

Supporting Information

Multiple Ethylene Activation by Heteroleptic L(Cl)Ga-substituted Germylenes

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I. Spectroscopic Characterization

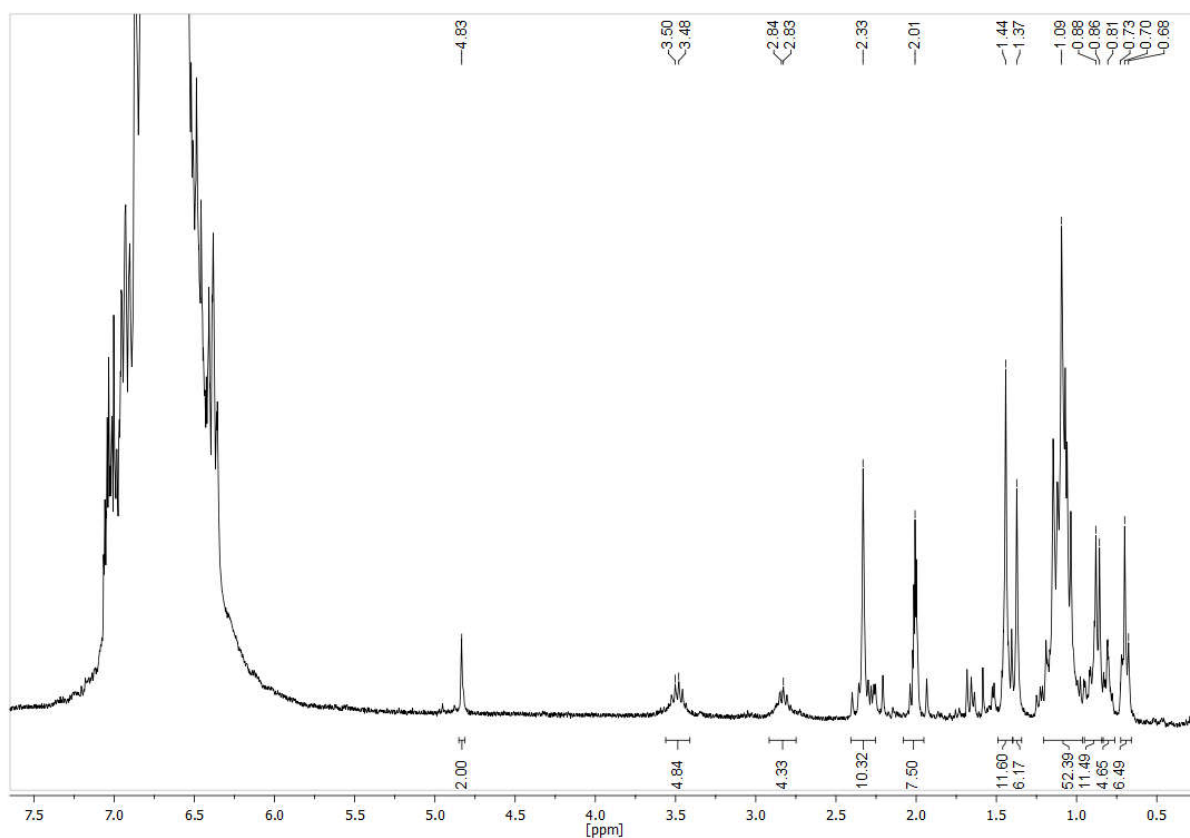


Figure S1. ¹H NMR spectrum of **3** in toluene-*d*₈ and 1,2-difluorobenzene at 90 °C. The low resolution is caused by the low solubility and thermal instability of compound **3**.

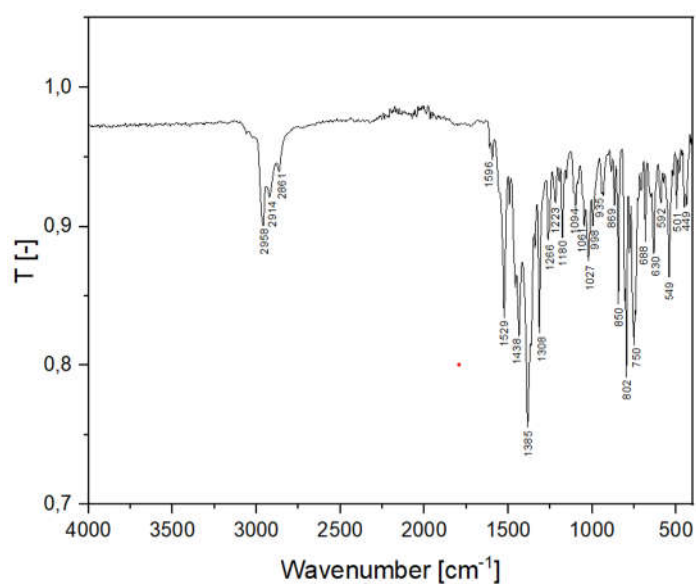


Figure S2. IR spectrum of **3**.

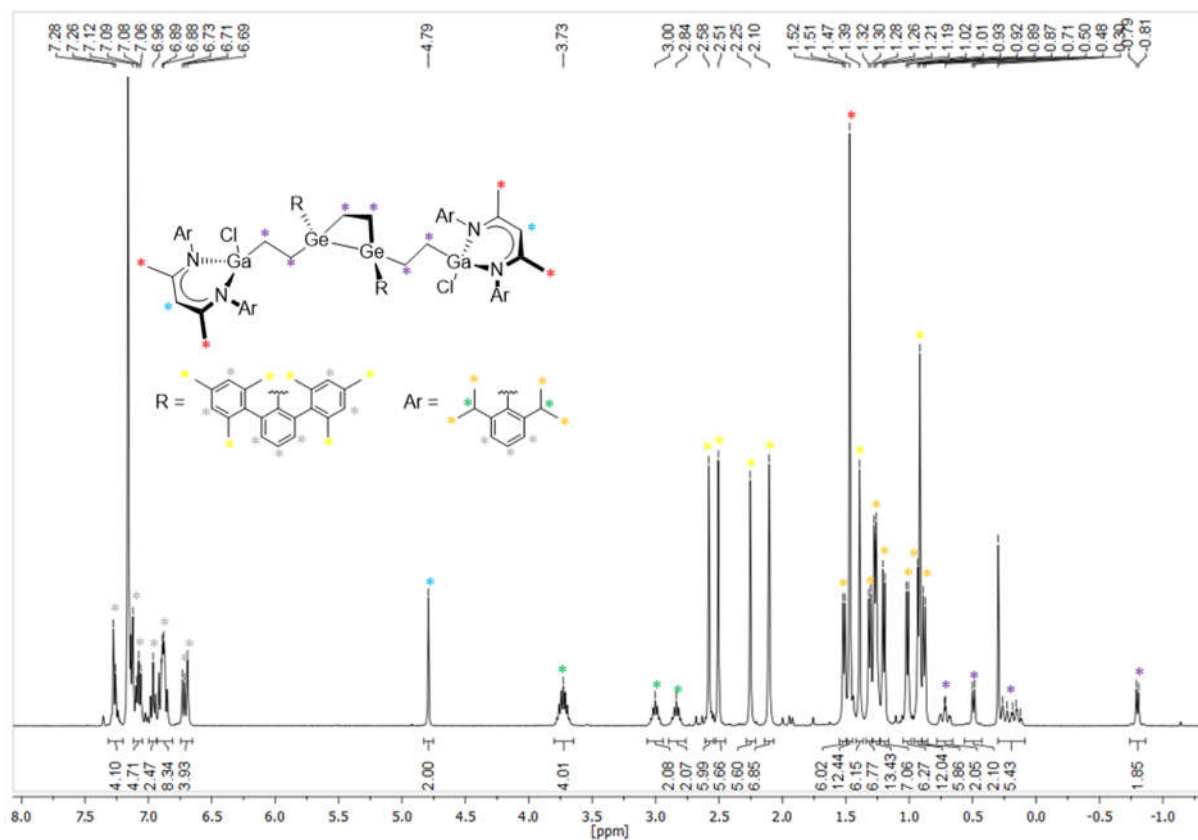


Figure S3. ¹H NMR spectrum of **4** in C₆D₆ at r.t.

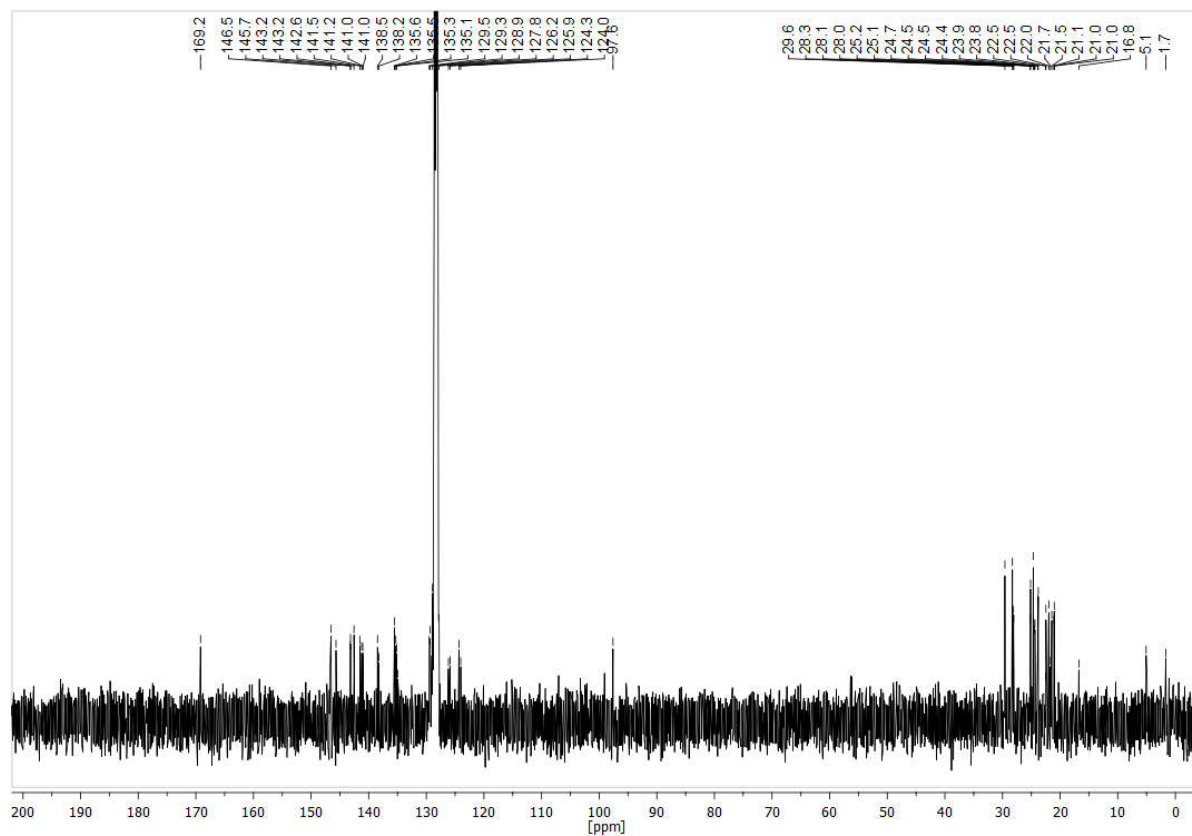


Figure S4. ¹³C NMR spectrum of **4** in C₆D₆ at r.t.

