441
H	0.405776	-1.385761	4.109649
Si	-1.568767	0.893320	-4.088760
Si	-0.872752	3.113616	-1.999953
Si	3.477071	2.107683	-1.952253
Si	3.076307	0.083121	-4.263266
C	-3.400171	0.556070	-3.740376
H	-3.931206	1.456074	-3.395833
H	-3.533254	-0.225659	-2.975141
H	-3.899584	0.208391	-4.661608
C	-1.524954	2.301115	-5.355103

H	-1.946571	3.248299	-4.990009
H	-2.136906	1.978486	-6.216525
H	-0.515257	2.506646	-5.739824
C	-0.936655	-0.601455	-5.049170
H	-1.253212	-1.554419	-4.604405
H	0.154444	-0.616953	-5.160095
H	-1.369721	-0.554511	-6.063679
C	2.197674	1.236208	-5.482090
H	2.896694	1.992087	-5.873053
H	1.364061	1.772609	-5.009697
H	1.792708	0.679974	-6.342697
C	2.876120	-1.686475	-4.897528
H	3.431074	-1.737235	-5.851218
H	1.843689	-1.991846	-5.101852
H	3.327522	-2.429450	-4.221214
C	4.947207	0.304936	-4.487886
H	5.293637	1.344258	-4.418303
H	5.208856	-0.064822	-5.494844
H	5.522723	-0.291051	-3.761454
C	3.506522	3.410994	-3.330015
H	3.719332	4.387440	-2.859369
H	2.560936	3.514256	-3.873549
H	4.300724	3.224040	-4.068245
C	5.297642	1.688814	-1.596439
H	5.612723	2.164553	-0.654751
H	5.953419	2.067257	-2.395470
H	5.484773	0.613146	-1.500469
C	2.883930	3.051153	-0.426366
H	3.770764	3.491156	0.063016
H	2.379926	2.414938	0.315444
H	2.205908	3.875822	-0.688501
C	-2.702683	3.611102	-2.121258
H	-3.113009	3.612190	-3.141073
H	-2.801275	4.637359	-1.724203
H	-3.341063	2.958423	-1.500442

C	-0.469708	3.619933	-0.216083
H	0.241853	2.964856	0.303323
H	-1.398925	3.673740	0.382159
H	-0.040980	4.637398	-0.213175
C	0.091833	4.258641	-3.155653
H	0.970819	4.690133	-2.655773
H	-0.559321	5.095321	-3.461643
H	0.436139	3.765442	-4.073143
Si	2.003140	-2.706233	5.350685
Si	2.049636	0.312499	4.604246
Si	3.356134	-4.478270	0.916027
Si	4.767723	-1.662170	1.301644
C	3.823206	-3.181367	5.336049
H	4.471852	-2.355353	5.660093
H	4.166801	-3.516948	4.351800
H	3.973454	-4.016889	6.041992
C	1.647232	-2.025162	7.087300
H	1.824036	-2.849283	7.800651
H	0.598285	-1.710411	7.207481
H	2.291107	-1.188800	7.389527
C	1.029016	-4.326661	5.448731
H	1.310306	-4.790640	6.410619
H	1.242265	-5.057288	4.661038
H	-0.059681	-4.159149	5.478450
C	0.791804	0.862811	5.925113
H	1.079282	0.600030	6.952032
H	-0.208917	0.433206	5.742297
H	0.690986	1.960382	5.879435
C	3.795021	0.301956	5.344526
H	4.522065	-0.210873	4.697238
H	3.851238	-0.160402	6.341096
H	4.131887	1.347969	5.444785
C	2.062768	1.845439	3.496129
H	2.515170	2.649799	4.108701
H	1.046345	2.164570	3.223449

H	2.628614	1.760591	2.563550
C	3.593042	-5.442281	2.520414
H	4.597227	-5.268206	2.938298
H	3.512056	-6.522295	2.307308
H	2.864849	-5.200735	3.304715
C	1.960774	-5.248679	-0.111964
H	2.379145	-6.077300	-0.708429
H	1.531548	-4.524242	-0.818789
H	1.138613	-5.658350	0.489205
C	4.892844	-4.901423	-0.108613
H	5.841827	-4.663412	0.394311
H	4.893153	-4.413098	-1.095537
H	4.875950	-5.992209	-0.282715
C	5.727513	-1.807415	-0.332205
H	6.427951	-0.958694	-0.395826
H	5.079300	-1.770855	-1.222854
H	6.328543	-2.724030	-0.395682
C	5.930909	-2.313347	2.637691
H	6.933432	-1.888322	2.453545
H	6.034436	-3.409307	2.636479
H	5.628798	-2.004883	3.647509
C	4.616855	0.190509	1.574774
H	5.592597	0.653541	1.347433
H	4.357265	0.459588	2.605508
H	3.864753	0.637811	0.909987

(Tbt)2Tl-Sb

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Tl	1.666902	1.372511	0.713318
Sb	-1.085404	0.489654	0.356972
C	2.742346	1.928199	-1.316016

C	4.275999	2.171143	-3.742899
C	3.381234	3.170135	-1.645176
C	2.771338	0.852183	-2.282874
C	3.557158	1.001701	-3.449769
C	4.163888	3.228453	-2.830637
H	3.592720	0.184123	-4.173934
H	4.673526	4.165448	-3.064891
C	2.452830	1.420513	2.930920
C	3.466314	2.723775	5.297386
C	3.816400	1.226388	3.345869
C	1.550720	2.017526	3.879526
C	2.093810	2.677427	5.014286
C	4.291482	1.949635	4.466144
H	1.398008	3.136956	5.721065
H	5.345159	1.849844	4.739653
C	1.955955	-0.454108	-2.200381
H	1.492060	-0.553192	-1.205689
C	3.251765	4.557583	-0.974010
H	3.560647	5.229269	-1.798509
C	5.043119	2.295816	-5.047376
H	5.027235	1.294577	-5.521253
C	4.783355	0.099764	2.902641
H	5.456202	0.037993	3.782315
C	0.007356	1.881948	3.958917
H	-0.143237	2.068193	5.046517
C	4.042167	3.408829	6.524347
H	5.140318	3.434056	6.386031
Si	2.851193	-2.153278	-2.420679
Si	0.404036	-0.381212	-3.383396
Si	4.127030	3.402884	-6.315117
Si	6.909034	2.668189	-4.885053
Si	1.532971	5.352473	-0.749684
Si	4.576646	5.150476	0.266832
Si	-1.166367	3.326147	3.458299
Si	-0.806340	0.118588	4.022454

