Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

A Single-Step Conversion of Silathiogermylene to Germaacid Anhydrides: An Unusual Reactivity

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Experimental procedures

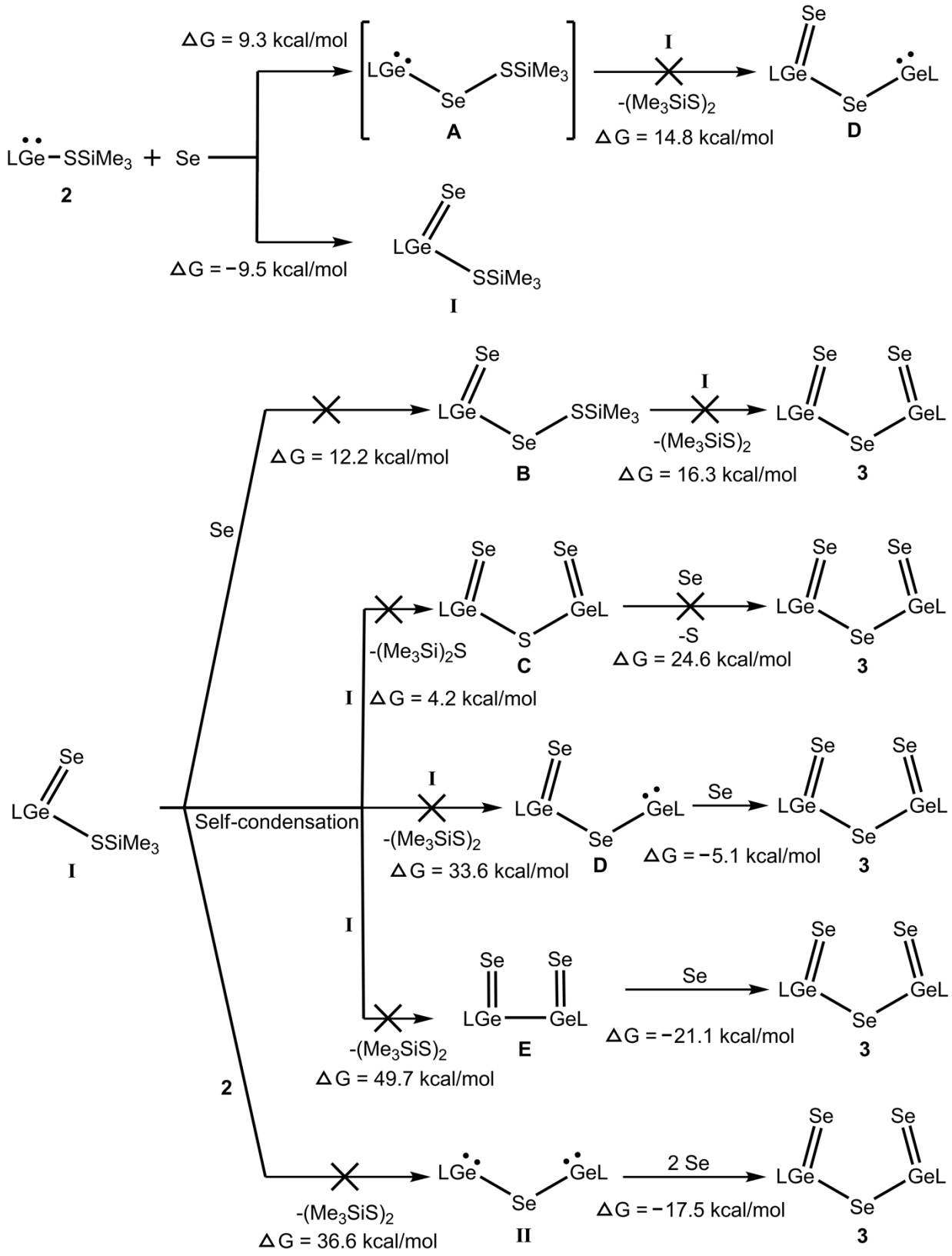
All the air and moisture sensitive compounds were manipulated under a dry N_2 atmosphere using either glovebox [Jacomax (GP Concept)-T2 workstation] or standard Schlenk techniques. All the solvents were dried prior to use. Hexane, THF, toluene, and C_6D_6 were dried over potassium. $CDCl_3$, DMSO-d_6, and acetonitrile were dried over 4 Å molecular sieves and P_2O_5, respectively. Elemental selenium, sulfur, and tellurium were purchased from Aldrich and used as such. Compound **1** and lithium trimethylsilyl thiolate·tetrahydrofuran adduct (1:0.82) ($LiSSiMe_3$·thf) were prepared according to the literature procedures.[S1,S2] Melting points were recorded using an Ambassador melting point apparatus by sealing the samples in glass capillaries. Elemental analyses were performed on a Perkin-Elmer CHN analyzer. The ^1H, ^{13}C, ^{29}Si, ^{77}Se, and ^{125}Te NMR spectra were recorded on a 300 MHz Bruker DPX-300 spectrometer. The chemical shifts δ are reported in ppm and referenced internally with respect to the residual solvent (^1H NMR) and solvent (^{13}C NMR) resonances.[S3] In the ^{29}Si ^{77}Se, and ^{125}Te NMR spectroscopic studies, tetramethylsilane (TMS), dimethylselenide (Me_2Se), and dimethyltelluride (Me_2Te) were used as external references, respectively.

Synthesis of (Bu^i_2ATI)GeSSiMe$_3$ (2). To a suspension of compound **1** (2.00 g, 5.89 mmol) in hexane (80 ml), a solution of lithium trimethylsilyl thiolate·tetrahydrofuran (1:0.82) adduct (1.01 g, 5.89 mmol) in hexane (10 ml) was added at 0 °C, allowed to come to room temperature, and stirred for 8 h. The resulting red solution was filtered through a G4 sintered funnel with celite. Removal of all the volatiles from the filtrate under reduced pressure afforded an analytically pure sample of compound **2** as a red solid. Yield: 2.36 g (5.77 mmol, 98%). Mp: 94 ºC. Anal. Calcd for $C_{18}H_{32}GeN_2SSi$ (M = 409.25): C, 52.8; H, 7.9; N, 6.9. Found: C, 52.7; H, 7.9; N, 6.8. ^{1}H NMR (300 MHz, C_6D_6): δ 0.63 (S, 9H, Si(CH_3)$_3$), 0.83 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$), 0.93 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$), 2.09-2.22 (m, 2H, CH(CH$_3$)$_2$), 3.17 (dd, J_{HH} = 13.8, 6.3 Hz, 2H, CH_2), 3.41 (dd, J_{HH} = 13.8, 8.1 Hz, 2H, CH_2), 6.09-6.15 (m, 1H, CH_{ring}), 6.26 (d, J_{HH} = 11.4 Hz, 2H, CH_{ring}), 6.59-6.66 (m, 2H, CH_{ring}). ^{13}C{^{1}H} NMR (75 MHz, C_6D_6): δ 5.35 (Si(*C*H$_3$)$_3$), 21.07 (CH(*C*H$_3$)$_2$), 21.32 (CH(*C*H$_3$)$_2$), 28.03 (*C*H(CH$_3$)$_2$), 54.13 (*C*H$_2$), 115.41, 120.50, 136.72, 161.54 (*C*H$_{ring}$). ^{29}Si{^{1}H} NMR (60 MHz, C_6D_6): δ 10.16 (S-*Si*(CH$_3$)$_3$).

Synthesis of {(Bu^i_2ATI)Ge(Se)}$_2$Se (3). To a solution of compound **2** (1.00 g, 2.44 mmol) in tetrahydrofuran (20 ml), elemental selenium (0.29 g, 3.67 mmol) was added at room temperature and stirred for 12 h. The resulting yellow solution was filtered through a G4 sintered funnel with celite. Removal of all the volatiles under reduced pressure led to the formation of a yellow paste. This was washed twice with cold hexane (5 ml) and dried under vacuum to get an analytically pure sample of compound **3** as a yellow solid. Slow cooling of a hot solution of compound **3** in acetonitrile to room temperature afforded single crystals suitable for X-ray diffraction studies. Yield: 0.99 g, (1.17 mmol, 95.8%). Mp: 198 ^{o}C (decomp). Anal. Calcd for $C_{30}H_{46}Ge_2N_4Se_3$ (M = 844.87): C, 42.7; H, 5.5; N, 6.6. Found: C, 42.6; H, 5.5; N, 6.7. ^{1}H NMR (300 MHz, (CD$_3$)$_2$SO): δ 0.98 (d, $^3J_{HH}$ = 5.7 Hz, 24H, CH(CH_3)$_2$), 2.33-2.43 (m, 4H, CH(CH$_3$)$_2$), 3.52-3.76 (m, 8H, CH_2), 6.97-7.05 (m, 2H,CH_{ring}), 7.24-7.30 (m, 4H, CH_{ring}), 7.53-7.60 (m, 4H, CH_{ring}). ^{13}C{^{1}H} NMR (75 MHz, (CD$_3$)$_2$SO): δ 20.70 (CH(*C*H$_3$)$_2$), 27.33 (*C*H(CH$_3$)$_2$), 51.90 (*C*H$_2$), 117.79, 126.28, 138.59, 156.49 (Ring). ^{77}Se{^{1}H} NMR (57 MHz, (CD$_3$)$_2$SO): δ –370.42, –324.06 (Ge=*Se*, Ge-*Se*-Ge).