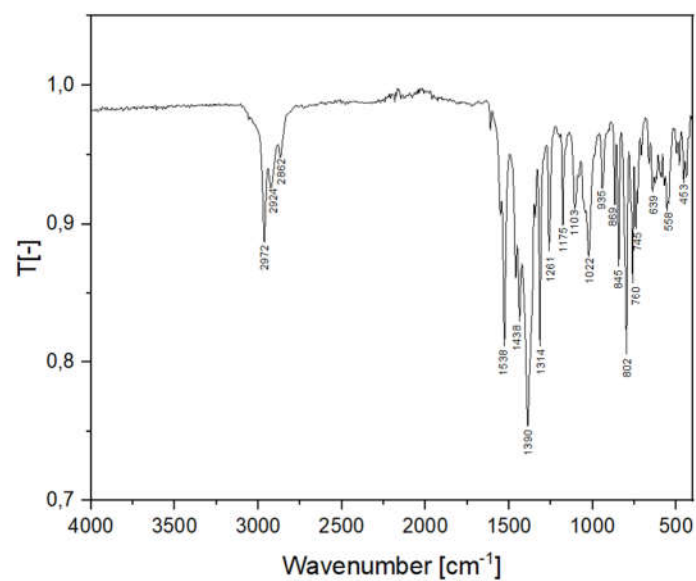


Figure S5. IR spectrum of 4.

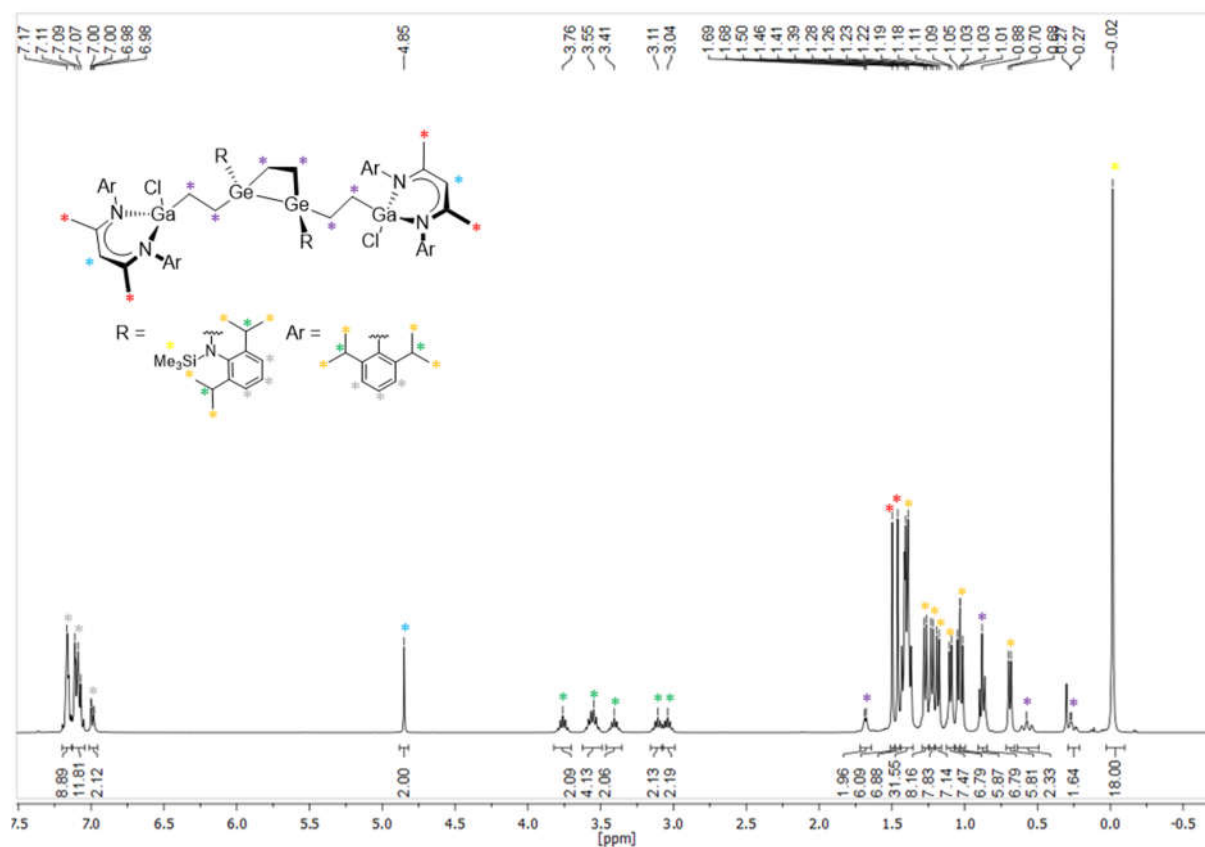


Figure S6. ^1H NMR spectrum of 5 in C_6D_6 at r.t.

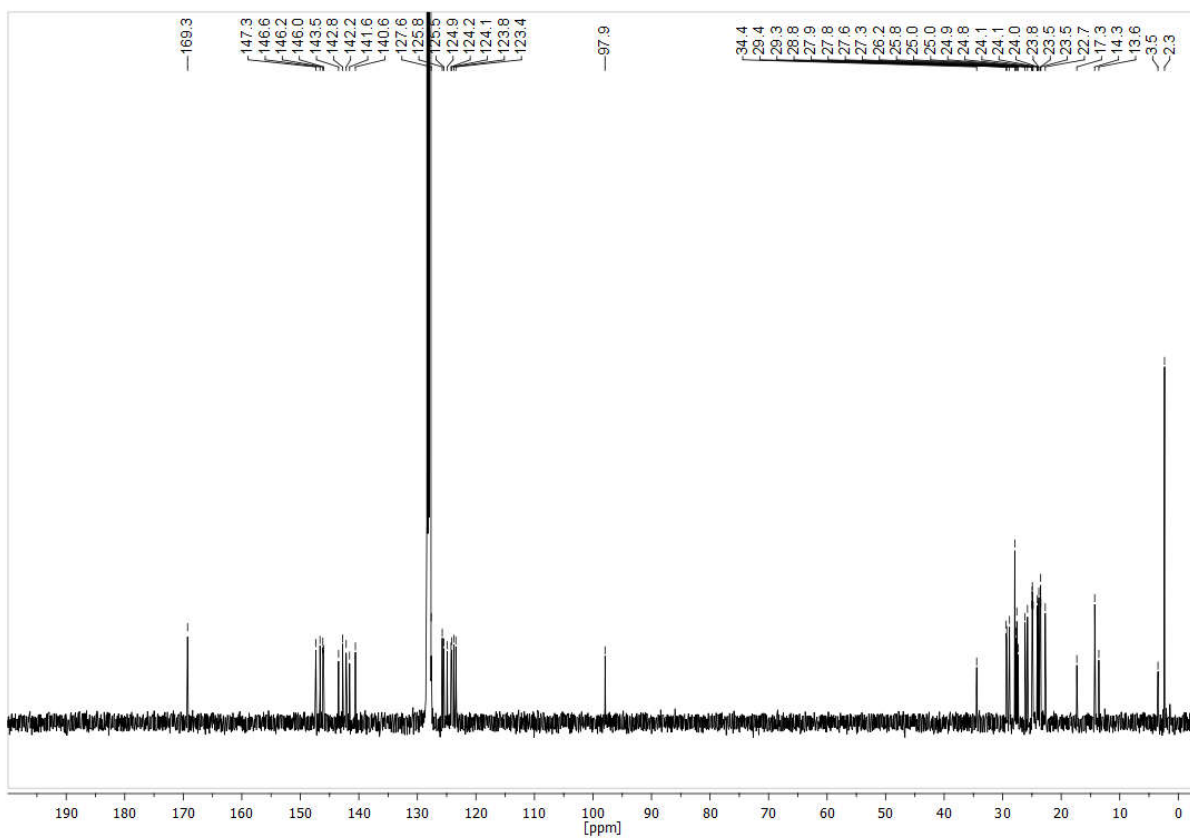


Figure S7. ^{13}C NMR spectrum of **5** in C_6D_6 at r.t.

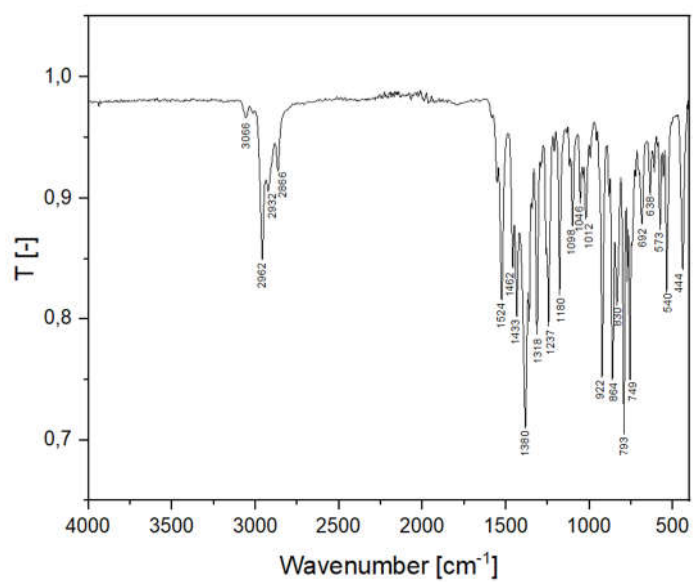


Figure S8. IR spectrum of **5**.