Si	3.812741	2.334735	8.098003
Si	3.594234	5.248281	6.771589
Si	4.105403	-1.674195	3.127113
Si	6.173025	0.384921	1.637203
C	3.007993	-2.773119	-4.198987
H	3.373836	-2.001483	-4.890919
H	2.056113	-3.160795	-4.587716
H	3.731235	-3.604356	-4.220689
C	1.882871	-3.469186	-1.465813
H	2.547394	-4.310724	-1.223939
H	1.050116	-3.866611	-2.056958
H	1.478056	-3.084047	-0.530483
C	4.611288	-2.096411	-1.762791
H	5.213477	-1.354816	-2.305569
H	5.081063	-3.083487	-1.895691
H	4.639904	-1.850834	-0.697433
C	-0.852714	-1.715407	-2.903751
H	-0.558788	-2.707894	-3.273070
H	-1.837674	-1.474371	-3.347294
H	-0.990694	-1.776648	-1.817160
C	0.803502	-0.588287	-5.223110
H	1.766385	-0.132896	-5.496280
H	0.023270	-0.077142	-5.816752
H	0.814120	-1.641466	-5.538805
C	-0.424936	1.318010	-3.285742
H	0.279315	2.112694	-3.596815
H	-0.782075	1.550127	-2.257030
H	-1.310767	1.355803	-3.957057
C	2.447795	2.621568	-6.670342
H	2.563318	1.598611	-7.064812
H	1.896757	3.213451	-7.420882
H	1.833888	2.568956	-5.756360
C	5.058382	3.499691	-7.954094
H	5.979949	4.097236	-7.882737
H	4.415961	3.974679	-8.714743

H	5.326660	2.498177	-8.326243
C	3.824502	5.151409	-5.679896
H	4.752813	5.664879	-5.390725
H	3.151111	5.143297	-4.808969
H	3.342480	5.752727	-6.469435
C	1.564269	7.070169	-1.542337
H	2.208096	7.774104	-0.999159
H	0.545233	7.486666	-1.554946
H	1.915864	7.013946	-2.584443
C	0.208074	4.401582	-1.668876
H	0.061533	3.391845	-1.278027
H	0.482060	4.304301	-2.729861
H	-0.748207	4.937692	-1.612018
C	1.040673	5.561062	1.044226
H	-0.007761	5.869890	1.119694
H	1.644996	6.327381	1.546633
H	1.163971	4.630547	1.606762
C	-0.360636	4.940688	4.026365
H	0.686069	5.031861	3.720644
H	-0.394834	5.001266	5.125760
H	-0.916214	5.800329	3.626210
C	-1.698157	3.425172	1.653016
H	-2.206010	4.376895	1.478138
H	-2.415917	2.631130	1.434360
H	-0.872666	3.361035	0.956550
C	-2.755866	3.261351	4.503530
H	-2.568214	2.861633	5.516754
H	-3.550073	2.659044	4.035436
H	-3.144556	4.286202	4.620980
C	-2.674568	0.058092	3.635389
H	-3.292545	0.463489	4.462042
H	-2.966417	-1.008855	3.501349
H	-2.950355	0.583087	2.690158
C	-0.676801	-0.391730	5.858492
H	0.377642	-0.436899	6.183123

H	-1.129712	-1.389035	6.014051
H	-1.207734	0.327477	6.513406
C	0.010489	-1.275479	3.021217
H	0.930407	-0.921875	2.562547
H	-0.659611	-1.646973	2.235355
H	0.255594	-2.121081	3.686669
C	2.006170	1.910739	8.414642
H	1.918483	1.316563	9.340489
H	1.590696	1.309309	7.590824
H	1.378492	2.806866	8.532997
C	4.760542	0.723329	7.845022
H	5.824033	0.920948	7.635180
H	4.344083	0.152899	7.002096
H	4.702238	0.095291	8.749275
C	4.527662	3.159385	9.637776
H	5.560966	3.502699	9.472820
H	4.549998	2.429511	10.464674
H	3.930269	4.019467	9.976814
C	4.951786	6.091606	7.780504
H	5.950828	5.816473	7.405774
H	4.908802	5.840286	8.849195
H	4.852640	7.185844	7.691478
C	3.544246	6.124419	5.106852
H	4.514596	6.039539	4.595898
H	3.327149	7.195040	5.249850
H	2.773138	5.701141	4.450428
C	1.942348	5.513359	7.636648
H	1.692139	6.586951	7.639051
H	1.966054	5.176390	8.684509
H	1.123574	4.984047	7.126849
C	4.521527	7.033446	0.465449
H	4.586851	7.548205	-0.505408
H	5.392376	7.349173	1.063957
H	3.622142	7.390801	0.985715
C	6.289291	4.788040	-0.436818

H	6.425226	5.294015	-1.405436
H	6.457405	3.714011	-0.585847
H	7.063262	5.164209	0.251535
C	4.426570	4.373951	1.953354
H	3.450411	4.553316	2.418905
H	4.569212	3.290511	1.889034
H	5.197735	4.769410	2.631664
C	7.581450	1.823565	-3.342470
H	8.682060	1.879034	-3.327002
H	7.289922	0.762114	-3.315905
H	7.199223	2.307540	-2.433187
C	7.309484	4.505200	-4.767278
H	8.383678	4.639433	-4.558347
H	6.751743	4.990707	-3.952282
H	7.085345	5.040993	-5.702496
C	7.820952	1.933436	-6.366662
H	8.907105	1.943418	-6.178242
H	7.639282	2.488622	-7.297815
H	7.520787	0.885817	-6.531399
C	3.050982	-1.681611	4.692569
H	3.703464	-1.589815	5.575011
H	2.506564	-2.635198	4.777787
H	2.327184	-0.857838	4.718416
C	5.504218	-2.887830	3.527363
H	6.016236	-3.268421	2.635074
H	5.077808	-3.753153	4.059444
H	6.255629	-2.432218	4.190246
C	3.151544	-2.372588	1.667322
H	3.814652	-2.965100	1.026350
H	2.692920	-1.601143	1.047149
H	2.355874	-3.038356	2.017422
C	5.606830	0.932186	-0.044192
H	6.446876	0.905365	-0.752842
H	5.216909	1.954053	-0.019068
H	4.821939	0.288326	-0.447624

C	7.317092	1.712560	2.343169
H	8.160866	1.884313	1.656019
H	7.729377	1.397222	3.315211
H	6.791372	2.666489	2.485719
C	7.263958	-1.135556	1.381412
H	8.097729	-0.847383	0.720322
H	6.731270	-1.963042	0.892874
H	7.699034	-1.504949	2.320615