Synthesis of {(Bu$^i_2$ATI)Ge(S)}$_2$S (4). To a solution of compound **2** (1.00 g, 2.44 mmol) in tetrahydrofuran (20 mL), elemental sulfur (0.08 g, 2.49 mmol) was added at room temperature and stirred for 6 h. Removal of all the volatiles from the resulting yellow solution under reduced pressure led to the formation of a yellow solid. This solid was washed twice with cold hexane (5 mL) and dried to get an analytically pure sample of compound **4** as a yellow solid. Cooling a hot solution of compound **4** in acetonitrile to room temperature slowly afforded single crystals suitable for X-ray diffraction studies. Yield: 0.84 g, (1.19 mmol, 97.7%). Mp: 181 ^{o}C (decomp). Anal. Calcd for $C_{30}H_{46}Ge_2N_4S_3$ (M = 704.19): C, 51.2; H, 6.5; N, 8.0. Found: C, 51.2; H, 6.6; N, 7.9. ^{1}H NMR (300 MHz, C_6D_6): δ 1.02 (d, $^3J_{HH}$ = 6.6 Hz, 24H, CH(CH_3)$_2$), 2.50-2.64 (m, 4H, CH(CH$_3$)$_2$), 3.80 (d, $^3J_{HH}$ = 7.2 Hz, 8H, CH_2), 6.18-6.25 (m, 2H,CH_{ring}), 6.54 (d, $^3J_{HH}$ = 11.1 Hz, 4H, CH_{ring}), 6.64-6.71 (m, 4H, CH_{ring}). ^{13}C{^{1}H} NMR (75 MHz, C_6D_6):δ 21.24 (CH(CH$_3$)$_2$), 28.25 (CH(CH$_3$)$_2$), 53.46 (CH$_2$), 116.49, 124.11, 137.72, 157.48 (CH$_{ring}$).

Synthesis of {(Bu$^i_2$ATI)Ge(Te)}$_2$Te (5). To a solution of compound **2** (70 mg, 0.17 mmol) in DMSO-d$_6$ (1 mL), elemental tellurium (37 mg, 0.29 mmol) was added at room temperature and stirred for 12 h. After that, with no color change being observed, the red reaction mixture (with trace amount of tellurium particles) was analyzed by NMR spectroscopic studies that revealed the quantitative formation of compound **5**. The reaction was performed also in tetrahydrofuran as a solvent that afforded the same product quantitatively as in DMSO-d$_6$. ^{125}Te{^{1}H} NMR (94.62 MHz, (CD$_3$)$_2$SO): δ –933.2, –217.9 (Ge=*Te*, Ge-*Te*-Ge).



Scheme S1. Various reaction pathways and their thermochemical feasibility for the formation of compound **3** from compound **2** and elemental selenium.

Table S1. Thermochemical variables for reactants, products, and reaction steps shown in scheme S1

S. No.	Variable	Reactant (Hartree/particle)	Product (Hartree/particle)	Reaction (kcal/mol)
1.	$E+H_{corr}$	**2** + 1/8$\mathbf{Se}_8$ = -5980.7696085	**A** = -5980.755986	ΔH = 8.5
	$E+G_{corr}$	-5980.87216375	-5980.857335	ΔG = 9.3
2.	$E+H_{corr}$	**2**+1/8$\mathbf{Se}_8$ = -5980.7696085	**I** = -5980.789785	ΔH = -12.7
	$E+G_{corr}$	-5980.87216375	-5980.887354	ΔG = -9.5
3.	$E+H_{corr}$	**I**+**A** = -11961.545771	**D**+$(Me_3SiS)_2$ = -11961.522431	ΔH = 14.6
	$E+G_{corr}$	-11961.744689	-11961.72111	ΔG = 14.8
4.	$E+H_{corr}$	**A**+**A** = - 11961.511972	**D**+$(Me_3SiS)_2$ = - 11961.522431	ΔH = -6.6
	$E+G_{corr}$	-11961.71467	-11961.72111	ΔG = -4.0
5	$E+H_{corr}$	**A**+**A** = - 11961.511972	**E**+$(Me_3SiS)_2$ = - 11961.499701	ΔH = 7.7
	$E+G_{corr}$	-11961.71467	-11961.695548	ΔG = 12.0
6	$E+H_{corr}$	**A**+**2** = - 9559.871855	**II**+$(Me_3SiS)_2$ = - 9559.844547	ΔH = 17.1
	$E+G_{corr}$	-9560.067829	-9560.039583	ΔG= 17.7
7	$E+H_{corr}$	**A**+**B** = - 14363.179968	**3**+$(Me_3SiS)_2$ = - 14363.188829	ΔH = -5.6
	$E+G_{corr}$	-14363.38684	-14363.390882	ΔG= -2.5
8	$E+H_{corr}$	**A**+1/8$\mathbf{Se}_8$ = -8382.4097255	**B** = -8382.423982	ΔH = -8.9
	$E+G_{corr}$	-8382.51900475	-8382.529505	ΔG= -6.6
9	$E+H_{corr}$	**I**+1/8$\mathbf{Se}_8$ = -8382.4435245	**B** = -8382.423982	ΔH = 12.3
	$E+G_{corr}$	-8382.54902375	-8382.529505	ΔG= 12.2
10	$E+H_{corr}$	**I**+**B** = -14363.213767	**3**+$(Me_3SiS)_2$ = - 14363.188829	ΔH = 15.6
	$E+G_{corr}$	-14363.416859	-14363.390882	ΔG= 16.3
11	$E+H_{corr}$	**I**+**2** = -9559.905654	**II**+$(Me_3SiS)_2$ = - 9559.844547	ΔH = 38.3
	$E+G_{corr}$	-9560.097848	-9560.039583	ΔG= 36.6
12	$E+H_{corr}$	**I**+**I** = -11961.57957	**D**+$(Me_3SiS)_2$ = - 11961.522431	ΔH = 35.9

	$E+G_{corr}$	-11961.774708	-11961.72111	ΔG= 33.6
13	$E+H_{corr}$	**I**+**I** = -11961.57957	**E**+$(Me_3SiS)_2$ = - 11961.499701	ΔH = 50.1
	$E+G_{corr}$	-11961.774708	-11961.695548	ΔG= 49.7
14	$E+H_{corr}$	**I**+**I** = -11961.57957	**C**+$(Me_3Si)_2S$ = -11961.571809	ΔH = 4.9
	$E+G_{corr}$	-11961.774708	-11961.768079	ΔG= 4.2
15	$E+H_{corr}$	**D**+1/8$\mathbf{Se}_8$ = -12748.4312085	**3** = -12748.443867	ΔH = -7.9
	$E+G_{corr}$	-12748.56972575	-12748.577828	ΔG= -5.1
16	$E+H_{corr}$	**C**+1/8$\mathbf{Se}_8$ = -13146.6681235	**3**+1/8$\mathbf{S}_8$ = -13146.630218125	ΔH = 23.8
	$E+G_{corr}$	-13146.80973475	-13146.770553625	ΔG= 24.6
17	$E+H_{corr}$	**E**+1/8$\mathbf{Se}_8$ = -12748.4084785	**3** = -12748.443867	ΔH = -22.2
	$E+G_{corr}$	-12748.54416375	-12748.577828	ΔG= -21.1
18	$E+H_{corr}$	**II**+1/4$\mathbf{Se}_8$ = -12748.407064	**3** = -12748.443867	ΔH = -23.1
	$E+G_{corr}$	-12748.5498685	-12748.577828	ΔG= -17.5

X-ray data collection for compounds 3 and 4. Suitable single crystals of compounds **3** and **4** were coated with a cryoprotectant and mounted on a glass fiber. The data were collected at low temperature on a Bruker SMART APEX CCD diffractometer with a 3-axis goniometer.[S4] SAINT and SADABS software were used for data integration and empirical absorption correction, respectively.[S5] The structure of these compounds were solved by patterson methods and refined by full matrix least-squares on F^2 using SHELXTL.[S6] All the non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated using a riding model and refined isotropically. Detailed crystallographic data for these compounds are given in Table S1.