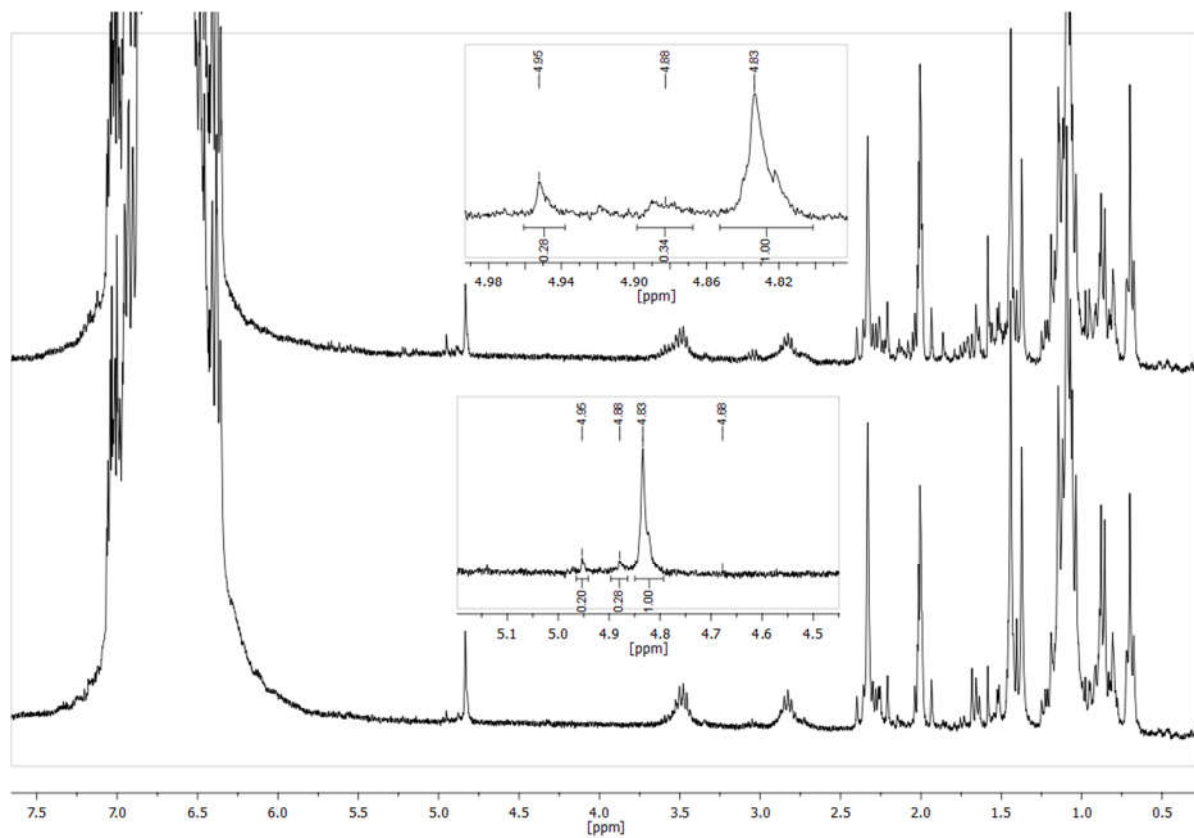


Figure S9. Time-dependent ^1H NMR spectra of **3** in $\text{toluene-}d_8$ and 1,2-difluorobenzene at 90°C .

II. Crystallographic Data

Table S1. Crystallographic details of compounds **3–5**.

Identification code	3	4	5
Empirical formula	C ₁₃₄ H ₁₆₀ Cl ₂ F ₄ Ga ₂ Ge ₂ N ₄	C ₁₃₆ H ₁₆₈ Cl ₂ Ga ₂ Ge ₂ N ₄	C ₁₀₄ H ₁₇₀ Cl ₂ Ga ₂ Ge ₂ N ₆ Si ₂
<i>M</i>	2258.17	2214.25	1916.15
Crystal size [mm]	0.304×0.259×0.105	0.243×0.177×0.040	0.252×0.157×0.138
<i>T</i> [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	monoclinic
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	36.693(5)	14.0575(8)	27.3921(14)
<i>b</i> [Å]	15.536(2)	20.5970(12)	14.6446(7)
<i>c</i> [Å]	20.813(3)	23.6061(14)	29.8421(15)
<i>α</i> [°]	90	115.356(2)	90
<i>β</i> [°]	92.735(4)	97.878(2)	113.082(2)
<i>γ</i> [°]	90	94.810(2)	90
<i>V</i> [Å ³]	11851(3)	6040.1(6)	11012.7(10)
<i>Z</i>	4	2	4
<i>D</i> _{calc} [g·cm ⁻³]	1.266	1.217	1.156
<i>μ</i> (MoK _α [mm ⁻¹])	1.054	1.863	2.168
Transmissions	0.75/0.60	0.75/0.58	0.75/0.63
<i>F</i> (000)	4752	2344	4096
Index ranges	-52 ≤ <i>h</i> ≤ 52	-17 ≤ <i>h</i> ≤ 18	-33 ≤ <i>h</i> ≤ 34
	-22 ≤ <i>k</i> ≤ 22	-26 ≤ <i>k</i> ≤ 26	-18 ≤ <i>k</i> ≤ 18
	-29 ≤ <i>l</i> ≤ 29	-30 ≤ <i>l</i> ≤ 30	-38 ≤ <i>l</i> ≤ 38
<i>θ</i> _{max} [°]	30.507	81.182	80.083
Reflections collected	188073	387670	617598
Independent reflections	18092	26310	23964
<i>R</i> _{int}	0.0522	0.0579	0.0865
Refined parameters	747	1136	1054
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0445	0.0427	0.0426
<i>wR</i> ₂ [all data]	0.1147	0.1170	0.1056
GooF	1.090	1.011	1.106
<i>Δρ</i> _{final} (max/min) [e·Å ⁻³]	2.901/-1.152	2.195/-1.093	1.132/-0.547

III. Computational Details

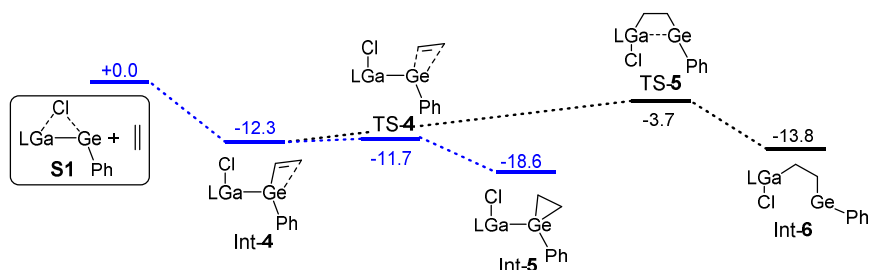


Figure S10. Gibbs energies for the reaction of germylene **S1** with ethylene calculated by means of PBE0-D3BJ(SMD,benzene as solvent)//def2-TZVP//PBE0-D3BJ/def2-SVP. The values are given in kcal/mol. L = HC(C(Me)NPh)₂.

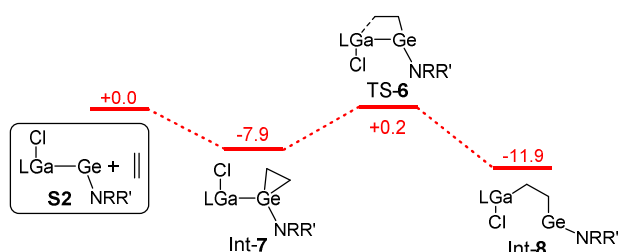


Figure S11. Gibbs energies for the reaction of germylene **S2** with ethylene calculated by means of PBE0-D3BJ(SMD,benzene as solvent)//def2-TZVP//PBE0-D3BJ/def2-SVP. The values are given in kcal/mol. L = HC(C(Me)NPh)₂; NRR' = N(SiMe₃)(Ph).

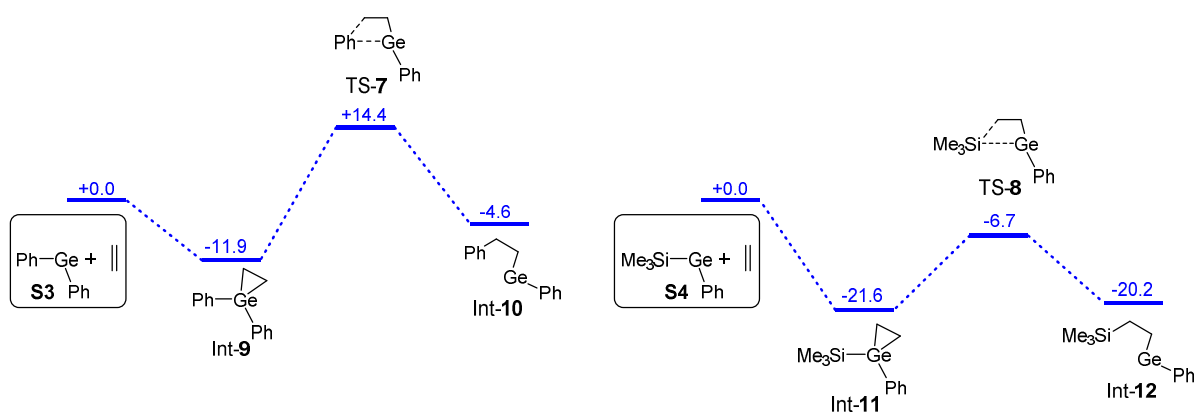


Figure S12. Gibbs energies for the reaction of germylene **S3** with ethylene calculated by means of PBE0-D3BJ(SMD,benzene as solvent)//def2-TZVP//PBE0-D3BJ/def2-SVP. The values are given in kcal/mol.

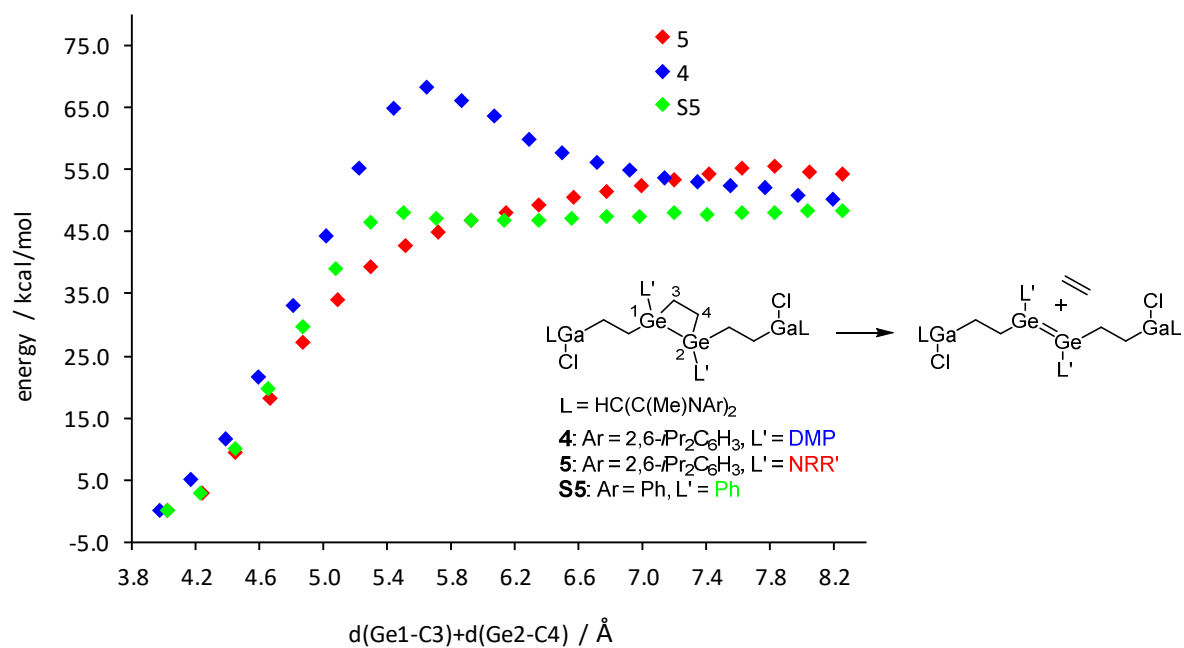


Figure S13. Energy scan for the elimination of ethylene from 1,2-digermacyclobutanes **4**, **5** and **S5** calculated by means of PBE0-D3BJ/def2-SVP. The sum of the two Ge–C distances ($d(Ge1-C3)$ and $d(Ge2-C4)$) was used as reaction coordinate. While a transition state is found for system **4**, the elimination of ethylene from **5** proceeds without a barrier. DMP = 2,6-Mes₂C₆H₃, Mes = 2,4,6-Me₃C₆H₂; NRR' = N(SiMe₃)(Ar).