Tbt-Tl-Sb-Tbt

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	-0.825229	-1.165206	-0.016720
Sb	0.903552	0.846311	-0.941760
C	2.916658	0.427035	-0.388734
C	5.623272	-0.029446	0.350133
C	3.668587	1.479270	0.223312
C	3.530314	-0.835850	-0.679376
C	4.870976	-1.029357	-0.294194
C	5.004779	1.215217	0.586146
H	5.348748	-1.989657	-0.502299
H	5.579454	2.010165	1.065502
C	-3.134294	-0.668767	0.216182
C	-5.746468	0.308160	0.729798
C	-3.689415	-0.805323	1.518904
C	-3.863539	-0.053080	-0.841870
C	-5.162245	0.427200	-0.543373
C	-4.989692	-0.301739	1.744743
H	-5.740777	0.887404	-1.347578
H	-5.436483	-0.407388	2.739033
C	2.801166	-1.971036	-1.390758
H	1.738771	-1.678101	-1.494272

C	3.161859	2.908699	0.459484
H	4.061336	3.440676	0.833576
C	7.055648	-0.296881	0.754664
H	7.275085	-1.350345	0.487595
C	-3.030958	-1.493895	2.724132
H	-3.850905	-1.521476	3.469862
C	-3.437374	0.149346	-2.310772
H	-4.413014	0.326064	-2.807684
C	-7.159379	0.767324	1.008234
H	-7.382557	0.498491	2.060597
Si	2.713842	-3.608013	-0.423548
Si	3.313095	-2.131124	-3.224576
Si	8.276666	0.687111	-0.324508
Si	7.315765	-0.259767	2.641474
Si	2.818480	3.983338	-1.100365
Si	2.052661	3.257927	1.989442
Si	-2.655961	1.853674	-2.792184
Si	-2.987279	-1.344288	-3.403046
Si	-8.454578	-0.226311	0.024595
Si	-7.302350	2.664235	1.014218
Si	-2.740929	-3.386923	2.606567
Si	-1.829592	-0.489754	3.838233
C	4.165633	-4.768186	-0.756670
H	5.134066	-4.286873	-0.546104
H	4.184309	-5.118984	-1.801051
H	4.090587	-5.659500	-0.109733
C	1.137417	-4.558394	-0.879924
H	1.037511	-5.446520	-0.231532
H	1.142627	-4.908978	-1.922754
H	0.220072	-3.959332	-0.744125
C	2.663267	-3.250078	1.426128
H	3.640095	-2.891788	1.784573
H	2.399582	-4.159169	1.993301
H	1.926590	-2.467774	1.669530
C	2.348977	-3.524322	-4.066418

H	2.667464	-4.527437	-3.740260
H	2.514429	-3.466700	-5.156690
H	1.264783	-3.437612	-3.895101
C	5.155166	-2.457505	-3.430639
H	5.747094	-1.616526	-3.039716
H	5.393936	-2.566568	-4.502850
H	5.486192	-3.373251	-2.918144
C	2.901997	-0.531417	-4.124823
H	3.533028	0.294989	-3.764600
H	1.853020	-0.237926	-3.965472
H	3.071513	-0.642613	-5.210003
C	8.002149	0.175090	-2.117826
H	8.108699	-0.915052	-2.245945
H	8.733736	0.665035	-2.783480
H	6.992368	0.455652	-2.459206
C	10.051108	0.258294	0.155751
H	10.331073	0.677959	1.135398
H	10.753719	0.664114	-0.592279
H	10.205960	-0.832712	0.200727
C	8.042330	2.555013	-0.213039
H	8.102298	2.932581	0.819098
H	7.070312	2.861051	-0.631472
H	8.830742	3.059077	-0.799047
C	3.877195	5.539070	-0.946182
H	3.592597	6.142973	-0.069461
H	3.759826	6.173757	-1.841673
H	4.947161	5.287584	-0.850434
C	3.339249	3.075212	-2.665933
H	2.658484	2.246725	-2.915957
H	4.351415	2.651754	-2.563364
H	3.338476	3.773735	-3.520424
C	1.031782	4.554882	-1.325325
H	0.695515	5.218689	-0.512727
H	0.326309	3.713265	-1.379819
H	0.947265	5.116910	-2.272173

C	-2.435897	2.907158	-1.249344
H	-1.732123	2.469337	-0.525783
H	-3.404648	3.028637	-0.738641
H	-2.065096	3.909844	-1.520384
C	-1.081824	1.786787	-3.836571
H	-0.265081	1.210430	-3.378436
H	-0.706719	2.815622	-3.981290
H	-1.275340	1.363340	-4.835588
C	-3.906284	2.729482	-3.907359
H	-4.885149	2.861317	-3.418019
H	-4.064551	2.170369	-4.844621
H	-3.528769	3.730170	-4.182066
C	-3.512766	-0.886901	-5.162859
H	-4.559166	-0.539133	-5.194465
H	-3.438561	-1.774562	-5.814952
H	-2.884770	-0.099641	-5.609573
C	-4.034710	-2.805482	-2.848691
H	-3.774335	-3.124615	-1.828400
H	-3.900741	-3.667006	-3.524874
H	-5.104505	-2.537598	-2.846110
C	-1.180053	-1.891841	-3.503540
H	-0.888305	-2.574468	-2.687978
H	-0.469389	-1.053070	-3.501658
H	-1.037657	-2.452623	-4.444303
C	-8.812889	0.496847	-1.680691
H	-9.492839	-0.171156	-2.237359
H	-7.896483	0.610218	-2.282200
H	-9.298748	1.483884	-1.615054
C	-7.840061	-1.995945	-0.190217
H	-7.587597	-2.451985	0.781963
H	-6.937809	-2.040082	-0.820429
H	-8.620579	-2.617971	-0.662472
C	-10.053789	-0.278114	1.025471
H	-9.856651	-0.598768	2.062928
H	-10.760874	-1.001361	0.584202

H	-10.558687	0.699110	1.069411
C	-9.053746	3.159198	1.511835
H	-9.378141	2.633629	2.425603
H	-9.788049	2.938264	0.720226
H	-9.100325	4.242585	1.716065
C	-6.091792	3.321145	2.301087
H	-6.288222	2.883781	3.294900
H	-6.173035	4.417929	2.394987
H	-5.051202	3.078345	2.030544
C	-6.887419	3.450170	-0.647763
H	-7.029912	4.543167	-0.585146
H	-7.525802	3.077643	-1.463173
H	-5.838342	3.270092	-0.928714
C	2.362794	5.066516	2.462852
H	3.435725	5.302686	2.556588
H	1.887398	5.276570	3.437245
H	1.925145	5.768165	1.733442
C	2.679839	2.168045	3.392376
H	3.742215	2.369501	3.608122
H	2.585714	1.100925	3.140273
H	2.104309	2.354875	4.315570
C	0.178726	3.101997	1.887326
H	-0.246336	3.712139	1.077189
H	-0.144006	2.068117	1.718401
H	-0.256087	3.456683	2.839166
C	5.775855	-0.935111	3.492540
H	5.938120	-0.999418	4.582838
H	5.533351	-1.947477	3.128647
H	4.896754	-0.296820	3.313473
C	7.662013	1.470836	3.308407
H	7.720809	1.444489	4.410340
H	6.864881	2.182000	3.037976
H	8.617720	1.874801	2.936585
C	8.764970	-1.391305	3.072148
H	8.809960	-1.560538	4.161686