Table S2. Crystal data and refinement parameters for compounds 3 and 4

	3	**4**
empirical formula	$C_{30}H_{46}Ge_2N_4Se_3$	$C_{30}H_{46}Ge_2N_4S_3$
fw	844.81	704.14
temperature, k	100(2)	150(2)
wavelength, Å	0.71073	0.71073
cryst syst	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$
unit cell dimens	a = 16.736(3) Å	a = 16.400(4) Å
	b = 11.336(2) Å	b = 11.364(3) Å
	c = 18.978(3) Å	c = 18.733(5) Å
	β = 106.354(3)°	β = 106.005(4)°
volume, Å^3	3454.8(10)	3355.9(15)
Z	4	4
density (calcd), Mg/m^3	1.565	1.394
absorption coefficient, mm^{-1}	4.511	2.003
F(000)	1626.6	1464.0
cryst size, mm^3	0.461 x 0.387 x 0.266	0.474 x 0.339 x 0.255
θ range for data collection, deg	1.27 to 25.00	1.29 to 25.00
limiting indices	$-10 \le h \le 19$,	$-19 \le h \le 19$,
	$-13 \le k \le 13$,	$-13 \le k \le 13$,
	$-22 \le l \le 22$	$-22 \le l \le 22$
no. of reflns collected	17739	17191
no. of indep reflns	6084 (R_{int} = 0.0461)	5904 (R_{int} = 0.0503)
abs corr	semiempirical	semiempirical
refinement method	full-matrix	full-matrix
	least-squares on F^2	least-squares on F^2
no. of data / restraints / params	6068 / 0 / 361	5903 / 0 / 360
goodness-of-fit on F^2	1.066	1.025
final R indices [$I>2\sigma(I)$]	R_1 = 0.0419, wR_2 = 0.1169	R_1 = 0.0426, wR_2 = 0.0921
R indices (all data)	R_1 = 0.0545, wR_2 = 0.1329	R_1 = 0.0599, wR_2 = 0.0981
largest diff peak and hole, e Å^{-3}	0.973 and −0.763	0.774 and −0.359

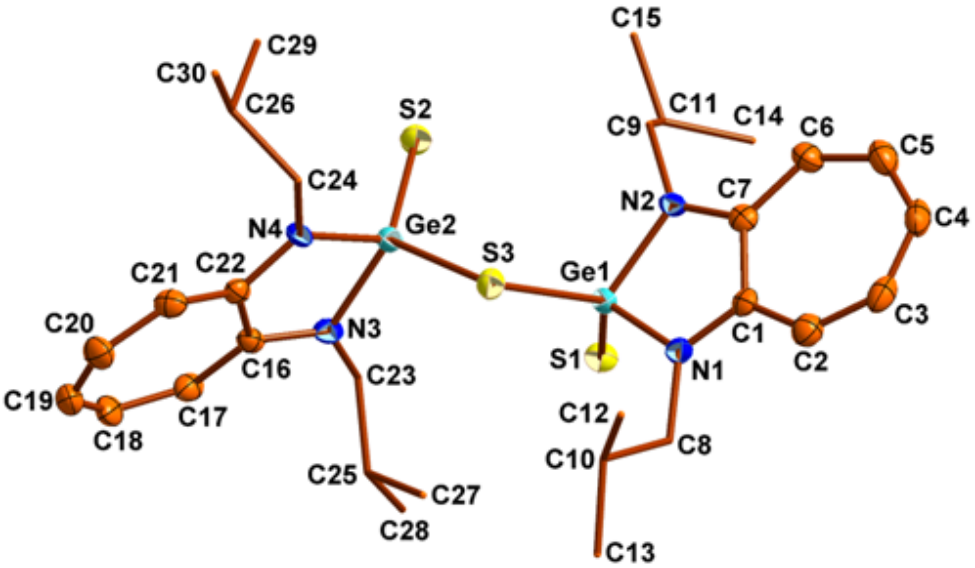


Figure S1. Molecular structure of $\{(Bu^{i}_{2}ATI)Ge(S)\}_2S$ (**4**). All the hydrogen atoms and thermal ellipsoids of isobutyl groups are omitted for clarity. Thermal ellipsoids are drawn at 50% probability. Selected bond lengths (Å) and angles (°): Ge(1)-S(1) 2.082(1), Ge(2)-S(2) 2.077(1), Ge(1)-S(3) 2.219(1), Ge(2)-S(3) 2.221(1), Ge(1)-N(1) 1.896(3), Ge(1)-N(2) 1.886(3), Ge(2)-N(3) 1.894(3), Ge(2)-N(4) 1.895(3); S(1)-Ge(1)-S(3) 123.4(1), S(2)-Ge(2)-S(3) 118.3(1), Ge(1)-S(3)-Ge(2) 105.7(1), N(1)-Ge(1)-N(2) 84.2(1), N(3)-Ge(2)-N(4) 84.2(1).

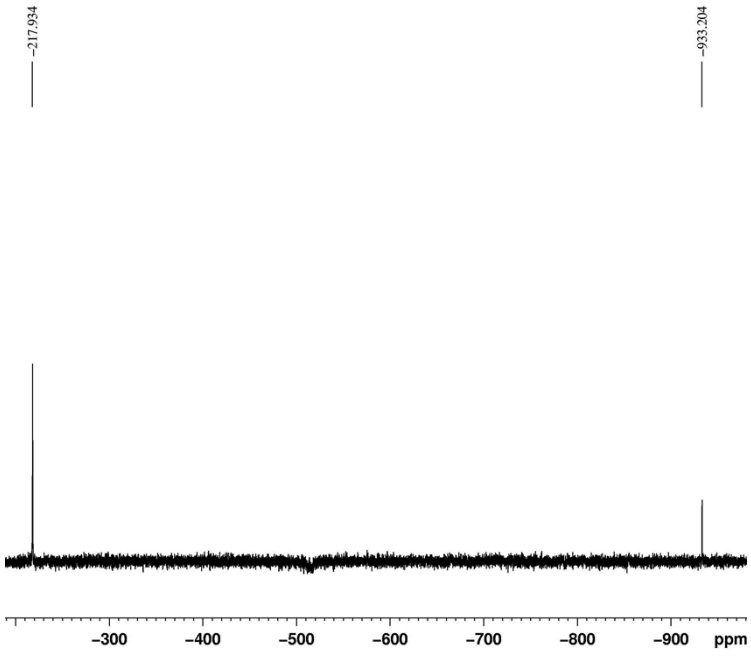


Figure S2: ^{125}Te NMR Spectrum of compound **5**

Computational details. GAUSSIAN-09 programs[S7] were used for doing all the computational work. The geometry optimizations of all the compounds (input coordinates taken from Single-crystal diffraction studies) and model compounds were done using basis sets cc-PVQZ for germanium and selenium, and TZV for rest of the elements at the B3LYP level of theory. The thermochemical variables for S and Se atoms were taken as 1/8 of those of S_8 and Se_8 (The grey selenium used in the reaction has a polymeric structure and is the most dense form of elemental selenium. As this form cannot be used for calculations, among the discrete forms of elemental selenium that is most dense (Se_8 ring) is used in calculations.[S8] Further, this approach gives uniformity with S_8 which has to be used for elemental sulfur), respectively.

Coordinates of the optimized geometry of compound I

6	**3.370395000**	**-1.275661000**	**-1.196751000**
6	**4.687717000**	**-0.890754000**	**-1.402999000**
6	**5.346657000**	**0.282281000**	**-1.043606000**
6	**4.775675000**	**1.371598000**	**-0.396901000**
6	**3.458597000**	**1.590792000**	**-0.006831000**
6	**2.298455000**	**0.795812000**	**-0.119921000**
6	**2.273257000**	**-0.608103000**	**-0.608333000**
7	**1.068693000**	**-1.198737000**	**-0.456117000**
7	**1.089152000**	**1.243110000**	**0.293335000**
6	**0.902115000**	**2.546856000**	**0.966305000**
1	**-0.050511000**	**2.489743000**	**1.496202000**
1	**1.669303000**	**2.658167000**	**1.738438000**
6	**0.727030000**	**-2.579348000**	**-0.856565000**
1	**-0.282960000**	**-2.534416000**	**-1.269258000**

1	**1.372753000**	**-2.919150000**	**-1.668158000**
6	**0.901655000**	**3.795030000**	**0.047090000**
1	**1.769416000**	**3.739183000**	**-0.617127000**
6	**1.046464000**	**5.055573000**	**0.919264000**
1	**1.974653000**	**5.045790000**	**1.495925000**
1	**1.045566000**	**5.954068000**	**0.299972000**
1	**0.215160000**	**5.137880000**	**1.624405000**
6	**-0.357112000**	**3.873834000**	**-0.829462000**
1	**-0.483311000**	**2.982352000**	**-1.441760000**
1	**-1.251838000**	**3.980400000**	**-0.209970000**
1	**-0.305672000**	**4.739682000**	**-1.493225000**
6	**0.740704000**	**-3.607661000**	**0.301829000**
1	**0.076969000**	**-3.220764000**	**1.079651000**
6	**2.133211000**	**-3.805489000**	**0.919247000**
1	**2.836172000**	**-4.221089000**	**0.191077000**
1	**2.543130000**	**-2.869160000**	**1.298797000**
1	**2.076826000**	**-4.501913000**	**1.757990000**
6	**0.165711000**	**-4.940207000**	**-0.210078000**
1	**0.788418000**	**-5.359970000**	**-1.005754000**
1	**0.121584000**	**-5.672468000**	**0.597631000**
1	**-0.845647000**	**-4.814840000**	**-0.602084000**
32	**-0.313042000**	**-0.076832000**	**0.282371000**
16	**-1.560232000**	**0.264163000**	**-1.574492000**
14	**-3.775106000**	**0.123981000**	**-0.975856000**
6	**-4.198420000**	**1.469953000**	**0.291118000**