IV. Absolute Energies and Cartesian Coordinates for the Calculated Compounds

Table S2. Absolute energies [au] calculated by means of different methods.

Compound	E^a	G^a	E^b
ethylene	-78.427381	-78.398546	-78.515329
1	-6625.889435	-6624.929430	-6628.824709
TS-1a	-6704.322406	-6703.310303	-6707.341665
Int-1a	-6704.367304	-6703.352573	-6707.384412
TS-2a	-6704.349038	-6703.335377	-6707.366449
Int-2a	-6704.367908	-6703.357474	-6707.388093
3	-13408.827801	-13406.768222	-13414.848352
TS-3a	-13487.212881	-13485.107264	-13493.324953
4	-13487.318209	-13485.205498	-13493.425276
2	-6628.149981	-6627.226112	-6630.896152
TS-1b	-6706.571656	-6705.595263	-6709.403964
Int-1b	-6706.608215	-6705.628406	-6709.438392
TS-2b	-6706.594786	-6705.614708	-6709.426473
Int-2b	-6706.619922	-6705.647165	-6709.450257
Int-3b	-13413.286522	-13411.307260	-13418.938043
5	-13491.806592	-13489.771104	-13497.539674
S1	-5458.241481	-5457.908667	-5459.966869
Int-4	-5536.712686	-5536.329716	-5538.523175
TS-4	-5536.712216	-5536.328279	-5538.523058
Int-5	-5536.721033	-5536.338576	-5538.532698
TS-5	-5536.701165	-5536.316713	-5538.510968
Int-6	-5536.719254	-5536.334515	-5538.527250
S5	-11152.009529	-11151.157539	-11155.699364
S2	-5921.784977	-5921.348822	-5923.804580
Int-7	-6000.253070	-5999.763668	-6002.356877
TS-6	-6000.243265	-5999.751809	-6002.346112
Int-8	-6000.266635	-5999.774154	-6002.366337
S3	-2538.893378	-2538.751175	-2539.648239
Int-9	-2617.363115	-2617.170892	-2618.203669
TS-7	-2617.323474	-2617.129154	-2618.163919
Int-10	-2617.375486	-2617.180602	-2618.213640
S4	-2716.499710	-2716.340917	-2717.239331
Int-11	-2794.984567	-2794.775193	-2795.810825
TS-8	-2794.964681	-2794.751177	-2795.791255
Int-12	-2794.983301	-2794.773898	-2795.808654

^a PBE0-D3BJ/def2-SVP.

^b PBE0-D3BJ(benzene as solvent)/def2-TZVP//PBE0-D3BJ/def2-SVP

Cartesian coordinates of the optimized geometry of ethylene at PBE0-D3BJ/def2-SVP level of theory:

C	-0.66528900	0.00000000	-0.00007200
C	0.66528900	0.00000000	0.00007700
H	-1.24015400	0.93114600	0.00045300
H	-1.24015500	-0.93114600	-0.00023000
H	1.24015500	0.93114600	-0.00047000
H	1.24015600	-0.93114600	0.00021300

Cartesian coordinates of the optimized geometry of **1** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.38268600	-0.11248800	0.82191200
Ga	0.60433700	0.52266600	-0.49199200
Cl	-1.43822100	0.07824500	-1.77566400
N	0.45914700	2.52338900	-0.62503700
N	2.00499800	0.38471100	-1.84975500
C	0.91024300	3.20387100	-1.66123200

C	1.61661700	2.60702800	-2.72902600
H	1.86037300	3.26984600	-3.55855500
C	2.17997400	1.33482800	-2.78305200
C	0.72262500	4.69213800	-1.75440400
H	-0.00967000	4.91922700	-2.54384700
H	1.66917200	5.17124300	-2.04111700
H	0.36429500	5.12633100	-0.81392500
C	3.07869300	1.03018700	-3.94826900
H	2.72084400	0.13890500	-4.48296500
H	4.09881500	0.79829000	-3.61067700
H	3.11765100	1.87512500	-4.64536000
C	-0.22861900	3.14541500	0.45963600
C	0.44874100	3.23994100	1.69745800
C	-0.23586000	3.76855300	2.79270300
H	0.26904000	3.84751000	3.75626400
C	-1.55479400	4.19541300	2.67699700
H	-2.07573000	4.60577300	3.54523700
C	-2.20736900	4.08898000	1.45784800
H	-3.24798300	4.41139800	1.37514600
C	-1.57317700	3.55628300	0.33022300
C	1.89827000	2.80805700	1.82361400
H	2.01988100	1.89569300	1.21136600
C	2.84011100	3.86914800	1.25123500
H	2.63101900	4.07685500	0.19292200
H	3.88911600	3.54282500	1.32701700
H	2.73748000	4.81457300	1.80724400
C	2.30262200	2.43503600	3.24363000
H	2.32124800	3.31242300	3.90925200
H	3.31421800	2.00469900	3.24676100
H	1.62077900	1.68575000	3.66996300
C	-2.37061800	3.43259400	-0.95609600
H	-1.73528500	2.93450600	-1.70319800
C	-2.78787200	4.80299200	-1.49622500
H	-3.29133500	4.69383600	-2.46957900
H	-1.93578200	5.48427700	-1.62687900
H	-3.49811200	5.29548100	-0.81299900
C	-3.60807800	2.55305000	-0.76926100
H	-4.34695500	3.03416600	-0.10812900
H	-3.35430300	1.57654800	-0.33670300
H	-4.09403000	2.36816900	-1.73925100
C	2.89529600	-0.73233100	-1.84277000
C	4.12273800	-0.60372200	-1.15539100
C	5.00618400	-1.68625400	-1.16110100
H	5.96134000	-1.60118600	-0.63630300
C	4.69501600	-2.86344300	-1.83319700
H	5.39933900	-3.69868800	-1.83207100
C	3.48308100	-2.97375100	-2.50354300
H	3.24081300	-3.90206100	-3.02654600
C	2.56279700	-1.92070400	-2.52272000
C	4.51801200	0.68147100	-0.44973000
H	3.68663500	1.39247900	-0.56318900
C	5.75293400	1.32005900	-1.08625700
H	5.60598500	1.51438300	-2.15892400
H	6.63876700	0.67335800	-0.98317400
H	5.98336000	2.28091300	-0.59992200
C	4.72477400	0.45938900	1.04580700
H	3.81430700	0.06440000	1.51779500
H	4.99342100	1.40408900	1.54332300
H	5.53888400	-0.25773200	1.23840300
C	1.25741800	-2.08429200	-3.27676700
H	0.73528500	-1.11588900	-3.26246600
C	1.48825700	-2.47462200	-4.73736600
H	0.53385200	-2.47718600	-5.28581800
H	1.92113000	-3.48356300	-4.82613500
H	2.17041000	-1.77842000	-5.24894500
C	0.34227100	-3.09574000	-2.58856500
H	0.01317500	-2.73915800	-1.60167600
H	0.84405400	-4.06708200	-2.45380800
H	-0.55882500	-3.26624800	-3.19486100

C	-1.54060600	-2.10939100	0.93411800
C	-0.62684200	-2.91404500	1.64604200
C	-0.85736600	-4.29090400	1.76244000
H	-0.14367400	-4.90472300	2.31837500
C	-1.99310500	-4.87185500	1.20731600
H	-2.16188600	-5.94726700	1.30374300
C	-2.93924900	-4.06909500	0.57574000
H	-3.86692900	-4.50636400	0.19650100
C	-2.73888000	-2.68957600	0.45681200
C	0.54421200	-2.33241400	2.36464900
C	0.34625700	-1.55441300	3.52271800
C	1.46062700	-1.06821300	4.21639500
H	1.29752800	-0.47516800	5.12164000
C	2.76467600	-1.33575400	3.80598800
C	2.93845900	-2.11843100	2.66104000
H	3.95046800	-2.34948400	2.31559100
C	1.85724500	-2.62213000	1.93844800
C	-1.02584900	-1.24999400	4.05826000
H	-1.73505700	-2.06342600	3.85457200
H	-1.44551200	-0.33385600	3.60554300
H	-0.98923600	-1.07871400	5.14356700
C	3.94799300	-0.82412100	4.57463900
H	3.64566000	-0.10598000	5.34981700
H	4.67076900	-0.32392700	3.91115700
H	4.48572700	-1.64786500	5.07193100
C	2.10896600	-3.46999400	0.72840500
H	1.96646200	-4.54048800	0.94789700
H	3.13334600	-3.33385400	0.35890500
H	1.41692600	-3.22186000	-0.08512600
C	-3.85107500	-1.84392100	-0.07871300
C	-4.64795800	-1.10595800	0.82313600
C	-5.68154400	-0.30920400	0.32457500
H	-6.29033100	0.26348800	1.03095300
C	-5.96114000	-0.22899100	-1.03970100
C	-5.19513000	-1.00702000	-1.90862900
H	-5.40971000	-0.98092900	-2.98123900
C	-4.15680100	-1.82148700	-1.45337500
C	-4.41756500	-1.16715400	2.30546100
H	-5.30052600	-0.80942100	2.85319200
H	-3.56606500	-0.52990700	2.59822200
H	-4.18534900	-2.18860300	2.63993300
C	-7.03604900	0.68297200	-1.55484400
H	-7.42384500	0.34428900	-2.52652600
H	-6.64603200	1.70552400	-1.69438100
H	-7.88004700	0.75094400	-0.85241400
C	-3.38568500	-2.66449100	-2.42334900
H	-3.60334100	-3.73615900	-2.28860800
H	-2.30756000	-2.52990900	-2.27628300
H	-3.62948400	-2.39602200	-3.46073300

Cartesian coordinates of the optimized geometry of **2** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.06841700	0.12652300	0.65492600
Ga	1.18562800	0.32333000	-0.54308700
Cl	1.83090400	0.53213600	-2.69639900
Si	-1.94202000	-1.78854700	-1.90587100
N	2.78255500	-0.66569000	0.10936600
N	1.80464600	2.06644900	0.17638700
N	-2.24407000	-0.79996900	-0.42992400
C	3.94471900	-0.04138000	0.25779000
C	4.10111500	1.35666600	0.18720500
H	5.12830300	1.71638200	0.23772900
C	3.10619900	2.34359700	0.21784400
C	5.19440900	-0.83772700	0.51412900
H	5.71148400	-1.02010200	-0.44072800
H	4.97561600	-1.81452900	0.96375200
H	5.88185800	-0.28056000	1.16330500
C	3.54615500	3.77859500	0.29000000