H	9.735124	-0.976848	2.758201
H	8.650915	-2.377028	2.588973
C	-3.416374	-4.075026	0.990884
H	-4.431598	-3.696548	0.793459
H	-3.457755	-5.176603	1.040795
H	-2.793442	-3.804771	0.124177
C	-3.704690	-4.166305	4.029965
H	-3.326775	-3.835907	5.010905
H	-3.636686	-5.267085	3.997393
H	-4.772664	-3.894354	3.974003
C	-0.942586	-3.946719	2.778527
H	-0.522593	-3.695022	3.765647
H	-0.265877	-3.524748	2.018550
H	-0.894330	-5.044391	2.670505
C	0.018708	-0.553203	3.460632
H	0.546962	-0.036382	4.280739
H	0.314446	-0.040383	2.532017
H	0.409410	-1.580703	3.426451
C	-2.402713	1.299830	3.858113
H	-1.756803	1.903190	4.518664
H	-3.437375	1.376079	4.230481
H	-2.371659	1.746832	2.853659
C	-2.022834	-1.189627	5.587480
H	-1.490958	-0.543162	6.307386
H	-1.604511	-2.204224	5.691468
H	-3.080736	-1.228108	5.898166

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Tl-Sb(Tbt)2

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Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

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Tl	6.461853	-0.834895	0.441057
Sb	3.462869	0.343300	0.857679
C	3.403803	1.614840	-1.102981
C	2.533687	2.572737	-3.718101
C	3.568040	2.994681	-1.480196
C	2.981578	0.711821	-2.158399
C	2.516267	1.206182	-3.391650
C	3.092939	3.420064	-2.753771
H	2.174909	0.488526	-4.142440
H	3.223533	4.472292	-3.011283
C	3.113042	1.181310	2.906303
C	2.997082	2.863187	5.243768
C	4.110385	1.065682	3.946777
C	1.896882	1.873850	3.246528
C	1.910197	2.752855	4.361183
C	4.041703	1.944327	5.048467
H	1.002029	3.318433	4.575501
H	4.808046	1.869125	5.827143
C	3.148596	-0.810357	-2.107135
H	3.530734	-1.104231	-1.112828
C	4.378572	4.126529	-0.803073
H	4.929110	4.540676	-1.674347
C	2.112619	3.053724	-5.096483
H	1.638112	2.192585	-5.609908
C	5.108473	-0.104661	4.200883
H	5.085521	-0.085505	5.311985
C	0.477678	1.633789	2.669988
H	-0.143437	1.991754	3.520897
C	2.982446	3.754426	6.471056
H	3.903197	3.518673	7.043861
Si	4.554984	-1.372226	-3.262401
Si	1.548084	-1.855448	-2.165903
Si	0.746248	4.383422	-5.122599

Si	3.655313	3.412304	-6.161652
Si	3.479518	5.755159	-0.303628
Si	5.885590	3.774790	0.269751
Si	-0.283436	2.883181	1.443637
Si	-0.260556	-0.149581	2.701498
Si	1.590334	3.248112	7.672728
Si	3.212451	5.596997	6.055429
Si	4.355229	-1.862127	4.213901
Si	7.032406	0.009750	4.177551
C	4.086538	-1.602206	-5.075196
H	3.562862	-2.554506	-5.246293
H	5.000720	-1.606443	-5.692867
H	3.445375	-0.791905	-5.447950
C	5.197112	-3.036239	-2.626800
H	4.484749	-3.848782	-2.843738
H	5.354771	-3.036065	-1.533343
H	6.157378	-3.301730	-3.101071
C	5.965882	-0.114651	-3.208570
H	5.587000	0.917870	-3.236007
H	6.641181	-0.260863	-4.068303
H	6.592284	-0.208820	-2.305138
C	0.126244	-0.838061	-1.491737
H	-0.745600	-1.473396	-1.264115
H	-0.181332	-0.075722	-2.224355
H	0.426988	-0.317338	-0.573884
C	1.840994	-3.382851	-1.093409
H	2.512299	-4.104518	-1.587467
H	0.890150	-3.903134	-0.886346
H	2.288647	-3.113439	-0.124242
C	1.031077	-2.456382	-3.880459
H	0.969534	-1.639731	-4.617328
H	0.026363	-2.909281	-3.806576
H	1.708237	-3.225537	-4.283261
C	-0.430444	4.100038	-3.687416
H	-0.793234	3.059240	-3.663220

H	-1.306856	4.766751	-3.761444
H	0.067881	4.295946	-2.729622
C	-0.242435	4.204191	-6.722340
H	0.340723	4.458453	-7.620204
H	-1.124513	4.867651	-6.697665
H	-0.611972	3.170954	-6.842638
C	1.423696	6.144266	-5.024747
H	2.004081	6.413861	-5.922071
H	2.075726	6.293556	-4.149969
H	0.591315	6.864483	-4.940672
C	4.339373	7.178959	-1.209715
H	5.365982	7.358304	-0.854936
H	3.769066	8.113563	-1.064960
H	4.388206	6.988414	-2.296051
C	1.696984	5.791004	-0.897662
H	1.159120	4.864199	-0.675574
H	1.658821	5.946930	-1.984916
H	1.159078	6.627656	-0.421556
C	3.570582	6.168163	1.537323
H	3.235673	5.355986	2.194137
H	2.933772	7.043449	1.749359
H	4.596586	6.424696	1.842630
C	0.324974	4.584775	1.956385
H	1.416197	4.668809	1.938587
H	-0.012723	4.803792	2.981766
H	-0.092044	5.363998	1.300212
C	-0.024745	2.556982	-0.377207
H	1.028845	2.482540	-0.678580
H	-0.496024	3.366998	-0.954512
H	-0.524689	1.625372	-0.674732
C	-2.156136	2.986704	1.739928
H	-2.424772	2.787832	2.791661
H	-2.737087	2.299907	1.108332
H	-2.491408	4.012690	1.507248
C	-1.881835	-0.260302	1.729938