1	**-3.639561000**	**1.315889000**	**1.213164000**
1	**-3.961584000**	**2.459125000**	**-0.101219000**
1	**-5.265552000**	**1.441908000**	**0.525664000**
6	**-4.635455000**	**0.451642000**	**-2.641126000**
1	**-4.347878000**	**-0.292347000**	**-3.384256000**
1	**-5.720412000**	**0.408606000**	**-2.519319000**
1	**-4.376523000**	**1.436323000**	**-3.030643000**
6	**-4.156916000**	**-1.622217000**	**-0.342194000**
1	**-3.915078000**	**-2.368847000**	**-1.099194000**
1	**-3.580403000**	**-1.835212000**	**0.556968000**
1	**-5.219010000**	**-1.711989000**	**-0.100648000**
1	**3.150120000**	**-2.276268000**	**-1.534525000**
1	**5.297963000**	**-1.635205000**	**-1.902720000**
1	**6.400091000**	**0.347269000**	**-1.282527000**
1	**5.450859000**	**2.189717000**	**-0.170968000**
1	**3.294562000**	**2.552117000**	**0.454396000**
34	**-1.205542000**	**-0.525955000**	**2.274118000**

Coordinates of the optimized geometry of compound A

6	**-3.711637000**	**1.351899000**	**-0.919032000**
6	**-5.031673000**	**0.990086000**	**-1.131728000**
6	**-5.724653000**	**-0.159087000**	**-0.747255000**
6	**-5.182991000**	**-1.248243000**	**-0.076961000**
6	**-3.870582000**	**-1.496482000**	**0.315295000**
6	**-2.692660000**	**-0.723398000**	**0.203581000**

6	**-2.640231000**	**0.681856000**	**-0.271746000**
7	**-1.443947000**	**1.257733000**	**-0.056921000**
7	**-1.488190000**	**-1.182980000**	**0.619633000**
6	**-1.301311000**	**-2.541807000**	**1.168731000**
1	**-0.309566000**	**-2.558190000**	**1.627564000**
1	**-2.018066000**	**-2.716498000**	**1.979587000**
6	**-1.070536000**	**2.628932000**	**-0.453983000**
1	**-0.062349000**	**2.566916000**	**-0.869373000**
1	**-1.709077000**	**3.000806000**	**-1.256610000**
6	**-1.384158000**	**-3.717284000**	**0.160806000**
1	**-2.373413000**	**-3.708749000**	**-0.304811000**
6	**-1.236500000**	**-5.040104000**	**0.934864000**
1	**-2.000042000**	**-5.142732000**	**1.709816000**
1	**-1.327568000**	**-5.893161000**	**0.260522000**
1	**-0.257339000**	**-5.101937000**	**1.417421000**
6	**-0.340419000**	**-3.612160000**	**-0.959366000**
1	**-0.467540000**	**-2.701031000**	**-1.543661000**
1	**0.674363000**	**-3.609026000**	**-0.555697000**
1	**-0.428942000**	**-4.460400000**	**-1.641644000**
6	**-1.060066000**	**3.642825000**	**0.716103000**
1	**-0.413640000**	**3.226456000**	**1.495863000**
6	**-2.454221000**	**3.871165000**	**1.319971000**
1	**-3.129047000**	**4.324804000**	**0.588677000**
1	**-2.903202000**	**2.938298000**	**1.662942000**
1	**-2.393050000**	**4.546013000**	**2.176204000**

6	**-0.436200000**	**4.964523000**	**0.235141000**
1	**-1.035691000**	**5.413890000**	**-0.561766000**
1	**-0.380508000**	**5.684259000**	**1.053692000**
1	**0.574435000**	**4.810548000**	**-0.147184000**
32	**-0.052638000**	**0.158191000**	**0.844032000**
1	**-3.459803000**	**2.332609000**	**-1.292477000**
1	**-5.619195000**	**1.731340000**	**-1.663276000**
1	**-6.778079000**	**-0.202619000**	**-0.991318000**
1	**-5.879819000**	**-2.044135000**	**0.164106000**
1	**-3.731206000**	**-2.453857000**	**0.793608000**
14	**4.636728000**	**-0.105211000**	**0.190704000**
16	**2.971554000**	**1.222162000**	**-0.649851000**
34	**1.358818000**	**-0.290972000**	**-1.220578000**
6	**6.003176000**	**1.143015000**	**0.635963000**
1	**5.655736000**	**1.853851000**	**1.386082000**
1	**6.876210000**	**0.624941000**	**1.039580000**
1	**6.320647000**	**1.705357000**	**-0.242474000**
6	**4.016026000**	**-1.029091000**	**1.729304000**
1	**3.677892000**	**-0.327544000**	**2.491543000**
1	**3.180824000**	**-1.681656000**	**1.476575000**
1	**4.813798000**	**-1.643666000**	**2.153554000**
6	**5.202767000**	**-1.310736000**	**-1.162289000**
1	**4.363665000**	**-1.907577000**	**-1.519651000**
1	**5.616172000**	**-0.767206000**	**-2.011863000**
1	**5.969107000**	**-1.989495000**	**-0.780534000**

Coordinates of the optimized geometry of compound B

6	**3.856382000**	**-1.137408000**	**-1.228882000**
6	**5.150305000**	**-0.699253000**	**-1.464125000**
6	**5.781743000**	**0.483612000**	**-1.081105000**
6	**5.196588000**	**1.528150000**	**-0.378781000**
6	**3.881775000**	**1.692207000**	**0.049901000**
6	**2.745852000**	**0.867238000**	**-0.068035000**
6	**2.756202000**	**-0.526770000**	**-0.582351000**
7	**1.581744000**	**-1.165038000**	**-0.403601000**
7	**1.525688000**	**1.269096000**	**0.369998000**
6	**1.298731000**	**2.555731000**	**1.064705000**
1	**0.337709000**	**2.464256000**	**1.574446000**
1	**2.047442000**	**2.670273000**	**1.854863000**
6	**1.271802000**	**-2.546423000**	**-0.830417000**
1	**0.246298000**	**-2.528611000**	**-1.205491000**
1	**1.899211000**	**-2.840854000**	**-1.673584000**
6	**1.281364000**	**3.830129000**	**0.183924000**
1	**2.237201000**	**3.910274000**	**-0.342020000**
6	**1.143059000**	**5.056558000**	**1.104804000**
1	**1.955059000**	**5.107538000**	**1.833841000**
1	**1.157305000**	**5.979009000**	**0.522116000**
1	**0.199587000**	**5.025118000**	**1.655627000**
6	**0.168604000**	**3.807626000**	**-0.873402000**
1	**0.285528000**	**2.975896000**	**-1.568140000**

1	**-0.814898000**	**3.717006000**	**-0.407011000**
1	**0.180467000**	**4.730895000**	**-1.456480000**
6	**1.360599000**	**-3.605331000**	**0.296083000**
1	**0.712919000**	**-3.263040000**	**1.107242000**
6	**2.780574000**	**-3.773406000**	**0.856924000**
1	**3.469540000**	**-4.146856000**	**0.093264000**
1	**3.174386000**	**-2.834666000**	**1.247914000**
1	**2.777106000**	**-4.493315000**	**1.677500000**
6	**0.808809000**	**-4.940003000**	**-0.235161000**
1	**1.413027000**	**-5.315249000**	**-1.066660000**
1	**0.819580000**	**-5.696908000**	**0.550697000**
1	**-0.220524000**	**-4.835068000**	**-0.583194000**
32	**0.187989000**	**-0.115357000**	**0.425024000**
1	**3.658552000**	**-2.134164000**	**-1.591313000**
1	**5.769469000**	**-1.403573000**	**-2.008917000**
1	**6.825192000**	**0.591111000**	**-1.346900000**
1	**5.852329000**	**2.357537000**	**-0.137308000**
1	**3.700004000**	**2.629320000**	**0.552349000**
14	**-4.637931000**	**0.166495000**	**-0.312701000**
16	**-2.925589000**	**-1.148411000**	**-1.120295000**
34	**-1.253636000**	**0.333637000**	**-1.488379000**
6	**-5.906260000**	**-1.138369000**	**0.238611000**
1	**-5.506301000**	**-1.748022000**	**1.048528000**
1	**-6.817811000**	**-0.653803000**	**0.595915000**
1	**-6.177691000**	**-1.800113000**	**-0.584360000**

6	**-4.036049000**	**1.245164000**	**1.121641000**
1	**-3.475371000**	**0.655577000**	**1.845536000**
1	**-3.382109000**	**2.039900000**	**0.763921000**
1	**-4.889232000**	**1.706471000**	**1.625570000**
6	**-5.290624000**	**1.217971000**	**-1.754459000**
1	**-4.505174000**	**1.865533000**	**-2.145311000**
1	**-5.642558000**	**0.584644000**	**-2.568682000**
1	**-6.119383000**	**1.849910000**	**-1.426184000**
34	**-0.590211000**	**-0.676693000**	**2.428966000**