H	3.44287400	4.22855300	-0.71085700
H	4.59451400	3.86373100	0.60015600
H	2.91379100	4.36710900	0.96801400
C	2.64809600	-2.07646700	0.25481400
C	2.03324900	-2.56151600	1.43283200
C	1.82460700	-3.93540100	1.56328400
H	1.35076500	-4.32488900	2.46569000
C	2.21141600	-4.81703600	0.55889500
H	2.04044200	-5.88974000	0.67541100
C	2.80679200	-4.32667200	-0.59437800
H	3.09708200	-5.02171900	-1.38594700
C	3.03127300	-2.95736100	-0.77896300
C	1.64040400	-1.60585000	2.54157900
H	1.31784500	-0.67064900	2.05322500
C	2.83702600	-1.24868100	3.42397000
H	3.64596400	-0.78044200	2.84652900
H	3.24298100	-2.15044200	3.90941100
H	2.53860500	-0.54158500	4.21380000
C	0.47070200	-2.09985200	3.38079800
H	0.11341400	-1.30033500	4.04566300
H	0.74930000	-2.95478900	4.01707500
H	-0.37283200	-2.41051400	2.74864600
C	3.64772900	-2.48832500	-2.08349300
H	3.76281700	-1.39576500	-2.03357100
C	5.02368600	-3.11539800	-2.31627000
H	5.49642100	-2.68083300	-3.21065800
H	4.94757300	-4.20196400	-2.48114400
H	5.70012000	-2.96157400	-1.46277800
C	2.72342400	-2.77642500	-3.26718400
H	1.75523200	-2.27402900	-3.14598800
H	2.54752100	-3.85792100	-3.38476000
H	3.17277300	-2.40207900	-4.19980000
C	0.82774200	3.04703800	0.51889500
C	0.41098600	3.13065400	1.87025800
C	-0.56405100	4.07128600	2.20881600
H	-0.89789300	4.14865800	3.24507700
C	-1.12489800	4.90492100	1.24666500
H	-1.88897000	5.63222800	1.53085800
C	-0.72048200	4.79867500	-0.07714100
H	-1.17318300	5.44577400	-0.83248600
C	0.25275400	3.87314300	-0.46841400
C	1.02120600	2.23580900	2.93341500
H	1.36612100	1.32696500	2.41555300
C	2.25276500	2.87802800	3.57562900
H	1.98826800	3.83323800	4.05710200
H	3.04557000	3.07646000	2.84229100
H	2.67453000	2.21468000	4.34711300
C	0.02177200	1.81074900	4.00465500
H	-0.28243400	2.65529100	4.64270300
H	0.47781400	1.05974900	4.66806100
H	-0.88167800	1.37147800	3.55592400
C	0.63730700	3.76480700	-1.92906700
H	1.47965900	3.06276000	-2.00432000
C	1.08837600	5.10200100	-2.51378900
H	0.26829000	5.83722400	-2.53854100
H	1.44005200	4.96697700	-3.54825000
H	1.91010900	5.54419100	-1.92993300
C	-0.50832600	3.16459800	-2.74413900
H	-1.37782100	3.84138300	-2.77163200
H	-0.84015700	2.20593300	-2.31874800
H	-0.18845600	2.96976100	-3.77861700
C	-3.60300600	-0.76023200	0.02288700
C	-4.09092100	-1.71591200	0.94179000
C	-5.44274600	-1.67390600	1.29864900
H	-5.83036100	-2.41399600	2.00386500
C	-6.29951700	-0.71056300	0.78260200
H	-7.35304600	-0.69881500	1.07175100
C	-5.80187600	0.24834000	-0.09275700
H	-6.46992400	1.02095700	-0.48065400

C	-4.46135900	0.24378500	-0.48354300
C	-3.19558900	-2.75403900	1.59081500
H	-2.18594000	-2.62212500	1.17312000
C	-3.63125500	-4.18644500	1.28665400
H	-4.63626600	-4.39757700	1.68519100
H	-2.93495900	-4.90679000	1.74432600
H	-3.65458700	-4.38245900	0.20486600
C	-3.11298400	-2.51439400	3.09933000
H	-2.74266500	-1.50149400	3.31855200
H	-2.43737000	-3.24063300	3.57776700
H	-4.10192200	-2.61828300	3.57280000
C	-3.93010700	1.34421000	-1.38039800
H	-2.97125700	0.99472500	-1.78712200
C	-3.63722800	2.59476600	-0.55052900
H	-3.23346300	3.40295400	-1.17871700
H	-2.89927500	2.39117400	0.24361300
H	-4.55111800	2.96324500	-0.05751400
C	-4.83728700	1.65603600	-2.56608900
H	-5.79623000	2.09823100	-2.25263700
H	-5.06116700	0.74954000	-3.14931100
H	-4.34999800	2.38047400	-3.23716200
C	-3.55516600	-2.63163500	-2.37227700
H	-4.32924900	-1.89039300	-2.62316900
H	-3.95517500	-3.26606100	-1.56921200
H	-3.38674800	-3.26305300	-3.25984700
C	-0.65045000	-3.07860400	-1.47997600
H	0.27729900	-2.62787200	-1.09676300
H	-0.38541800	-3.67769400	-2.36509700
H	-1.02824100	-3.76474600	-0.70608300
C	-1.43101900	-0.73912100	-3.36869100
H	-2.23972900	-0.04932700	-3.65572300
H	-1.24351000	-1.40561200	-4.22697700
H	-0.51195800	-0.16115100	-3.19858500

Cartesian coordinates of the optimized geometry of **3** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.96508700	-0.48007900	0.39386900
Ga	-5.62361500	0.54229400	0.31880200
Cl	-5.91501600	1.39858200	2.36319000
N	-7.21017200	-0.58576800	0.08023700
N	-6.22633900	2.01063000	-0.83407600
C	-8.38533500	-0.02678800	-0.19936700
C	-8.53079600	1.30712600	-0.61210200
H	-9.55455100	1.63825400	-0.77768000
C	-7.53184700	2.21946300	-0.99599700
C	-9.63358800	-0.85413500	-0.08537900
H	-10.49564000	-0.33341700	-0.51784300
H	-9.84336700	-1.06117200	0.97497700
H	-9.51353200	-1.83016700	-0.57558100
C	-7.99405100	3.48761600	-1.65473000
H	-7.87713000	4.33275400	-0.96123100
H	-9.04896400	3.41812600	-1.94400300
H	-7.38665500	3.72021000	-2.53999300
C	-7.11384100	-1.99690700	0.27359700
C	-7.34371000	-2.57274500	1.54003800
C	-7.27273600	-3.96549600	1.65492200
H	-7.45075100	-4.42776000	2.62883400
C	-6.98050700	-4.76900800	0.56011600
H	-6.93865500	-5.85503800	0.67191000
C	-6.72200600	-4.18294300	-0.67446600
H	-6.47340800	-4.81497000	-1.52982500
C	-6.76902300	-2.79658700	-0.83844900
C	-7.62878800	-1.73945900	2.77392900
H	-7.73585000	-0.69136400	2.45794300
C	-8.91727300	-2.16125400	3.47955400
H	-9.13638200	-1.47678900	4.31338100
H	-8.83812300	-3.17596600	3.90076900
H	-9.78333800	-2.15545200	2.80017800

C	-6.44219100	-1.79048600	3.73680800
H	-6.61874200	-1.13243100	4.60109100
H	-5.52061500	-1.44909500	3.24798200
H	-6.27487500	-2.81345300	4.11120400
C	-6.48665500	-2.17908900	-2.19424400
H	-6.24863500	-1.11897800	-2.02006500
C	-7.72374900	-2.21873400	-3.09263300
H	-8.56040600	-1.65212100	-2.65932000
H	-8.06150000	-3.25585800	-3.24889800
H	-7.50257600	-1.78246100	-4.07902200
C	-5.28390700	-2.81373600	-2.88613000
H	-4.40741800	-2.84746800	-2.22281500
H	-5.01344700	-2.23606100	-3.78328300
H	-5.49451500	-3.84301400	-3.21677300
C	-5.28115100	2.93732100	-1.37766200
C	-4.97507700	4.13322500	-0.69466900
C	-4.06420100	5.01706500	-1.28365900
H	-3.81825900	5.94825100	-0.76775200
C	-3.45234600	4.72436800	-2.49277600
H	-2.73052200	5.41937700	-2.92758100
C	-3.73971300	3.52701500	-3.13914200
H	-3.22991300	3.29553300	-4.07385400
C	-4.65489800	2.61611600	-2.60572200
C	-5.55521900	4.48254500	0.66297600
H	-6.29177400	3.71119400	0.93052500
C	-6.25186800	5.84394600	0.67291900
H	-6.73345400	6.01769900	1.64753200
H	-7.02468100	5.92880800	-0.10577500
H	-5.53612500	6.66532000	0.51060000
C	-4.46542700	4.44419300	1.73444900
H	-4.90329000	4.58505800	2.73435200
H	-3.72739200	5.24598300	1.57141900
H	-3.93415600	3.48335400	1.73920400
C	-4.96772000	1.32095600	-3.33876600
H	-4.96662400	0.52018300	-2.57901300
C	-6.35145000	1.33093400	-3.99496400
H	-7.17025500	1.37557400	-3.26595200
H	-6.49393500	0.41355900	-4.58688700
H	-6.44799800	2.18791000	-4.68054900
C	-3.92176000	0.96040400	-4.38737800
H	-2.89856800	0.99913400	-3.99120400
H	-3.97399400	1.63739700	-5.25503300
H	-4.10247900	-0.05769100	-4.76251800
C	-0.65153000	-1.39260400	2.12100900
C	-0.60311000	-2.80206000	2.11408100
C	-0.14161900	-3.49020200	3.24159400
H	-0.10970400	-4.58269000	3.22142400
C	0.25700700	-2.79314600	4.37855800
H	0.62812300	-3.33482700	5.25267000
C	0.13317600	-1.40687700	4.41843400
H	0.37885300	-0.85698500	5.33084600
C	-0.33820300	-0.69682400	3.30640800
C	-1.16159400	-3.58091500	0.96746100
C	-2.53966700	-3.88851800	0.98352100
C	-3.08701100	-4.62572200	-0.06846700
H	-4.15982500	-4.83288400	-0.05795300
C	-2.29754600	-5.12038400	-1.10852100
C	-0.92986500	-4.85067700	-1.07542600
H	-0.28335100	-5.25096600	-1.86027400
C	-0.35070300	-4.06425800	-0.07587300
C	-3.41891100	-3.48776900	2.13278800
H	-3.19321000	-2.47719300	2.49570800
H	-3.26491200	-4.16016200	2.99348000
H	-4.48053800	-3.53642100	1.85480000
C	-2.90317400	-5.89169800	-2.24511400
H	-3.06861700	-5.23857000	-3.11927500
H	-3.87745800	-6.32085900	-1.96954800
H	-2.24665100	-6.71143200	-2.57354300
C	1.09993500	-3.71377800	-0.17601000