H	-2.694003	0.316633	2.195677
H	-2.190675	-1.320663	1.724745
H	-1.791747	0.056831	0.680608
C	-0.745006	-0.451271	4.507082
H	0.089999	-0.281509	5.202383
H	-1.095108	-1.487626	4.655622
H	-1.566775	0.224778	4.802797
C	0.744147	-1.624157	2.108646
H	1.549245	-1.891662	2.803015
H	1.201735	-1.451241	1.126136
H	0.060915	-2.490982	2.028733
C	-0.074892	4.025032	7.242613
H	-0.859559	3.642122	7.918049
H	-0.387420	3.796719	6.211298
H	-0.050411	5.121947	7.350271
C	1.441300	1.370779	7.616201
H	2.400138	0.892115	7.878937
H	1.170088	1.025436	6.608020
H	0.675622	1.007749	8.322812
C	2.057580	3.751252	9.431287
H	3.073855	3.405535	9.687795
H	1.361005	3.295268	10.156200
H	2.027784	4.841326	9.581708
C	3.276530	6.615394	7.643956
H	3.996991	6.206516	8.371888
H	2.292149	6.665974	8.137311
H	3.584564	7.650583	7.415091
C	4.864821	5.763440	5.164370
H	5.700485	5.481157	5.828118
H	5.037519	6.799192	4.825493
H	4.903579	5.109026	4.281565
C	1.839382	6.278741	4.969778
H	2.048082	7.331888	4.713839
H	0.860380	6.242907	5.472817
H	1.754710	5.721481	4.028324

C	6.997587	5.309103	0.270232
H	7.206109	5.672426	-0.750060
H	7.966358	5.039320	0.728229
H	6.586443	6.148127	0.851759
C	6.920727	2.451429	-0.596531
H	7.379918	2.857978	-1.513375
H	6.272061	1.619533	-0.906622
H	7.741965	2.075938	0.039327
C	5.484954	3.356465	2.049104
H	4.460795	3.645879	2.313242
H	5.550638	2.281540	2.237119
H	6.171856	3.874050	2.735561
C	4.609193	1.805889	-6.395910
H	5.525541	1.975198	-6.987750
H	4.005009	1.050980	-6.925888
H	4.907518	1.375320	-5.429121
C	4.814378	4.660408	-5.351244
H	5.657262	4.879694	-6.029742
H	5.233135	4.259258	-4.414512
H	4.315437	5.613717	-5.118949
C	3.158803	4.046806	-7.869442
H	4.049952	4.128817	-8.515797
H	2.687058	5.041090	-7.826623
H	2.451428	3.360913	-8.365064
C	2.695524	-1.668343	5.079125
H	2.871574	-1.445552	6.145347
H	2.076893	-2.578359	5.024353
H	2.122657	-0.831370	4.663983
C	5.386610	-2.955713	5.367816
H	6.377717	-3.225118	4.975222
H	4.833765	-3.898311	5.529617
H	5.526111	-2.491588	6.358174
C	4.231105	-2.829172	2.596614
H	5.232517	-3.118146	2.228459
H	3.705734	-2.293250	1.791973

H	3.682451	-3.769413	2.779923
C	7.907639	-1.538902	3.480941
H	7.256914	-2.239437	2.934381
H	8.350297	-2.116767	4.309310
H	8.738527	-1.255757	2.811121
C	7.845535	1.498972	3.361650
H	8.928501	1.433241	3.572287
H	7.475783	2.441960	3.788429
H	7.721666	1.558329	2.270195
C	7.544374	0.117643	5.996743
H	8.643235	0.129461	6.101385
H	7.163535	-0.739214	6.577309
H	7.155716	1.038117	6.465431

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(Ar*)2Tl-Sb

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Atomic Number	Coordinates (Angstroms) X	Y	Z

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Tl	-0.376376	-0.507347	8.517925
Sb	-2.285884	1.777014	8.442431
H	0.336036	-0.999414	3.084422
C	0.806011	-0.622114	3.994555
C	1.926106	0.405390	6.346771
C	0.269470	-1.022134	5.241862
C	1.890860	0.253270	3.905870
C	2.447399	0.756531	5.082792
C	0.835759	-0.504401	6.447874
H	2.289104	0.545911	2.931857
H	3.287942	1.450553	5.038849

C	-0.876876	-2.000488	5.121009
C	-3.040058	-3.818996	4.625056
C	-2.234507	-1.543284	5.107337
C	-0.621215	-3.370299	4.794964
C	-1.705493	-4.240997	4.560888
C	-3.279001	-2.464075	4.884509
H	-1.506975	-5.285101	4.308361
H	-4.307563	-2.096408	4.873121
C	2.621127	1.083673	7.499520
C	4.040287	2.556190	9.496781
C	2.143635	2.349732	7.951029
C	3.881301	0.614247	7.978251
C	4.545366	1.353268	8.980983
C	2.849256	3.048631	8.945409
H	5.505918	0.976400	9.344144
H	2.485480	4.020301	9.283400
C	-2.592611	-0.059113	5.121695
H	-1.792722	0.470797	5.682121
C	-3.945388	0.263469	5.782713
H	-4.800699	-0.057339	5.162472
H	-4.034452	1.358004	5.921244
H	-4.042126	-0.214361	6.768447
C	-2.582602	0.510281	3.682592
H	-1.609715	0.356928	3.187970
H	-2.792858	1.597217	3.699536
H	-3.360743	0.022975	3.065876
C	0.791592	-3.915561	4.570861
H	1.498525	-3.269233	5.112609
C	0.977996	-5.358840	5.075903
H	0.478220	-6.085876	4.414829
H	0.580409	-5.486404	6.086205
H	2.046971	-5.617692	5.090481
C	1.150333	-3.888672	3.068093
H	1.086311	-2.881792	2.636692
H	0.462350	-4.541264	2.504277

H	2.176080	-4.263178	2.913500
C	-4.187385	-4.786083	4.364462
H	-3.748063	-5.792641	4.254787
C	-5.176707	-4.832063	5.545936
H	-5.687352	-3.864623	5.675778
H	-4.657534	-5.067582	6.486945
H	-5.950730	-5.597659	5.373551
C	-4.917620	-4.447796	3.048242
H	-4.213647	-4.422925	2.201285
H	-5.406598	-3.461322	3.107903
H	-5.697092	-5.196891	2.830806
C	0.972365	3.047178	7.258349
H	0.353365	2.292958	6.753034
C	1.514235	3.999984	6.173318
H	2.117404	4.800245	6.630447
H	0.681585	4.470086	5.627731
H	2.144895	3.469561	5.449298
C	0.054965	3.846140	8.195772
H	-0.341738	3.223878	9.013465
H	-0.798134	4.236003	7.627519
H	0.561621	4.706420	8.655125
C	4.775090	3.344621	10.573158
H	4.096699	4.150750	10.902802
C	6.046278	4.010157	10.006840
H	5.804493	4.648214	9.142593
H	6.772549	3.251462	9.673281
H	6.535296	4.634406	10.773051
C	5.105094	2.483592	11.807490
H	5.839897	1.699676	11.564869
H	4.203050	1.988603	12.199448
H	5.535584	3.107509	12.607999
C	4.683037	-0.572105	7.422411
H	5.333858	-0.880885	8.254298
C	5.646049	-0.104838	6.306780
H	6.334542	-0.923698	6.037995