Coordinates of the optimized geometry of compound C

32	**-1.687651000**	**-0.628290000**	**-0.345188000**
32	**1.820687000**	**0.599846000**	**-0.417106000**
34	**1.662728000**	**1.699290000**	**-2.340755000**
34	**-1.320234000**	**-2.051908000**	**-2.011366000**
7	**2.874473000**	**-0.994725000**	**-0.242857000**
7	**-2.972499000**	**0.762336000**	**-0.704029000**
6	**3.843284000**	**-0.935419000**	**0.696827000**
7	**-2.906438000**	**-1.074302000**	**1.078774000**
7	**3.057384000**	**1.296514000**	**0.875964000**
6	**-5.260230000**	**1.419324000**	**-0.287118000**
1	**-5.207634000**	**1.930488000**	**-1.236421000**
6	**-3.999073000**	**-0.281127000**	**1.157769000**
6	**-4.092345000**	**0.696126000**	**0.045089000**
6	**3.950288000**	**0.396801000**	**1.352998000**

6	**4.665630000**	**-2.046520000**	**0.992254000**
1	**4.455322000**	**-2.919892000**	**0.395886000**
6	**4.889793000**	**0.735845000**	**2.347514000**
1	**4.802526000**	**1.748373000**	**2.708514000**
6	**-6.116092000**	**0.280363000**	**2.470337000**
1	**-6.572875000**	**0.043127000**	**3.425009000**
6	**-4.894822000**	**-0.346364000**	**2.245077000**
1	**-4.579360000**	**-1.002147000**	**3.042949000**
6	**-6.850546000**	**1.124626000**	**1.645297000**
1	**-7.819130000**	**1.444668000**	**2.006801000**
6	**-6.458381000**	**1.590895000**	**0.392011000**
1	**-7.185231000**	**2.206015000**	**-0.127153000**
6	**6.276983000**	**-1.321001000**	**2.791148000**
1	**7.093644000**	**-1.685613000**	**3.400444000**
6	**5.705073000**	**-2.220609000**	**1.894419000**
1	**6.140375000**	**-3.213990000**	**1.887521000**
6	**5.894937000**	**0.002384000**	**2.969787000**
1	**6.456274000**	**0.556667000**	**3.714149000**
6	**2.546836000**	**-2.178422000**	**-1.070996000**
1	**1.459113000**	**-2.204743000**	**-1.171348000**
1	**2.832331000**	**-3.097330000**	**-0.556220000**
6	**3.070789000**	**2.747536000**	**1.158934000**
1	**2.874156000**	**3.234858000**	**0.200643000**
1	**4.068668000**	**3.060875000**	**1.471314000**
6	**-2.811170000**	**1.659350000**	**-1.872093000**

1	**-3.611934000**	**1.462017000**	**-2.592592000**
1	**-1.880442000**	**1.366116000**	**-2.359252000**
6	**-2.599129000**	**-2.134715000**	**2.061284000**
1	**-2.607044000**	**-1.705847000**	**3.068746000**
1	**-1.572138000**	**-2.449919000**	**1.871054000**
6	**3.157131000**	**-2.145440000**	**-2.494208000**
1	**2.801008000**	**-1.226560000**	**-2.967285000**
6	**-2.754214000**	**3.177403000**	**-1.563721000**
1	**-3.712614000**	**3.489661000**	**-1.138735000**
6	**-3.517534000**	**-3.382481000**	**2.020001000**
1	**-4.555820000**	**-3.052387000**	**2.117695000**
6	**2.014951000**	**3.237832000**	**2.178710000**
1	**1.035245000**	**2.929909000**	**1.803737000**
6	**-1.650354000**	**3.536638000**	**-0.558612000**
1	**-0.668505000**	**3.272501000**	**-0.954750000**
1	**-1.781287000**	**3.013631000**	**0.389056000**
1	**-1.661524000**	**4.610557000**	**-0.357623000**
6	**-2.559524000**	**3.930865000**	**-2.893179000**
1	**-1.603962000**	**3.664254000**	**-3.349218000**
1	**-2.560921000**	**5.009352000**	**-2.725412000**
1	**-3.353546000**	**3.701504000**	**-3.608316000**
6	**2.609120000**	**-3.341785000**	**-3.291905000**
1	**2.977590000**	**-3.315720000**	**-4.319078000**
1	**1.519091000**	**-3.327326000**	**-3.323218000**
1	**2.926403000**	**-4.290960000**	**-2.848696000**

6	4.693376000	-2.125207000	-2.505779000
1	5.108224000	-3.044065000	-2.080699000
1	5.094343000	-1.276747000	-1.949569000
1	5.057705000	-2.044403000	-3.531879000
6	-3.390192000	-4.159382000	0.701812000
1	-3.591967000	-3.530282000	-0.163974000
1	-4.089472000	-4.998384000	0.686848000
1	-2.380838000	-4.558380000	0.579049000
6	-3.187935000	-4.278497000	3.227904000
1	-3.827878000	-5.162340000	3.236598000
1	-3.329654000	-3.752166000	4.175219000
1	-2.150677000	-4.621414000	3.185402000
6	2.047237000	4.775976000	2.225306000
1	1.278682000	5.155764000	2.900696000
1	1.869564000	5.208277000	1.238816000
1	3.014297000	5.139403000	2.585061000
6	2.192828000	2.634928000	3.580489000
1	2.167433000	1.545025000	3.555914000
1	1.388304000	2.968114000	4.239176000
1	3.138242000	2.950529000	4.031441000
16	-0.001673000	0.214990000	0.940632000

Coordinates of the optimized geometry of compound D

32	-1.584320000	-0.449750000	-0.378159000
32	1.954788000	0.495641000	-1.014792000

34	**-1.166998000**	**-1.813365000**	**-2.103117000**
34	**0.178517000**	**0.505616000**	**0.870728000**
7	**3.040348000**	**-0.992893000**	**-0.296373000**
7	**-2.991060000**	**0.830375000**	**-0.770805000**
6	**4.101138000**	**-0.676179000**	**0.470550000**
7	**-2.803905000**	**-0.968431000**	**1.035365000**
7	**3.325275000**	**1.507172000**	**-0.001866000**
6	**-5.233540000**	**1.527204000**	**-0.196549000**
1	**-5.227602000**	**2.066178000**	**-1.131613000**
6	**-3.898009000**	**-0.188641000**	**1.164592000**
6	**-4.057033000**	**0.784418000**	**0.054502000**
6	**4.273595000**	**0.791415000**	**0.644877000**
6	**4.955001000**	**-1.660851000**	**1.029794000**
1	**4.673427000**	**-2.674009000**	**0.789792000**
6	**5.323669000**	**1.402968000**	**1.365846000**
1	**5.272848000**	**2.479965000**	**1.392142000**
6	**-5.957613000**	**0.344890000**	**2.581071000**
1	**-6.371635000**	**0.086897000**	**3.549902000**
6	**-4.748977000**	**-0.275247000**	**2.289250000**
1	**-4.399639000**	**-0.947319000**	**3.058582000**
6	**-6.727042000**	**1.210865000**	**1.809932000**
1	**-7.674307000**	**1.529584000**	**2.225132000**
6	**-6.391523000**	**1.700934000**	**0.550809000**
1	**-7.133639000**	**2.340277000**	**0.084802000**
6	**6.773121000**	**-0.443997000**	**2.285059000**

1	**7.661067000**	**-0.617985000**	**2.878911000**
6	**6.097322000**	**-1.567005000**	**1.809482000**
1	**6.532288000**	**-2.522849000**	**2.082121000**
6	**6.405278000**	**0.877624000**	**2.065341000**
1	**7.050688000**	**1.624575000**	**2.515563000**
6	**2.611734000**	**-2.367884000**	**-0.629060000**
1	**1.520834000**	**-2.377170000**	**-0.581679000**
1	**2.965589000**	**-3.083334000**	**0.115062000**
6	**3.327304000**	**2.978894000**	**-0.126173000**
1	**2.988369000**	**3.197891000**	**-1.142908000**
1	**4.342449000**	**3.376249000**	**-0.050845000**
6	**-2.971620000**	**1.618864000**	**-2.021085000**
1	**-3.889673000**	**1.417702000**	**-2.581802000**
1	**-2.156030000**	**1.219104000**	**-2.626475000**
6	**-2.447452000**	**-2.028462000**	**2.000206000**
1	**-2.444163000**	**-1.615187000**	**3.013870000**
1	**-1.417025000**	**-2.315217000**	**1.785367000**
6	**3.021897000**	**-2.831402000**	**-2.048470000**
1	**2.590025000**	**-2.111809000**	**-2.751536000**
6	**-2.785709000**	**3.148596000**	**-1.862574000**
1	**-3.528696000**	**3.520151000**	**-1.150377000**
6	**-3.338701000**	**-3.295023000**	**1.953648000**
1	**-4.382240000**	**-2.987975000**	**2.071171000**
6	**2.391237000**	**3.733477000**	**0.850857000**
1	**1.392261000**	**3.305982000**	**0.729443000**