H	1.53269300	-3.42467700	0.78978200
H	1.22361300	-2.86838700	-0.87261800
H	1.68527600	-4.55084300	-0.57907500
C	-0.64727800	0.75483900	3.47625600
C	-1.97118600	1.09247900	3.83933000
C	-2.29702600	2.42843000	4.07353200
H	-3.33020000	2.67817800	4.33019800
C	-1.33502400	3.44086400	4.00936600
C	-0.03032700	3.07970300	3.68300300
H	0.74628900	3.84725000	3.64346100
C	0.32717300	1.76043500	3.38662500
C	-3.02081200	0.03139700	3.99112000
H	-3.96759900	0.45667000	4.34434300
H	-2.69560900	-0.75971700	4.68385600
H	-3.22626900	-0.46026800	3.02904300
C	-1.70014500	4.87678100	4.24853800
H	-0.87186900	5.43248900	4.71278400
H	-2.58382200	4.96860400	4.89640300
H	-1.94233500	5.38278300	3.29857300
C	1.73940500	1.48144700	2.97209600
H	2.44492100	1.69886400	3.78925400
H	2.01008400	2.12424900	2.11903200
H	1.87968400	0.43791100	2.66620000
C	-3.89907800	-0.36570300	0.06105100
H	-3.92263500	-1.21084500	0.76809500
H	-3.86358500	-0.82774900	-0.93811500
C	-2.67761300	0.52334200	0.29522700
H	-2.76993000	1.10080300	1.22926100
H	-2.56580200	1.25748200	-0.51720000
Ge	0.96522300	0.48026000	-0.39386800
Ga	5.62365500	-0.54235500	-0.31891300
Cl	5.91484100	-1.39876800	-2.36327700
N	7.21033200	0.58555500	-0.08044300
N	6.22628700	-2.01072300	0.83395600
C	8.38544400	0.02646700	0.19916700
C	8.53079600	-1.30745800	0.61191300
H	9.55452400	-1.63866700	0.77749500
C	7.53177200	-2.21970000	0.99584200
C	9.63377600	0.85369900	0.08518700
H	10.49577400	0.33290000	0.51766000
H	9.84358200	1.06071300	-0.97516600
H	9.51381000	1.82974500	0.57538400
C	7.99385500	-3.48789300	1.65458000
H	7.87683000	-4.33302600	0.96108900
H	9.04878200	-3.41851000	1.94382800
H	7.38645500	-3.72041200	2.53985900
C	7.11412100	1.99671400	-0.27376600
C	7.34397000	2.57261700	-1.54018800
C	7.27306500	3.96538000	-1.65497800
H	7.45106600	4.42769500	-2.62886900
C	6.98093100	4.76884200	-0.56010900
H	6.93913500	5.85488000	-0.67183800
C	6.72244800	4.18271700	0.67444600
H	6.47392100	4.81470500	1.52985300
C	6.76939200	2.79634600	0.83833700
C	7.62895900	1.73942200	-2.77416000
H	7.73601100	0.69129800	-2.45827300
C	8.91740800	2.16125200	-3.47982900
H	9.13643900	1.47686700	-4.31374300
H	8.83826000	3.17601100	-3.90093200
H	9.78352100	2.15535300	-2.80051700
C	6.44231000	1.79057400	-3.73696900
H	6.61877600	1.13256600	-4.60130400
H	5.52074300	1.44920500	-3.24811200
H	6.27503000	2.81357600	-4.11128900
C	6.48702600	2.17876700	2.19409800
H	6.24894400	1.11868200	2.01983800
C	7.72414300	2.21826600	3.09245900
H	8.56075700	1.65163900	2.65907900

H	8.06196100	3.25535700	3.24880800
H	7.50296500	1.78192300	4.07881600
C	5.28433300	2.81343000	2.88606000
H	4.40782800	2.84726900	2.22277200
H	5.01386700	2.23570700	3.78318000
H	5.49501500	3.84267100	3.21677200
C	5.28099000	-2.93727900	1.37758500
C	4.97464500	-4.13306200	0.69450800
C	4.06363900	-5.01678600	1.28347100
H	3.81746900	-5.94786600	0.76748200
C	3.45189900	-4.72407500	2.49264000
H	2.72995400	-5.41897500	2.92741800
C	3.73951500	-3.52682500	3.13908600
H	3.22979200	-3.29532400	4.07383700
C	4.65486000	-2.61605800	2.60571500
C	5.55455600	-4.48231200	-0.66325200
H	6.29107600	-3.71095000	-0.93087500
C	6.25119100	-5.84371700	-0.67338000
H	6.73263400	-6.01741900	-1.64807300
H	7.02411200	-5.92863100	0.10520200
H	5.53546300	-6.66509200	-0.51100800
C	4.46457600	-4.44388900	-1.73453300
H	4.90226100	-4.58466900	-2.73452600
H	3.72658600	-5.24570900	-1.57143500
H	3.93328400	-3.48306200	-1.73911700
C	4.96791000	-1.32101900	3.33888700
H	4.96716900	-0.52019300	2.57919100
C	6.35149200	-1.33139200	3.99538400
H	7.17044600	-1.37621500	3.26655700
H	6.49408900	-0.41407300	4.58736900
H	6.44766600	-2.18841700	4.68096100
C	3.92183800	-0.96026300	4.38731400
H	2.89871800	-0.99867400	3.99092700
H	3.97370600	-1.63735000	5.25491900
H	4.10276700	0.05774800	4.76258200
C	0.65174700	1.39283700	-2.12097600
C	0.60346100	2.80229000	-2.11400400
C	0.14209000	3.49050700	-3.24152000
H	0.11026600	4.58299600	-3.22132200
C	-0.25658500	2.79351200	-4.37851000
H	-0.62763200	3.33525400	-5.25261300
C	-0.13293900	1.40722700	-4.41840200
H	-0.37868300	0.85737100	-5.33081700
C	0.33836200	0.69710500	-3.30638300
C	1.16182000	3.58104000	-0.96725300
C	2.53993200	3.88849100	-0.98299200
C	3.08712700	4.62554500	0.06917900
H	4.15996800	4.83258400	0.05892300
C	2.29749500	5.12019300	1.10911500
C	0.92979700	4.85061300	1.07572000
H	0.28315900	5.25088000	1.86047900
C	0.35076700	4.06434300	0.07597100
C	3.41938900	3.48771500	-2.13208400
H	3.19367900	2.47717400	-2.49509400
H	3.26562400	4.16015100	-2.99278600
H	4.48096000	3.53625900	-1.85386600
C	2.90295800	5.89135000	2.24590100
H	3.06813800	5.23813700	3.12004800
H	3.87734700	6.32043100	1.97058300
H	2.24644900	6.71112700	2.57425000
C	-1.09991800	3.71395700	0.17578200
H	-1.53248600	3.42495000	-0.79012500
H	-1.22380500	2.86853000	0.87230900
H	-1.68528500	4.55104100	0.57876800
C	0.64721400	-0.75461200	-3.47619700
C	1.97102200	-1.09250300	-3.83942300
C	2.29658300	-2.42851700	-4.07365600
H	3.32967500	-2.67846200	-4.33046100
C	1.33440300	-3.44077300	-4.00936000

C	0.02982000	-3.07937100	-3.68281400
H	-0.74692400	-3.84678300	-3.64313800
C	-0.32739800	-1.76003800	-3.38639900
C	3.02084000	-0.03163700	-3.99137600
H	3.96748400	-0.45710800	-4.34474700
H	2.69569400	0.75954500	-4.68406300
H	3.22654700	0.45998700	-3.02933300
C	1.69922800	-4.87675700	-4.24858000
H	0.87080600	-5.43230200	-4.71276000
H	2.58283100	-4.96873800	-4.89652200
H	1.94140300	-5.38281900	-3.29864200
C	-1.73949600	-1.48079400	-2.97159200
H	-2.44522300	-1.69812400	-3.78858900
H	-2.01010200	-2.12352300	-2.11844800
H	-1.87953500	-0.43722600	-2.66569200
C	3.89920900	0.36577500	-0.06109100
H	3.92281000	1.21088000	-0.76818500
H	3.86377200	0.82787100	0.93805100
C	2.67769500	-0.52321700	-0.29521000
H	2.76999100	-1.10069300	-1.22923600
H	2.56586000	-1.25733700	0.51723000

Cartesian coordinates of the optimized geometry of **4** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.91797500	0.35998000	-0.86639500
Ge	0.92272500	0.37448500	0.87576500
Ga	-5.51339900	-0.62621200	-0.08954900
Ga	5.51383500	-0.62884100	0.08991400
Cl	-5.67163000	-2.26382700	-1.60277000
Cl	5.67327900	-2.25352100	1.61702700
N	-6.37715100	-1.39968100	1.49554500
N	-6.98609800	0.58295500	-0.57658300
N	6.37736700	-1.41887200	-1.48746800
N	6.98737900	0.58412600	0.56465500
C	-7.70376300	-1.39186500	1.60895300
C	-8.56008800	-0.66200600	0.76719300
H	-9.62379100	-0.78426200	0.96358400
C	-8.23092400	0.31700900	-0.18398000
C	-8.34874500	-2.18996600	2.70643500
H	-7.84577300	-2.02452200	3.66931000
H	-8.25971900	-3.26441300	2.48865700
H	-9.41142800	-1.93971500	2.80314700
C	-9.36653000	1.11080500	-0.76533200
H	-10.30267100	0.90817600	-0.23261200
H	-9.50120600	0.84969900	-1.82529700
H	-9.15677000	2.18913500	-0.73540200
C	-5.58749500	-2.03235300	2.50592300
C	-5.36190300	-3.42442900	2.48451000
C	-4.64517700	-3.99190500	3.54384500
H	-4.46384100	-5.06929400	3.54595700
C	-4.15008600	-3.21551900	4.58331500
H	-3.59235600	-3.68164100	5.39880200
C	-4.33581400	-1.83725200	4.56291100
H	-3.90949100	-1.22525800	5.35955000
C	0.30140200	0.41431600	2.78214000
C	-5.04403500	-1.22214000	3.52770300
C	-5.83465700	-4.31615100	1.35171300
H	-6.45794500	-3.71021900	0.67750800
C	-6.66773600	-5.49928100	1.84604700
H	-6.06284500	-6.20189200	2.44068000
H	-7.07556200	-6.06105900	0.99174200
H	-7.51248600	-5.18211900	2.47625200
C	-4.64462600	-4.81172200	0.52863200
H	-3.95398800	-5.40338000	1.15119400
H	-4.08690900	-3.97619700	0.08497300
H	-4.98871900	-5.44823400	-0.30099100
C	-5.24189400	0.28110800	3.52213500
H	-5.39885000	0.57668300	2.47360400