H	6.250259	0.754992	6.636898
H	5.101561	0.187286	5.397786
C	3.911558	-1.828965	6.990156
H	4.608488	-2.680917	6.957681
H	3.471308	-1.718635	5.990580
H	3.110122	-2.083175	7.694303
H	1.042241	-4.291983	12.435354
C	0.500400	-3.363158	12.249395
C	-0.913760	-1.018793	11.700145
C	0.557158	-2.803726	10.951105
C	-0.235736	-2.765934	13.272927
C	-0.938978	-1.593476	12.991472
C	-0.159265	-1.614406	10.647262
H	-0.270358	-3.213911	14.268248
H	-1.543293	-1.112122	13.762978
C	1.365247	-3.630594	9.996857
C	2.879934	-5.490754	8.473328
C	2.784718	-3.647372	10.095348
C	0.703533	-4.618255	9.219410
C	1.476500	-5.531667	8.479973
C	3.515400	-4.546175	9.296031
H	0.977685	-6.335076	7.933647
H	4.606274	-4.545534	9.361106
C	-1.790613	0.195291	11.586619
C	-3.562248	2.421740	11.730658
C	-3.177084	0.027588	11.316391
C	-1.295500	1.474002	11.971155
C	-2.187532	2.565149	12.015303
C	-4.035249	1.141088	11.399604
H	-1.803126	3.553001	12.296631
H	-5.100229	1.012866	11.200329
C	3.523689	-2.858578	11.179324
H	2.792073	-2.228416	11.703815
C	4.612659	-1.922244	10.639331
H	5.355715	-2.463062	10.032545

H	5.149537	-1.439064	11.472262
H	4.167753	-1.133109	10.023656
C	4.120351	-3.834762	12.217992
H	3.357926	-4.524593	12.610104
H	4.549752	-3.276936	13.066322
H	4.923987	-4.444076	11.773759
C	-0.805490	-4.836971	9.338614
H	-1.229304	-3.990433	9.894909
C	-1.537767	-4.904511	7.990229
H	-1.234493	-5.784206	7.402966
H	-1.347584	-4.015184	7.376129
H	-2.623998	-4.981030	8.153210
C	-1.079116	-6.108991	10.170495
H	-0.583334	-6.057974	11.151457
H	-0.707441	-7.007722	9.651873
H	-2.160996	-6.238100	10.335843
C	3.675670	-6.515257	7.674045
H	2.958133	-7.055106	7.033063
C	4.720030	-5.857324	6.753080
H	5.507228	-5.354709	7.337433
H	4.255249	-5.104523	6.098907
H	5.209453	-6.615457	6.119887
C	4.337318	-7.551383	8.606818
H	4.854241	-8.330878	8.022715
H	3.587109	-8.038896	9.249070
H	5.080823	-7.071527	9.263693
C	-3.772927	-1.345672	11.008793
H	-2.950648	-2.061369	10.888263
C	-4.597911	-1.367498	9.708898
H	-5.461696	-0.695097	9.763530
H	-4.976019	-2.381845	9.519243
H	-3.993328	-1.064879	8.849962
C	-4.627643	-1.829600	12.199842
H	-4.038878	-1.836909	13.127877
H	-5.005001	-2.848261	12.021569

H	-5.494406	-1.169826	12.355397
C	-4.509761	3.614675	11.770942
H	-5.504967	3.247318	11.462732
C	-4.087393	4.705193	10.764552
H	-3.991865	4.285474	9.748060
H	-3.112038	5.146282	11.035689
H	-4.829619	5.521892	10.738815
C	-4.644080	4.182964	13.198818
H	-4.951025	3.395708	13.906479
H	-5.394770	4.991110	13.230985
H	-3.685610	4.599039	13.553542
C	0.144034	1.665316	12.451955
H	0.737479	0.804076	12.102992
C	0.175822	1.667726	13.996600
H	-0.261898	0.748518	14.412929
H	-0.396464	2.525432	14.391461
H	1.213686	1.753550	14.361185
C	0.822848	2.941588	11.922892
H	1.873601	2.971228	12.254234
H	0.336378	3.855113	12.306248
H	0.814666	2.979816	10.826723

Ar*-Tl-Sb-Ar*

Atomic Number	Coordinates (Angstroms) X	Y	Z
Tl	1.524519	0.580398	-0.027187
Sb	-1.281738	0.009486	0.443780
H	-0.323932	-0.562762	5.686688
C	-0.995329	-0.778502	4.850518
C	-2.696815	-1.360792	2.695326
C	-0.626194	-0.351079	3.558222
C	-2.198975	-1.469905	5.075437

C	-3.048580	-1.764305	3.991199
C	-1.498940	-0.626150	2.471622
H	-2.471406	-1.779133	6.087443
H	-3.985439	-2.304400	4.152379
C	0.700136	0.330866	3.377091
C	3.257683	1.591713	3.223425
C	0.799090	1.748919	3.291392
C	1.883826	-0.455114	3.306236
C	3.135100	0.191138	3.233689
C	2.072376	2.351346	3.224056
H	4.048198	-0.411071	3.217586
H	2.138295	3.441762	3.197620
C	-3.565090	-1.642018	1.499251
C	-5.266637	-2.101494	-0.747130
C	-4.486334	-0.633124	1.064517
C	-3.474831	-2.871037	0.770668
C	-4.332435	-3.066818	-0.329008
C	-5.316717	-0.889413	-0.044546
H	-4.265184	-4.016836	-0.867311
H	-6.034396	-0.128196	-0.362779
C	-0.440952	2.639971	3.316908
H	-1.319474	1.985343	3.222275
C	-0.474861	3.636681	2.142215
H	0.360562	4.353849	2.184760
H	-1.410547	4.217452	2.164777
H	-0.432911	3.118148	1.173665
C	-0.547810	3.376500	4.668065
H	-0.541311	2.663620	5.507645
H	-1.480549	3.962940	4.714384
H	0.296594	4.072861	4.806164
C	1.849945	-1.980759	3.322898
H	0.798857	-2.290450	3.258620
C	2.586988	-2.593572	2.116794
H	3.657001	-2.332313	2.106869
H	2.154363	-2.264586	1.159858