6	**-1.394120000**	**3.512137000**	**-1.324624000**
1	**-0.615157000**	**3.187617000**	**-2.019892000**
1	**-1.195641000**	**3.039231000**	**-0.363532000**
1	**-1.304348000**	**4.593671000**	**-1.198915000**
6	**-3.046845000**	**3.822093000**	**-3.222169000**
1	**-2.343241000**	**3.459787000**	**-3.976278000**
1	**-2.924681000**	**4.903967000**	**-3.146179000**
1	**-4.058153000**	**3.622504000**	**-3.584593000**
6	**2.385285000**	**-4.203850000**	**-2.328612000**
1	**2.611970000**	**-4.532726000**	**-3.344559000**
1	**1.300691000**	**-4.160290000**	**-2.221742000**
1	**2.770497000**	**-4.962278000**	**-1.640044000**
6	**4.542588000**	**-2.866652000**	**-2.265564000**
1	**5.017367000**	**-3.609751000**	**-1.618590000**
1	**5.003876000**	**-1.898366000**	**-2.066712000**
1	**4.770146000**	**-3.137397000**	**-3.298802000**
6	**-3.212622000**	**-4.044615000**	**0.619307000**
1	**-3.434965000**	**-3.401772000**	**-0.231464000**
1	**-3.896697000**	**-4.895931000**	**0.594930000**
1	**-2.197523000**	**-4.422653000**	**0.478462000**
6	**-2.973473000**	**-4.204437000**	**3.140780000**
1	**-3.592959000**	**-5.102920000**	**3.142145000**
1	**-3.114685000**	**-3.697704000**	**4.098794000**
1	**-1.929172000**	**-4.522137000**	**3.079379000**
6	**2.336017000**	**5.217391000**	**0.446430000**

1	1.649038000	5.766474000	1.092647000
1	1.994702000	5.338903000	-0.583938000
1	3.320202000	5.687444000	0.533226000
6	2.790173000	3.576329000	2.325568000
1	2.830280000	2.528353000	2.622605000
1	2.059790000	4.072813000	2.967622000
1	3.765767000	4.029721000	2.524072000

Coordinates of the optimized geometry of compound E

32	-0.798182000	0.456189000	-1.060946000
32	1.071150000	0.912176000	0.588141000
34	1.246538000	2.947822000	1.496022000
34	-0.462964000	1.220886000	-3.138577000
7	2.595332000	0.138961000	-0.330535000
7	-2.547605000	0.911725000	-0.354486000
6	3.099049000	-0.984466000	0.223254000
7	-1.467098000	-1.356183000	-0.847033000
7	1.412236000	-0.537644000	1.832115000
6	-4.800457000	0.059288000	-0.145200000
1	-5.120560000	1.082717000	-0.265878000
6	-2.744942000	-1.446471000	-0.411156000
6	-3.403079000	-0.125990000	-0.261604000
6	2.420445000	-1.375302000	1.487568000
6	4.171167000	-1.696227000	-0.368938000
1	4.542689000	-1.252486000	-1.278743000

6	**2.786445000**	**-2.471880000**	**2.296463000**
1	**2.188169000**	**-2.580427000**	**3.187091000**
6	**-4.640162000**	**-3.008864000**	**0.291996000**
1	**-4.791015000**	**-4.057074000**	**0.526763000**
6	**-3.336500000**	**-2.681347000**	**-0.066842000**
1	**-2.659236000**	**-3.522405000**	**-0.089727000**
6	**-5.777101000**	**-2.210452000**	**0.349374000**
1	**-6.710656000**	**-2.700778000**	**0.592722000**
6	**-5.827751000**	**-0.838919000**	**0.105761000**
1	**-6.816075000**	**-0.393557000**	**0.140560000**
6	**4.681122000**	**-3.658346000**	**1.131344000**
1	**5.338852000**	**-4.512889000**	**1.221350000**
6	**4.842822000**	**-2.848822000**	**0.007876000**
1	**5.625089000**	**-3.154276000**	**-0.678621000**
6	**3.757472000**	**-3.458174000**	**2.148643000**
1	**3.782753000**	**-4.183193000**	**2.955068000**
6	**3.116444000**	**0.805091000**	**-1.549373000**
1	**2.247031000**	**1.175146000**	**-2.096221000**
1	**3.601247000**	**0.081889000**	**-2.207618000**
6	**0.763748000**	**-0.499294000**	**3.160191000**
1	**0.669550000**	**0.561534000**	**3.405807000**
1	**1.420676000**	**-0.935207000**	**3.915492000**
6	**-2.963591000**	**2.334936000**	**-0.293918000**
1	**-3.676375000**	**2.533769000**	**-1.101623000**
1	**-2.071662000**	**2.916638000**	**-0.527615000**

6	**-0.630215000**	**-2.543197000**	**-1.121147000**
1	**-0.611080000**	**-3.182534000**	**-0.232771000**
1	**0.390692000**	**-2.185930000**	**-1.267945000**
6	**4.066641000**	**1.994304000**	**-1.264692000**
1	**3.524977000**	**2.683350000**	**-0.611589000**
6	**-3.547329000**	**2.854765000**	**1.046678000**
1	**-4.555641000**	**2.452956000**	**1.179049000**
6	**-1.035543000**	**-3.392236000**	**-2.355850000**
1	**-2.116735000**	**-3.551870000**	**-2.320410000**
6	**-0.639004000**	**-1.143905000**	**3.240732000**
1	**-1.243116000**	**-0.701787000**	**2.441946000**
6	**-2.714051000**	**2.446640000**	**2.268667000**
1	**-1.684398000**	**2.796195000**	**2.179539000**
1	**-2.693502000**	**1.362590000**	**2.392833000**
1	**-3.144495000**	**2.876440000**	**3.176144000**
6	**-3.669833000**	**4.387436000**	**0.945011000**
1	**-2.682879000**	**4.848208000**	**0.866827000**
1	**-4.159435000**	**4.791731000**	**1.832636000**
1	**-4.255116000**	**4.688325000**	**0.072649000**
6	**4.362289000**	**2.715662000**	**-2.591742000**
1	**4.986184000**	**3.593996000**	**-2.416714000**
1	**3.442909000**	**3.046791000**	**-3.077103000**
1	**4.896820000**	**2.061546000**	**-3.287423000**
6	**5.365689000**	**1.586995000**	**-0.552683000**
1	**5.971893000**	**0.922864000**	**-1.176097000**

1	**5.169079000**	**1.085262000**	**0.395563000**
1	**5.966053000**	**2.472428000**	**-0.334434000**
6	**-0.702006000**	**-2.695854000**	**-3.683261000**
1	**-1.148166000**	**-1.704923000**	**-3.752747000**
1	**-1.058865000**	**-3.294575000**	**-4.524260000**
1	**0.378362000**	**-2.571609000**	**-3.795258000**
6	**-0.345955000**	**-4.766192000**	**-2.266763000**
1	**-0.609224000**	**-5.383150000**	**-3.127331000**
1	**-0.634155000**	**-5.309777000**	**-1.363258000**
1	**0.741993000**	**-4.656348000**	**-2.260172000**
6	**-1.284812000**	**-0.771770000**	**4.587381000**
1	**-2.293293000**	**-1.182868000**	**4.659430000**
1	**-1.352381000**	**0.310116000**	**4.710628000**
1	**-0.702949000**	**-1.171183000**	**5.422819000**
6	**-0.626420000**	**-2.667841000**	**3.042433000**
1	**-0.154979000**	**-2.951378000**	**2.100841000**
1	**-1.645441000**	**-3.059676000**	**3.037893000**
1	**-0.087607000**	**-3.163760000**	**3.854861000**

Coordinates of the optimized geometry of compound II

32	**1.779523000**	**-0.392561000**	**1.040231000**
32	**-1.872615000**	**0.188842000**	**1.157281000**
34	**-0.029280000**	**0.304103000**	**-0.531572000**
7	**-3.011028000**	**-1.137187000**	**0.202239000**
7	**3.253623000**	**0.915157000**	**0.711404000**

6	**-4.075814000**	**-0.674102000**	**-0.477427000**
7	**2.830369000**	**-1.347074000**	**-0.353906000**
7	**-3.201565000**	**1.384606000**	**0.291655000**
6	**5.458935000**	**1.240484000**	**-0.243065000**
1	**5.550941000**	**2.080296000**	**0.428589000**
6	**3.938921000**	**-0.745485000**	**-0.821285000**
6	**4.235903000**	**0.532297000**	**-0.130513000**
6	**-4.195619000**	**0.807477000**	**-0.416165000**
6	**-4.973233000**	**-1.530599000**	**-1.166266000**
1	**-4.714958000**	**-2.576745000**	**-1.110881000**
6	**-5.249634000**	**1.556305000**	**-0.994705000**
1	**-5.162107000**	**2.621873000**	**-0.854832000**
6	**5.912842000**	**-0.904292000**	**-2.443415000**
1	**6.240665000**	**-1.519124000**	**-3.275352000**
6	**4.696908000**	**-1.282883000**	**-1.894352000**
1	**4.251533000**	**-2.149074000**	**-2.360863000**
6	**6.784527000**	**0.119217000**	**-2.074118000**
1	**7.713791000**	**0.197302000**	**-2.623449000**
6	**6.564464000**	**1.050678000**	**-1.063734000**
1	**7.368122000**	**1.761775000**	**-0.901871000**
6	**-6.792561000**	**-0.079342000**	**-2.138752000**
1	**-7.705348000**	**-0.129655000**	**-2.718052000**
6	**-6.136114000**	**-1.280583000**	**-1.879863000**
1	**-6.606843000**	**-2.167422000**	**-2.291709000**
6	**-6.371588000**	**1.179481000**	**-1.722297000**