C	-6.49895700	0.68828700	4.29223900
H	-7.40889200	0.25987000	3.84853300
H	-6.61457300	1.78354200	4.29261700
H	-6.44040200	0.35379300	5.34038100
C	-4.01969800	1.03680100	4.03001600
H	-3.86487700	0.89762400	5.11089700
H	-4.14461400	2.11645300	3.86172300
H	-3.09711500	0.71502000	3.52458200
C	-6.73875400	1.72266100	-1.40261400
C	-6.90613200	1.65584100	-2.80142100
C	-6.73048600	2.82792000	-3.54507100
H	-6.86509800	2.79402400	-4.62883100
C	-6.38186900	4.02701400	-2.93720900
H	-6.25609300	4.93102500	-3.53777000
C	-6.16739900	4.06453600	-1.56365100
H	-5.86792900	5.00210300	-1.09082500
C	-6.33164000	2.92185400	-0.77699500
C	-7.21639100	0.36103100	-3.52570800
H	-7.40893500	-0.41411100	-2.76938900
C	-8.44230100	0.46465100	-4.43222500
H	-8.67476500	-0.51801300	-4.87039700
H	-8.27437500	1.16330600	-5.26703200
H	-9.33506200	0.81134100	-3.88976000
C	-5.99274300	-0.09154900	-4.32325300
H	-5.11291200	-0.18766800	-3.67431000
H	-5.75131900	0.62594200	-5.12416100
H	-6.17236800	-1.07465700	-4.78420100
C	-6.11151400	2.98817000	0.72120900
H	-5.90706000	1.96120700	1.05937000
C	-7.36958300	3.45613000	1.45400300
H	-8.21424000	2.77134300	1.29243300
H	-7.67336200	4.45811000	1.11075300
H	-7.18893200	3.50976700	2.53897700
C	-4.90522100	3.83971200	1.10116800
H	-4.69753300	3.74041900	2.17661300
H	-5.07441900	4.91010200	0.90368700
H	-4.00277500	3.53340600	0.55113500
C	7.70360400	-1.41223400	-1.60227700
C	8.56051200	-0.67442400	-0.76791100
H	9.62408900	-0.79856200	-0.96386800
C	8.23204700	0.31331600	0.17426000
C	8.34833100	-2.22131800	-2.69182900
H	8.27750500	-3.29251200	-2.45196200
H	9.40647100	-1.95842500	-2.80393800
H	7.83340400	-2.08161600	-3.65235500
C	9.36834600	1.11157300	0.74818600
H	9.50098000	0.86258600	1.81130200
H	9.16071800	2.18989700	0.70548400
H	10.30484100	0.90109900	0.21914800
C	5.58408300	-2.06163100	-2.48835400
C	5.36142500	-3.45389200	-2.45487300
C	4.63498500	-4.03007800	-3.50286900
H	4.45560300	-5.10777300	-3.49561800
C	4.12647700	-3.26164600	-4.54175500
H	3.55983800	-3.73426000	-5.34730700
C	4.31118000	-1.88307800	-4.53381800
H	3.87577600	-1.27761500	-5.33041800
C	5.03095500	-1.25980100	-3.51163900
C	5.84704000	-4.33703000	-1.32087400
H	6.47369700	-3.72477200	-0.65554900
C	6.67963000	-5.52039200	-1.81558000
H	7.09772300	-6.07533900	-0.96176000
H	7.51678100	-5.20445900	-2.45639000
H	6.07126400	-6.22881600	-2.39967500
C	4.66587400	-4.83172200	-0.48469400
H	5.01971900	-5.45999300	0.34716200
H	3.97336900	-5.43147100	-1.09745500
H	4.10812500	-3.99474800	-0.04397400
C	5.23395900	0.24270000	-3.52214500

H	5.39007600	0.54946000	-2.47665000
C	6.49425700	0.63611200	-4.29422700
H	7.40164700	0.20876100	-3.84445800
H	6.61444800	1.73080600	-4.30614800
H	6.43592400	0.29054800	-5.33877100
C	4.01659000	0.99813900	-4.04079600
H	3.09160900	0.68603100	-3.53384800
H	3.86361000	0.84792000	-5.12046900
H	4.14624000	2.07892800	-3.88404200
C	6.74228300	1.73215900	1.37983200
C	6.91036600	1.67838600	2.77912800
C	6.73850400	2.85801600	3.51158100
H	6.87382500	2.83420900	4.59552100
C	6.39258200	4.05212900	2.89243600
H	6.26964400	4.96222900	3.48432900
C	6.17717700	4.07696500	1.51875900
H	5.87999100	5.01075900	1.03709700
C	6.33802500	2.92635200	0.74299000
C	7.21727600	0.38962400	3.51547000
H	7.40852500	-0.39289900	2.76645800
C	8.44280200	0.49847600	4.42184900
H	8.27618600	1.20517800	5.25011500
H	9.33682300	0.83778300	3.87678000
H	8.67243400	-0.48072300	4.86917000
C	5.99184800	-0.05254200	4.31610400
H	6.16847100	-1.03181000	4.78627500
H	5.11234800	-0.15240500	3.66726500
H	5.75146000	0.67301800	5.11002200
C	6.11749700	2.97911000	-0.75568300
H	5.91135700	1.94937700	-1.08422700
C	7.37592800	3.43831400	-1.49338900
H	8.21944500	2.75343200	-1.32636800
H	7.68176900	4.44274600	-1.15924900
H	7.19462800	3.48269300	-2.57867600
C	4.91240200	3.82912100	-1.14282500
H	4.00992300	3.52979800	-0.58901000
H	4.70356100	3.71995900	-2.21709000
H	5.08368600	4.90102600	-0.95567300
C	-3.71846300	0.17025200	0.07622800
H	-3.81087600	1.24424100	-0.15749900
H	-3.40479800	0.11845700	1.13179600
C	-2.70063200	-0.49528200	-0.84201700
H	-3.05434700	-0.47764900	-1.88175900
H	-2.57424800	-1.56146100	-0.61515800
C	3.71743200	0.16349900	-0.08427800
H	3.81019900	1.24346200	0.11969000
H	3.39672300	0.08246000	-1.13591800
C	2.70640800	-0.47889700	0.85775200
H	3.06772600	-0.43646600	1.89422000
H	2.57890300	-1.55015900	0.65709300
C	-0.75984800	2.18412500	-0.10551400
H	-1.16884300	3.04160200	-0.65053400
H	-1.26799300	2.14025400	0.87083800
C	0.76004600	2.18709900	0.08864800
H	1.16725800	3.05328000	0.62103600
H	1.26815300	2.13023000	-0.88699800
C	-0.29249000	0.37215300	-2.77149100
C	-0.04127200	-0.86358300	-3.41201600
C	0.49528100	-0.90299600	-4.70480600
H	0.69080200	-1.87681000	-5.16141400
C	0.74170800	0.26901500	-5.40921600
H	1.15803100	0.23236600	-6.41921500
C	0.39935100	1.48690600	-4.83406200
H	0.51198800	2.41358000	-5.40291700
C	-0.12729200	1.55653900	-3.53718200
C	-0.44603100	-2.17314100	-2.81813000
C	0.46089900	-2.93773700	-2.06478500
C	0.07659900	-4.20050200	-1.61301200
H	0.79596100	-4.79302600	-1.04400700

C	-1.19446600	-4.71924900	-1.86988900
C	-2.08158800	-3.94336600	-2.61691100
H	-3.08377400	-4.32576500	-2.83179400
C	-1.72083400	-2.69033200	-3.12064500
C	1.83666300	-2.41827200	-1.79864800
H	1.80028000	-1.36989900	-1.47918000
H	2.45783100	-2.45260400	-2.70502400
H	2.34014300	-3.00450400	-1.02003200
C	-1.60124600	-6.06545900	-1.34414100
H	-2.09248500	-5.97730700	-0.36057100
H	-0.73252300	-6.72810900	-1.21829300
H	-2.31835100	-6.56051300	-2.01519800
C	-2.68068500	-1.96360200	-4.01859600
H	-3.71827200	-2.17018400	-3.72246600
H	-2.55319500	-2.29087700	-5.06445800
H	-2.52127900	-0.87787800	-4.00872600
C	-0.61380700	2.89317900	-3.08198100
C	0.27654900	3.92546300	-2.73654700
C	-0.23213300	5.12451100	-2.22702800
H	0.47044500	5.90271700	-1.91331200
C	-1.60182100	5.34654800	-2.09100100
C	-2.47155000	4.34964000	-2.53983700
H	-3.55162000	4.50909700	-2.48510700
C	-2.00386900	3.13156300	-3.03500300
C	1.75993600	3.77640600	-2.90384000
H	2.29778700	4.46526200	-2.23886400
H	2.06588600	4.00534600	-3.93865400
H	2.10025600	2.75458900	-2.69426700
C	-2.12989100	6.59825800	-1.45311100
H	-2.33197100	6.43101200	-0.38111000
H	-3.07502000	6.92113400	-1.91494700
H	-1.41076400	7.42714600	-1.52489600
C	-2.99324600	2.10007100	-3.49136100
H	-3.08023000	1.27756400	-2.76757500
H	-2.69395600	1.64615200	-4.44772500
H	-3.99372400	2.53735400	-3.60300000
C	0.13753900	1.60939200	3.53112600
C	-0.38696500	1.55828700	4.82975000
H	-0.49918000	2.49311400	5.38519400
C	-0.72750000	0.34873600	5.42329800
H	-1.14171600	0.32656200	6.43457000
C	-0.48273800	-0.83321700	4.73508400
H	-0.67853700	-1.80045600	5.20536700
C	0.05004000	-0.81188300	3.44038300
C	0.62134600	2.93962800	3.05532500
C	-0.27152000	3.96523700	2.69662800
C	0.23425200	5.15731700	2.16836500
H	-0.47010300	5.92984800	1.84475200
C	1.60341100	5.37921500	2.02596000
C	2.47567700	4.39033200	2.48739400
H	3.55541300	4.55061700	2.42786400
C	2.01086700	3.17902800	3.00167100
C	-1.75432800	3.81599200	2.86945600
H	-2.09311700	2.79035500	2.67648100
H	-2.29497500	4.49350100	2.19515300
H	-2.05845600	4.06031300	3.90129000
C	2.12784400	6.62219000	1.36826900
H	1.41118200	7.45347100	1.43726000
H	2.31891400	6.44196600	0.29634200
H	3.07810400	6.94837000	1.81699900
C	3.00243900	2.15531600	3.47064400
H	2.70216000	1.70927100	4.43035300
H	4.00119900	2.59689400	3.58047400
H	3.09426900	1.32651000	2.75464200
C	0.44186700	-2.12944800	2.85673600
C	-0.47839400	-2.89089400	2.11770800
C	-0.10723200	-4.15801400	1.66640200
H	-0.83555700	-4.74685400	1.10524200
C	1.16196200	-4.68460600	1.91291200

C	2.06243100	-3.91212500	2.64861600
H	3.06401200	-4.30081600	2.85540600
C	1.71607100	-2.65442300	3.14967000
C	-1.85298200	-2.36211800	1.86554900
H	-2.38021800	-2.96232300	1.11402600
H	-1.81068100	-1.32292300	1.51784400
H	-2.45504700	-2.36439900	2.78512600
C	1.55511100	-6.03737800	1.39335900
H	2.12824900	-6.60518900	2.14174300
H	2.19632900	-5.94974400	0.50075800
H	0.67429600	-6.63197500	1.11191200
C	2.68913100	-1.92876900	4.03409300
H	2.57064200	-2.25065300	5.08267700
H	2.53499600	-0.84224400	4.02073000
H	3.72259700	-2.14192000	3.72838900