H	2.517548	-3.691659	2.144814
C	2.423427	-2.520493	4.649579
H	1.885467	-2.096972	5.511879
H	3.489460	-2.257329	4.754995
H	2.339428	-3.619086	4.692020
C	4.637417	2.237624	3.291625
H	5.377607	1.419124	3.247988
C	4.918221	3.185141	2.112919
H	4.232155	4.045985	2.123022
H	4.798107	2.668445	1.148687
H	5.947434	3.577042	2.169496
C	4.827707	2.969107	4.638723
H	4.650617	2.290065	5.487717
H	4.123558	3.812559	4.729573
H	5.850899	3.372789	4.722123
C	-4.673085	0.675765	1.834689
H	-3.855986	0.755020	2.566583
C	-6.003444	0.639774	2.618569
H	-6.863622	0.593722	1.929626
H	-6.110950	1.549020	3.233538
H	-6.051388	-0.238454	3.281725
C	-4.608457	1.923193	0.932652
H	-3.637290	1.987295	0.420897
H	-4.734746	2.833571	1.540115
H	-5.402437	1.923177	0.167985
C	-6.239666	-2.374715	-1.887626
H	-6.738386	-1.417492	-2.121527
C	-7.329616	-3.373629	-1.438232
H	-7.848948	-3.013218	-0.535991
H	-6.885365	-4.354884	-1.202141
H	-8.077260	-3.522164	-2.235818
C	-5.540062	-2.868474	-3.168654
H	-5.077891	-3.857332	-3.016842
H	-4.749777	-2.171197	-3.486539
H	-6.268814	-2.966037	-3.990504

C	-2.587181	-4.068230	1.137326
H	-2.518518	-4.656314	0.205603
C	-3.306507	-4.958915	2.175723
H	-2.738259	-5.890237	2.340012
H	-4.321047	-5.225256	1.838150
H	-3.389694	-4.436643	3.141118
C	-1.139067	-3.791074	1.580250
H	-0.563521	-4.730615	1.528209
H	-1.094402	-3.426134	2.614381
H	-0.646791	-3.050104	0.935742
H	2.897841	-1.262444	-5.076812
C	2.382820	-0.447586	-4.559013
C	0.968845	1.614133	-3.231460
C	2.174069	-0.523087	-3.165098
C	1.924018	0.672152	-5.276204
C	1.194408	1.682168	-4.624282
C	1.527252	0.541165	-2.503603
H	2.114726	0.746857	-6.350341
H	0.801574	2.530107	-5.192759
C	2.546112	-1.772289	-2.411102
C	3.254088	-4.214072	-1.117709
C	1.653335	-2.883144	-2.432647
C	3.762944	-1.872415	-1.684079
C	4.095636	-3.091556	-1.060108
C	2.029095	-4.079593	-1.793517
H	5.046073	-3.177917	-0.524622
H	1.348931	-4.933435	-1.836495
C	0.085553	2.643937	-2.569040
C	-1.599632	4.680513	-1.490467
C	0.646091	3.761265	-1.896633
C	-1.335358	2.523373	-2.650817
C	-2.143291	3.543686	-2.115044
C	-0.204539	4.756743	-1.374902
H	-3.228490	3.455592	-2.200100
H	0.229998	5.632081	-0.883076

C	0.314248	-2.832260	-3.170051
H	0.146964	-1.793554	-3.489412
C	-0.869846	-3.229226	-2.267205
H	-0.790201	-4.272722	-1.920083
H	-1.819818	-3.135129	-2.819033
H	-0.925135	-2.577543	-1.382454
C	0.362770	-3.710589	-4.437832
H	1.195708	-3.413101	-5.094100
H	-0.577701	-3.623431	-5.007510
H	0.502904	-4.773071	-4.176012
C	4.748806	-0.706712	-1.616691
H	4.244126	0.179539	-2.032458
C	5.177400	-0.376613	-0.172403
H	5.739102	-1.206300	0.286115
H	4.313149	-0.180483	0.484618
H	5.823983	0.515656	-0.153224
C	5.981627	-0.988992	-2.499598
H	5.675843	-1.197749	-3.536469
H	6.537404	-1.865735	-2.127142
H	6.667873	-0.125355	-2.503984
C	3.706873	-5.544952	-0.526678
H	4.513020	-5.322260	0.195602
C	2.595274	-6.299056	0.226971
H	1.806377	-6.644582	-0.461074
H	2.121519	-5.664067	0.990913
H	3.009451	-7.191905	0.723929
C	4.308345	-6.437547	-1.636550
H	4.701236	-7.379108	-1.215923
H	5.127601	-5.920095	-2.160568
H	3.538995	-6.692497	-2.384543
C	2.157106	3.958588	-1.806290
H	2.636888	3.008542	-2.089957
C	2.622726	4.316429	-0.384099
H	2.214570	5.283158	-0.048685
H	3.720332	4.389468	-0.346717

H	2.305442	3.561152	0.353153
C	2.617776	5.025891	-2.819696
H	2.308130	4.752085	-3.840095
H	3.715430	5.134341	-2.804018
H	2.172528	6.006304	-2.581424
C	-2.476432	5.835089	-1.017264
H	-1.828620	6.516328	-0.436785
C	-3.627122	5.386400	-0.097960
H	-3.249778	4.819368	0.765387
H	-4.341478	4.742296	-0.634831
H	-4.185066	6.261905	0.274972
C	-3.020558	6.627049	-2.226940
H	-2.199829	6.973403	-2.875197
H	-3.597034	7.506710	-1.892878
H	-3.687319	5.994938	-2.836717
C	-2.003753	1.353217	-3.375724
H	-1.276091	0.527521	-3.413425
C	-2.351158	1.755557	-4.825873
H	-1.462886	2.099099	-5.374178
H	-3.088739	2.576193	-4.824319
H	-2.789487	0.902986	-5.371735
C	-3.274562	0.830506	-2.678232
H	-3.623870	-0.090041	-3.171452
H	-4.100074	1.559470	-2.725522
H	-3.101198	0.600698	-1.617781

Tl-Sb(Ar*)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Sb	3.156800	-3.537868	7.131543
Tl	1.165964	-1.716968	8.204300
H	-0.108454	-0.167465	3.296198

C	0.467081	0.135515	4.175622
C	1.842553	0.984257	6.472813
C	0.177688	-0.465757	5.424996
C	1.460907	1.106339	4.049387
C	2.126397	1.532682	5.196417
C	0.872007	-0.049855	6.605292
H	1.684570	1.551492	3.076667
H	2.867067	2.333927	5.123261
C	-0.975889	-1.421104	5.376835
C	-3.249231	-3.111456	5.009417
C	-2.301900	-0.897576	5.500703
C	-0.814311	-2.783424	4.994235
C	-1.951107	-3.597356	4.830127
C	-3.405455	-1.755033	5.329177
H	-1.825561	-4.633739	4.520373
H	-4.412957	-1.345807	5.416654
C	2.485739	1.755775	7.588752
C	3.614627	3.521252	9.534564
C	1.808218	2.963773	7.970157
C	3.783477	1.511578	8.112280
C	4.296150	2.383850	9.096708
C	2.381845	3.808380	8.935432
H	5.290565	2.184511	9.494020
H	1.876868	4.738582	9.202592
C	-2.567461	0.604228	5.661627
H	-1.619513	1.108637	5.890317
C	-3.525241	0.940613	6.812713
H	-4.526952	0.511023	6.662930
H	-3.644095	2.031348	6.898260
H	-3.131399	0.571809	7.763995
C	-3.091599	1.194422	4.336776
H	-2.404927	0.984066	3.503635
H	-3.202406	2.287418	4.421446
H	-4.076587	0.776220	4.075155
C	0.545155	-3.352210	4.576464