1	**-7.007571000**	**2.006683000**	**-2.020475000**
6	**-2.606692000**	**-2.550622000**	**0.284936000**
1	**-1.520134000**	**-2.565144000**	**0.166643000**
1	**-3.010599000**	**-3.133736000**	**-0.544469000**
6	**-3.121821000**	**2.827739000**	**0.591214000**
1	**-2.721361000**	**2.906525000**	**1.606064000**
1	**-4.117010000**	**3.279020000**	**0.620536000**
6	**3.381633000**	**2.102392000**	**1.580048000**
1	**4.333013000**	**2.056616000**	**2.122175000**
1	**2.595189000**	**2.025895000**	**2.335289000**
6	**2.347841000**	**-2.641073000**	**-0.867605000**
1	**2.330694000**	**-2.629181000**	**-1.961360000**
1	**1.306022000**	**-2.735140000**	**-0.554802000**
6	**-2.961398000**	**-3.235371000**	**1.628295000**
1	**-2.516578000**	**-2.627767000**	**2.423240000**
6	**3.257449000**	**3.481978000**	**0.883381000**
1	**3.925066000**	**3.493181000**	**0.017273000**
6	**3.135344000**	**-3.879769000**	**-0.371286000**
1	**4.190187000**	**-3.740320000**	**-0.626728000**
6	**-2.194692000**	**3.648672000**	**-0.340568000**
1	**-1.210367000**	**3.176163000**	**-0.300552000**
6	**1.832079000**	**3.749730000**	**0.381843000**
1	**1.131062000**	**3.793933000**	**1.220181000**
1	**1.488774000**	**2.967481000**	**-0.293495000**
1	**1.785303000**	**4.705913000**	**-0.144538000**

6	**3.717159000**	**4.581393000**	**1.857724000**
1	**3.094017000**	**4.590138000**	**2.756457000**
1	**3.640444000**	**5.565916000**	**1.392775000**
1	**4.754380000**	**4.438012000**	**2.170652000**
6	**-2.316612000**	**-4.631622000**	**1.674191000**
1	**-2.512386000**	**-5.116995000**	**2.631982000**
1	**-1.233934000**	**-4.575397000**	**1.543612000**
1	**-2.719208000**	**-5.275754000**	**0.887085000**
6	**-4.474745000**	**-3.315038000**	**1.879896000**
1	**-4.965065000**	**-3.949308000**	**1.136158000**
1	**-4.940593000**	**-2.329783000**	**1.845606000**
1	**-4.675600000**	**-3.744116000**	**2.863927000**
6	**3.034950000**	**-4.052197000**	**1.152311000**
1	**3.397072000**	**-3.170451000**	**1.681379000**
1	**3.624848000**	**-4.910235000**	**1.481863000**
1	**1.998634000**	**-4.221166000**	**1.457080000**
6	**2.626538000**	**-5.131966000**	**-1.106677000**
1	**3.177191000**	**-6.019174000**	**-0.788728000**
1	**2.740296000**	**-5.036506000**	**-2.189097000**
1	**1.567704000**	**-5.304922000**	**-0.895110000**
6	**-2.076028000**	**5.080683000**	**0.210357000**
1	**-1.382819000**	**5.668786000**	**-0.393429000**
1	**-1.709562000**	**5.085816000**	**1.239404000**
1	**-3.044422000**	**5.589665000**	**0.194512000**
6	**-2.645301000**	**3.657524000**	**-1.808940000**

1	-2.725308000	2.647435000	-2.210084000
1	-1.918671000	4.197320000	-2.419819000
1	-3.611690000	4.155711000	-1.928421000

Coordinates of the optimized geometry of compound Se_8

34	2.085025000	-1.701408000	-0.574271000
34	0.271151000	-2.677131000	0.574454000
34	-1.701345000	-2.084970000	-0.574347000
34	-2.677505000	-0.271197000	0.574177000
34	2.677506000	0.271198000	0.574172000
34	1.701344000	2.084969000	-0.574357000
34	-2.085026000	1.701406000	-0.574274000
34	-0.271151000	2.677133000	0.574446000

Coordinates of the optimized geometry of compound S_8

16	-2.931878000	0.001412000	-0.000100000
16	-1.698005000	-1.807857000	-0.548690000
16	-0.001131000	-2.276756000	0.871850000
16	1.695977000	-1.809103000	-0.548901000
16	2.931877000	-0.001413000	0.000067000
16	1.698005000	1.807854000	0.548690000
16	0.001133000	2.276778000	-0.871832000
16	-1.695977000	1.809085000	0.548916000

Coordinates of the optimized geometry of compound $(Me_3Si)_2S$

16	**0.000000000**	**1.261545000**	**0.000001000**
14	**1.866507000**	**-0.037890000**	**-0.001246000**
14	**-1.866507000**	**-0.037890000**	**0.001245000**
6	**3.242870000**	**1.179365000**	**-0.484159000**
1	**3.280042000**	**2.016620000**	**0.212874000**
1	**4.216324000**	**0.683899000**	**-0.474491000**
1	**3.072164000**	**1.581708000**	**-1.482490000**
6	**2.165520000**	**-0.736236000**	**1.742490000**
1	**1.371997000**	**-1.420099000**	**2.042444000**
1	**3.113512000**	**-1.278610000**	**1.779226000**
1	**2.205620000**	**0.071781000**	**2.472994000**
6	**-1.726969000**	**-1.445717000**	**1.274677000**
1	**-0.955036000**	**-2.165467000**	**1.001324000**
1	**-1.491748000**	**-1.052083000**	**2.263320000**
1	**-2.675604000**	**-1.984097000**	**1.340450000**
6	**-3.242870000**	**1.179367000**	**0.484152000**
1	**-3.072165000**	**1.581716000**	**1.482481000**
1	**-3.280043000**	**2.016618000**	**-0.212886000**
1	**-4.216324000**	**0.683900000**	**0.474488000**
6	**-2.165517000**	**-0.736241000**	**-1.742488000**
1	**-3.113511000**	**-1.278610000**	**-1.779226000**
1	**-2.205610000**	**0.071775000**	**-2.472994000**
1	**-1.371996000**	**-1.420108000**	**-2.042438000**
6	**1.726966000**	**-1.445720000**	**-1.274673000**
1	**0.955033000**	**-2.165469000**	**-1.001318000**

1	**1.491744000**	**-1.052089000**	**-2.263317000**
1	**2.675601000**	**-1.984101000**	**-1.340445000**

Coordinates of the optimized geometry of compound $(Me_3SiS)_2$

16	**0.736178000**	**-0.951318000**	**-0.872176000**
16	**-0.736178000**	**-0.951309000**	**0.872186000**
14	**2.497524000**	**0.188368000**	**0.068051000**
14	**-2.497524000**	**0.188366000**	**-0.068054000**
6	**3.787228000**	**0.166352000**	**-1.328106000**
1	**3.416695000**	**0.676336000**	**-2.217325000**
1	**4.700315000**	**0.671365000**	**-1.004945000**
1	**4.047179000**	**-0.855091000**	**-1.605616000**
6	**1.956018000**	**1.951162000**	**0.513822000**
1	**1.138726000**	**1.931207000**	**1.234166000**
1	**2.787940000**	**2.502556000**	**0.958288000**
1	**1.619983000**	**2.493500000**	**-0.369663000**
6	**-3.787214000**	**0.166398000**	**1.328117000**
1	**-3.416674000**	**0.676413000**	**2.217315000**
1	**-4.700305000**	**0.671399000**	**1.004947000**
1	**-4.047161000**	**-0.855036000**	**1.605664000**
6	**-1.956009000**	**1.951145000**	**-0.513876000**
1	**-1.138737000**	**1.931167000**	**-1.234241000**
1	**-2.787937000**	**2.502540000**	**-0.958330000**

1	**-1.619945000**	**2.493497000**	**0.369590000**
6	**3.075443000**	**-0.772629000**	**1.596997000**
1	**3.396112000**	**-1.777035000**	**1.321185000**
1	**3.912945000**	**-0.263375000**	**2.079505000**
1	**2.268061000**	**-0.864868000**	**2.323232000**
6	**-3.075465000**	**-0.772665000**	**-1.596970000**
1	**-3.396159000**	**-1.777054000**	**-1.321126000**
1	**-3.912953000**	**-0.263405000**	**-2.079494000**
1	**-2.268084000**	**-0.864948000**	**-2.323200000**