H	1.340244	-2.682744	4.962935
C	0.840502	-4.770221	5.095400
H	0.173578	-5.511626	4.644988
H	0.733705	-4.839280	6.171191
H	1.862511	-5.051835	4.824541
C	0.675334	-3.339356	3.037610
H	0.521630	-2.330640	2.623851
H	-0.062773	-4.010998	2.571847
H	1.680869	-3.682486	2.735502
C	-4.444410	-4.028434	4.793807
H	-4.054439	-5.034199	4.568982
C	-5.313420	-4.146985	6.056291
H	-5.751294	-3.177544	6.335318
H	-4.719383	-4.504932	6.907677
H	-6.139182	-4.855263	5.890693
C	-5.284020	-3.582062	3.583681
H	-4.662001	-3.509882	2.679557
H	-5.743187	-2.597073	3.756147
H	-6.093867	-4.301662	3.389316
C	0.550941	3.467611	7.246036
H	0.217344	2.705800	6.531597
C	0.874871	4.735268	6.429282
H	1.130666	5.584028	7.082657
H	0.003460	5.031732	5.823916
H	1.722535	4.567528	5.748725
C	-0.637138	3.717964	8.180941
H	-0.928948	2.793880	8.691181
H	-1.502928	4.073964	7.602030
H	-0.417321	4.480888	8.941912
C	4.223226	4.494444	10.534306
H	3.402675	5.117053	10.926247
C	5.222713	5.431459	9.830444
H	4.741801	5.970755	9.001538
H	6.066734	4.860933	9.414630
H	5.626969	6.172786	10.536591

C	4.884529	3.799573	11.735935
H	5.792051	3.255103	11.440253
H	4.199504	3.083473	12.209375
H	5.179684	4.544627	12.489356
C	4.782679	0.414297	7.701117
H	5.746463	0.944852	7.656476
C	4.652054	-0.225851	6.319488
H	5.510860	-0.892153	6.148601
H	4.651164	0.525565	5.516042
H	3.742855	-0.843914	6.206185
C	4.947159	-0.656234	8.793078
H	5.715584	-1.363844	8.492993
H	4.025463	-1.205516	8.969506
H	5.253582	-0.210065	9.741556
H	0.897520	-4.602069	12.698118
C	0.570432	-3.633581	12.308121
C	-0.407978	-1.251483	11.191572
C	0.860247	-3.310749	10.961008
C	-0.173193	-2.774423	13.109878
C	-0.669751	-1.609208	12.540141
C	0.396579	-2.087537	10.377787
H	-0.402874	-3.033606	14.144155
H	-1.306300	-0.953448	13.135506
C	1.493213	-4.453792	10.232166
C	2.625494	-6.812125	9.058795
C	2.892085	-4.734898	10.386322
C	0.668555	-5.402682	9.549711
C	1.257616	-6.530855	8.943057
C	3.420173	-5.919177	9.811226
H	0.627167	-7.236447	8.398509
H	4.495433	-6.132481	9.929069
C	-1.236426	-0.066489	10.796274
C	-3.186872	1.997087	10.711043
C	-2.585051	-0.358087	10.430340
C	-0.855894	1.272124	11.123238

C	-1.856784	2.264872	11.079901
C	-3.526600	0.685841	10.373667
H	-1.610282	3.288437	11.351798
H	-4.562660	0.462375	10.109831
C	3.839081	-3.828162	11.176613
H	3.363766	-2.835855	11.252532
C	5.217833	-3.637756	10.510474
H	5.845882	-4.537318	10.620017
H	5.753215	-2.806269	10.986462
H	5.122814	-3.429982	9.443666
C	4.039443	-4.369273	12.606974
H	3.084102	-4.467487	13.145151
H	4.693156	-3.695800	13.186228
H	4.516106	-5.366526	12.577792
C	-0.856838	-5.285993	9.532179
H	-1.145895	-4.361084	10.042190
C	-1.444087	-5.221864	8.114091
H	-1.200768	-6.115531	7.526902
H	-1.079030	-4.350958	7.567487
H	-2.538427	-5.145650	8.162858
C	-1.486449	-6.444663	10.330542
H	-1.073140	-6.490087	11.349641
H	-1.303398	-7.417203	9.848671
H	-2.576102	-6.308271	10.406954
C	3.225268	-8.042620	8.397620
H	2.401795	-8.577988	7.893280
C	4.256480	-7.663048	7.319672
H	5.129143	-7.151272	7.760627
H	3.816857	-6.986969	6.571660
H	4.620447	-8.564731	6.801165
C	3.828396	-9.001530	9.439438
H	4.176709	-9.929294	8.956863
H	3.082029	-9.268134	10.206050
H	4.691297	-8.544382	9.954292
C	-3.107081	-1.789362	10.250587

H	-2.274219	-2.490747	10.365467
C	-3.695780	-2.039465	8.855778
H	-4.551936	-1.383477	8.643263
H	-4.046337	-3.077475	8.773739
H	-2.944095	-1.873819	8.077251
C	-4.137627	-2.144945	11.341958
H	-3.731335	-1.968037	12.348025
H	-4.418110	-3.207460	11.268445
H	-5.059685	-1.551795	11.240679
C	-4.250290	3.085742	10.714473
H	-5.192870	2.626899	10.371633
C	-3.915982	4.224798	9.737726
H	-3.763016	3.836507	8.721275
H	-2.999835	4.755068	10.036636
H	-4.735209	4.959616	9.707405
C	-4.494396	3.628177	12.133960
H	-4.750613	2.813441	12.827335
H	-5.322213	4.354335	12.133130
H	-3.600950	4.136759	12.526960
C	0.585804	1.672317	11.521891
H	1.230292	1.437639	10.660618
C	1.160284	0.931894	12.753240
H	1.470246	-0.091878	12.526200
H	0.430558	0.903828	13.575163
H	2.052906	1.459221	13.123197
C	0.747880	3.178501	11.811223
H	1.802471	3.403353	12.013472
H	0.175958	3.473989	12.705272
H	0.435027	3.809185	10.973218