Coordinates of the optimized geometry of compound 2

6	**-3.168722000**	**-1.249633000**	**1.033048000**
6	**-4.445126000**	**-0.812804000**	**1.352413000**
6	**-5.067872000**	**0.409777000**	**1.104132000**
6	**-4.485606000**	**1.504668000**	**0.477406000**
6	**-3.192114000**	**1.678737000**	**-0.004059000**
6	**-2.074327000**	**0.812404000**	**-0.046125000**
6	**-2.083009000**	**-0.610229000**	**0.381651000**
7	**-0.932825000**	**-1.247033000**	**0.092470000**
7	**-0.887607000**	**1.200317000**	**-0.564890000**
6	**-0.690048000**	**2.539979000**	**-1.155111000**
1	**0.216613000**	**2.487475000**	**-1.763110000**
1	**-1.511657000**	**2.754997000**	**-1.846953000**
6	**-0.624602000**	**-2.646581000**	**0.439452000**
1	**0.400954000**	**-2.648308000**	**0.815316000**

1	**-1.249991000**	**-3.001945000**	**1.259739000**
6	**-0.541224000**	**3.716771000**	**-0.152539000**
1	**-1.303882000**	**3.603994000**	**0.623087000**
6	**-0.794911000**	**5.044163000**	**-0.889771000**
1	**-1.800108000**	**5.086003000**	**-1.316926000**
1	**-0.683711000**	**5.890567000**	**-0.209896000**
1	**-0.078766000**	**5.178649000**	**-1.705350000**
6	**0.832267000**	**3.722562000**	**0.534643000**
1	**1.040151000**	**2.776543000**	**1.032018000**
1	**1.626726000**	**3.898091000**	**-0.197018000**
1	**0.883820000**	**4.520629000**	**1.278641000**
6	**-0.718832000**	**-3.629121000**	**-0.753328000**
1	**-0.077529000**	**-3.231932000**	**-1.547577000**
6	**-2.144331000**	**-3.757909000**	**-1.311987000**
1	**-2.818677000**	**-4.193752000**	**-0.569538000**
1	**-2.549204000**	**-2.790672000**	**-1.611610000**
1	**-2.153769000**	**-4.408783000**	**-2.188769000**
6	**-0.162853000**	**-4.999638000**	**-0.328741000**
1	**-0.763994000**	**-5.433846000**	**0.475137000**
1	**-0.176345000**	**-5.698629000**	**-1.166910000**
1	**0.866817000**	**-4.921028000**	**0.025680000**
32	**0.486244000**	**-0.201743000**	**-0.817163000**
16	**1.791503000**	**0.033323000**	**1.167821000**
14	**3.909612000**	**-0.112237000**	**0.388777000**
6	**4.254093000**	**1.279382000**	**-0.866048000**

1	**3.592401000**	**1.199133000**	**-1.729291000**
1	**4.097469000**	**2.256134000**	**-0.407739000**
1	**5.285754000**	**1.230091000**	**-1.223167000**
6	**5.026242000**	**0.082830000**	**1.917951000**
1	**4.824645000**	**-0.702308000**	**2.647075000**
1	**6.080546000**	**0.026409000**	**1.636419000**
1	**4.853176000**	**1.043345000**	**2.403812000**
6	**4.195051000**	**-1.810742000**	**-0.426129000**
1	**3.997286000**	**-2.613835000**	**0.284573000**
1	**3.537771000**	**-1.948330000**	**-1.285504000**
1	**5.228178000**	**-1.905117000**	**-0.769727000**
1	**-2.975072000**	**-2.272645000**	**1.316162000**
1	**-5.055812000**	**-1.551387000**	**1.861161000**
1	**-6.095498000**	**0.513613000**	**1.427280000**
1	**-5.127786000**	**2.370626000**	**0.355345000**
1	**-3.010378000**	**2.659457000**	**-0.415362000**

Coordinates of the optimized geometry of compound 3

32	**-1.761335000**	**-0.627437000**	**-0.330431000**
32	**1.879465000**	**0.567020000**	**-0.448144000**
34	**1.683770000**	**1.632435000**	**-2.389340000**
34	**-1.391302000**	**-2.092560000**	**-1.961690000**
34	**0.002643000**	**0.240092000**	**1.063678000**
7	**2.899286000**	**-1.053104000**	**-0.286005000**
7	**-3.011297000**	**0.779204000**	**-0.754455000**

6	**3.907978000**	**-1.003980000**	**0.611179000**
7	**-3.033633000**	**-1.021832000**	**1.066526000**
7	**3.196013000**	**1.253733000**	**0.774700000**
6	**-5.295141000**	**1.491281000**	**-0.413571000**
1	**-5.209334000**	**1.973899000**	**-1.375335000**
6	**-4.108244000**	**-0.200480000**	**1.102077000**
6	**-4.150803000**	**0.753012000**	**-0.033688000**
6	**4.087011000**	**0.338866000**	**1.227480000**
6	**4.700315000**	**-2.137329000**	**0.906114000**
1	**4.429011000**	**-3.019866000**	**0.349267000**
6	**5.090766000**	**0.674574000**	**2.158184000**
1	**5.060634000**	**1.701203000**	**2.486978000**
6	**-6.239460000**	**0.445422000**	**2.351603000**
1	**-6.722773000**	**0.244291000**	**3.301514000**
6	**-5.030152000**	**-0.217845000**	**2.169205000**
1	**-4.750007000**	**-0.861838000**	**2.989682000**
6	**-6.934270000**	**1.285626000**	**1.489265000**
1	**-7.902038000**	**1.638920000**	**1.820727000**
6	**-6.503648000**	**1.708151000**	**0.232762000**
1	**-7.204373000**	**2.325009000**	**-0.319254000**
6	**6.421990000**	**-1.418804000**	**2.602563000**
1	**7.253289000**	**-1.795399000**	**3.184136000**
6	**5.772518000**	**-2.324110000**	**1.765958000**
1	**6.167436000**	**-3.334215000**	**1.774307000**
6	**6.100173000**	**-0.076191000**	**2.752759000**

1	**6.720578000**	**0.480555000**	**3.446669000**
6	**2.508144000**	**-2.241681000**	**-1.078955000**
1	**1.417918000**	**-2.234081000**	**-1.149808000**
1	**2.776210000**	**-3.159322000**	**-0.552538000**
6	**3.267291000**	**2.709866000**	**1.021000000**
1	**3.024036000**	**3.181696000**	**0.065746000**
1	**4.291340000**	**3.001534000**	**1.261914000**
6	**-2.803684000**	**1.645366000**	**-1.939144000**
1	**-3.589230000**	**1.443223000**	**-2.674898000**
1	**-1.866165000**	**1.325519000**	**-2.395537000**
6	**-2.782966000**	**-2.075237000**	**2.072280000**
1	**-2.801975000**	**-1.631172000**	**3.073101000**
1	**-1.762179000**	**-2.425518000**	**1.911454000**
6	**3.080563000**	**-2.258124000**	**-2.518534000**
1	**2.738667000**	**-1.339480000**	**-3.002313000**
6	**-2.729158000**	**3.169397000**	**-1.666454000**
1	**-3.689575000**	**3.505829000**	**-1.265283000**
6	**-3.737954000**	**-3.295027000**	**2.027587000**
1	**-4.767605000**	**-2.932659000**	**2.098568000**
6	**2.291936000**	**3.254587000**	**2.091858000**
1	**1.282649000**	**2.966535000**	**1.784600000**
6	**-1.637013000**	**3.537008000**	**-0.651796000**
1	**-0.652002000**	**3.253962000**	**-1.026546000**
1	**-1.788420000**	**3.035370000**	**0.304345000**
1	**-1.638620000**	**4.614928000**	**-0.473016000**

6	**-2.500469000**	**3.887106000**	**-3.010258000**
1	**-1.542837000**	**3.592550000**	**-3.444161000**
1	**-2.484784000**	**4.969175000**	**-2.868277000**
1	**-3.287178000**	**3.654758000**	**-3.732501000**
6	**2.476541000**	**-3.454953000**	**-3.274027000**
1	**2.815248000**	**-3.460808000**	**-4.311672000**
1	**1.386890000**	**-3.410641000**	**-3.273879000**
1	**2.780653000**	**-4.403006000**	**-2.819394000**
6	**4.615709000**	**-2.283385000**	**-2.572124000**
1	**5.015603000**	**-3.204734000**	**-2.138389000**
1	**5.055693000**	**-1.435394000**	**-2.045615000**
1	**4.953382000**	**-2.235134000**	**-3.609361000**
6	**-3.605772000**	**-4.093517000**	**0.722922000**
1	**-3.772907000**	**-3.471169000**	**-0.155122000**
1	**-4.327669000**	**-4.913091000**	**0.705106000**
1	**-2.605527000**	**-4.521489000**	**0.626170000**
6	**-3.461399000**	**-4.183091000**	**3.254560000**
1	**-4.128506000**	**-5.046623000**	**3.262103000**
1	**-3.606553000**	**-3.638752000**	**4.191135000**
1	**-2.434604000**	**-4.558258000**	**3.239149000**
6	**2.368604000**	**4.791779000**	**2.096342000**
1	**1.654579000**	**5.210178000**	**2.807763000**
1	**2.141625000**	**5.204335000**	**1.111529000**
1	**3.365993000**	**5.135514000**	**2.385631000**
6	**2.538776000**	**2.681171000**	**3.495460000**

1	**2.487727000**	**1.591735000**	**3.501270000**
1	**1.783343000**	**3.050088000**	**4.192071000**
1	**3.516707000**	**2.983601000**	**3.881279000**

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