Cartesian coordinates of the optimized geometry of **5** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.78349400	-0.94025700	1.01596700
Ga	-5.24230500	-0.11762600	-0.47475500
Cl	-6.31626900	-1.32006300	1.06081900
Si	1.03111100	-2.84137200	2.78752800
N	-5.86543500	-0.84369500	-2.19127800
C	-7.64215700	-1.26287000	-3.81661900
H	-7.92606200	-2.27859600	-3.50377700
H	-6.89816900	-1.37957100	-4.61722400
H	-8.52975100	-0.75742400	-4.21425400
C	-2.37099300	2.88507700	1.47919600
H	-3.38108900	2.89179600	1.91463000
H	-2.30023900	2.01668800	0.81313400
H	-2.27200200	3.78821200	0.86011500
C	-1.42894100	1.52168300	4.06785000
H	-0.70594900	1.54147000	4.89742000
H	-1.39694700	0.51432700	3.62671700
H	-2.43824400	1.67181700	4.48402000
Ge	0.78349900	0.94074100	1.01591000
Ga	5.24225000	0.11750100	-0.47479400
Cl	6.31637000	1.32033500	1.06042500
Si	-1.03097300	2.84194500	2.78761700
N	-6.26377800	1.55024000	-0.58232900
C	-7.06676700	-0.51160700	-2.65093200
N	-0.52158700	-2.49466500	2.01816300
C	-7.83999200	0.53326900	-2.11031000
H	-8.83369400	0.65312200	-2.53850900
N	0.52161500	2.49515700	2.01808400
C	-7.43642900	1.54201100	-1.22309300
N	5.86536000	0.84320900	-2.19151500
C	-8.38159900	2.69050000	-1.01221900
H	-8.66064400	2.75610600	0.04996800
H	-9.28925200	2.57156000	-1.61475000
H	-7.90519100	3.64852000	-1.26388100
N	6.26375900	-1.55030100	-0.58199800
C	-5.06969300	-1.81718900	-2.86895800
C	-4.03079300	-1.36675400	-3.71625400
C	-3.27640600	-2.31883400	-4.40605600
H	-2.47405600	-1.99105500	-5.06870200
C	-3.52700500	-3.67899800	-4.26003000
H	-2.92974000	-4.40822200	-4.81225000
C	-4.51486900	-4.10544900	-3.38404700
H	-4.68114400	-5.17558300	-3.23937100
C	-5.29113500	-3.19399000	-2.66036000
C	-3.74231600	0.11379100	-3.88571600
H	-3.98251000	0.59512300	-2.92456100
C	-2.27451700	0.40669400	-4.18196900
H	-2.08941700	1.48963200	-4.14610000
H	-1.97939000	0.06312700	-5.18582700
H	-1.60747400	-0.06963700	-3.44849500
C	-4.64716600	0.75017200	-4.94205400

H	-5.70956100	0.67555600	-4.67092700
H	-4.50841200	0.26234800	-5.92002100
H	-4.41118200	1.81936800	-5.06080300
C	-6.27736500	-3.71690400	-1.63466700
H	-6.84297400	-2.86226200	-1.23557900
C	-5.51793900	-4.33645200	-0.46050100
H	-4.79599900	-3.63311200	-0.02432200
H	-4.96261000	-5.23365800	-0.77657900
H	-6.21160900	-4.62796900	0.34237900
C	-7.27133700	-4.71866000	-2.22107200
H	-8.01134100	-5.00945500	-1.45984800
H	-6.76964300	-5.63983000	-2.55732500
H	-7.81793700	-4.31003200	-3.08484000
C	-5.83986200	2.75649400	0.05982000
C	-6.15692200	3.00392500	1.41147800
C	-5.78289900	4.23188500	1.96735800
H	-6.02511100	4.43702700	3.01286800
C	-5.11206300	5.19153600	1.21957200
H	-4.83480500	6.14647800	1.67198900
C	-4.77570300	4.91962400	-0.10076100
H	-4.22665000	5.66577600	-0.68059400
C	-0.95772300	4.53481100	3.59625600
H	-1.93787500	4.76353100	4.04514500
H	-0.73366300	5.31191500	2.85027000
H	-0.19247200	4.60489100	4.38178500
C	-5.11917000	3.70438200	-0.69884800
C	-6.84491700	1.97217600	2.28086300
H	-7.17519000	1.14757100	1.63298300
C	-5.84754000	1.37933500	3.27725500
H	-5.48191900	2.14641300	3.97964400
H	-4.97738100	0.94967100	2.76129600
H	-6.31268100	0.56964500	3.85896300
C	-8.07533800	2.52514100	2.99713800
H	-7.81135000	3.30458400	3.72933500
H	-8.58825700	1.72048900	3.54576400
H	-8.79696600	2.96527400	2.29155500
C	-4.72364300	3.44387000	-2.13981600
H	-4.97020000	2.39528300	-2.36102400
C	-3.22145200	3.62228600	-2.35201400
H	-2.90302900	4.65854900	-2.16018600
H	-2.94834100	3.38507700	-3.39120500
H	-2.63831000	2.96874500	-1.68679400
C	-5.52161700	4.31363500	-3.11165000
H	-5.33542700	5.38462500	-2.93224900
H	-6.60355300	4.14104300	-3.01638700
H	-5.23932700	4.09343500	-4.15308900
C	-3.28525300	-0.15581200	-0.33478200
H	-2.97037400	-0.84423200	-1.13605300
H	-2.89713300	0.83213500	-0.62709100
C	-2.73314800	-0.62007300	1.00598800
H	-3.18028500	-1.58591000	1.28881100
H	-2.98977100	0.07522300	1.81866700
C	-1.54574700	-3.48018500	2.04875700
C	-1.60031100	-4.47615100	1.04418000
C	-2.55447100	-5.49176800	1.14270200
H	-2.59011200	-6.26846200	0.37368700
C	-3.46457800	-5.52561700	2.19263700
H	-4.20496000	-6.32670800	2.25475300
C	-3.44381800	-4.51556300	3.14717800
H	-4.18103600	-4.52332700	3.95393400
C	-2.50294800	-3.48338700	3.09307700
C	-0.67248000	-4.43695700	-0.15386200
H	0.01511100	-3.59455600	0.00431700
C	0.17454800	-5.70058600	-0.28664900
H	0.77343900	-5.88128400	0.61863400
H	0.86743900	-5.61368700	-1.13868900
H	-0.44898600	-6.59280400	-0.45687100
C	-1.45880400	-4.15877500	-1.43431400
H	-2.07746500	-3.25353600	-1.34185000

H	-2.14075700	-4.98869400	-1.67675000
H	-0.78317600	-4.01850700	-2.29318900
C	-2.53873400	-2.38347700	4.13572700
H	-1.86304100	-1.59387200	3.77505100
C	-3.93469600	-1.78108200	4.29242800
H	-3.89012000	-0.87129500	4.91189200
H	-4.62366500	-2.48137500	4.79160000
H	-4.38285100	-1.51763300	3.32410900
C	-2.00551100	-2.85336500	5.48883400
H	-2.01929700	-2.02838500	6.21895600
H	-0.97286100	-3.22136900	5.41589900
H	-2.62308900	-3.67172200	5.89326800
C	1.42905200	-1.52111800	4.06778200
H	1.39749600	-0.51378400	3.62656900
H	2.43814700	-1.67148800	4.48436900
H	0.70571300	-1.54062800	4.89705600
C	2.37110800	-2.88445900	1.47907600
H	2.30061500	-2.01593600	0.81316200
H	2.27202500	-3.78748600	0.85985100
H	3.38115400	-2.89145300	1.91463700
C	0.95809400	-4.53425900	3.59615100
H	0.19372700	-4.60408800	4.38255600
H	1.93867800	-4.76336600	4.04389900
H	0.73288200	-5.31124300	2.85038100
C	-0.13008400	-0.75786900	-0.87745800
H	0.80468500	-1.32428900	-1.00996600
H	-0.83625800	-1.10308500	-1.64771500
C	0.13009800	0.75821300	-0.87752400
H	-0.80467500	1.32460600	-1.01012200
H	0.83630100	1.10338300	-1.64777700
C	1.54583400	3.48063800	2.04852800
C	1.60036400	4.47657100	1.04391400
C	2.55461000	5.49212300	1.14232200
H	2.59022600	6.26880000	0.37328900
C	3.46481200	5.52593600	2.19217200
H	4.20525700	6.32697600	2.25420000
C	3.44410500	4.51587700	3.14671500
H	4.18142000	4.52359200	3.95338000
C	2.50316300	3.48376400	3.09271600
C	0.67243200	4.43744900	-0.15405900
H	-0.01524400	3.59513400	0.00420500
C	1.45860000	4.15909400	-1.43457500
H	2.14067700	4.98888200	-1.67711600
H	0.78286100	4.01889800	-2.29337100
H	2.07710600	3.25374900	-1.34211800
C	-0.17443600	5.70118700	-0.28682600
H	-0.77333200	5.88193500	0.61843700
H	-0.86731100	5.61440200	-1.13889200
H	0.44922200	6.59333000	-0.45698500
C	2.53902100	2.38378700	4.13529000
H	1.86316400	1.59428000	3.77470100
C	2.00609900	2.85362400	5.48853300
H	2.62383900	3.67189600	5.89288900
H	2.01995400	2.02859600	6.21860100
H	0.97346300	3.22172600	5.41583500
C	3.93493400	1.78118000	4.29168300
H	4.62404100	2.48125600	4.79097200
H	4.38294400	1.51792700	3.32324200
H	3.89033100	0.87123300	4.91091000
C	2.73312800	0.62030800	1.00607700
H	3.18044400	1.58595600	1.28924700
H	2.98953400	-0.07528000	1.81857400
C	3.28522400	0.15647000	-0.33480900
H	2.97089300	0.84553100	-1.13576000
H	2.89658300	-0.83105300	-0.62787900
C	7.64197600	1.26200400	-3.81705400
H	6.89787000	1.37874800	-4.61754100
H	8.52942400	0.75634900	-4.21475200
H	7.92612300	2.27772000	-3.50439000

C	7.06665000	0.51103000	-2.65115500
C	7.83992600	-0.53369800	-2.11028000
H	8.83362200	-0.65363600	-2.53847500
C	7.43641200	-1.54219500	-1.22279200
C	8.38165900	-2.69052800	-1.01144300
H	8.66117400	-2.75518800	0.05068800
H	9.28906900	-2.57207900	-1.61444000
H	7.90514800	-3.64876300	-1.26206400
C	5.06950500	1.81645800	-2.86942000
C	4.03065900	1.36570200	-3.71660200
C	3.27612000	2.31752600	-4.40658700
H	2.47380100	1.98948900	-5.06914100
C	3.52652900	3.67776300	-4.26084700
H	2.92913100	4.40679700	-4.81317500
C	4.51438500	4.10452900	-3.38501300
H	4.68052900	5.17471700	-3.24058100
C	5.29080800	3.19332100	-2.66116800
C	3.74241300	-0.11492300	-3.88576000
H	3.98261600	-0.59600000	-2.92447600
C	2.27468500	-0.40812100	-4.18206700
H	1.60750000	0.06837300	-3.44883200
H	2.08972500	-1.49106900	-4.14584100
H	1.97962300	-0.06494100	-5.18607700
C	4.64745800	-0.75140000	-4.94187100
H	4.50872800	-0.26381900	-5.91996100
H	4.41163600	-1.82065600	-5.06040300
H	5.70981700	-0.67657800	-4.67066400
C	6.27707000	3.71658300	-1.63568600
H	6.84273200	2.86209500	-1.23634500
C	7.27096600	4.71818900	-2.22246400
H	6.76920600	5.63921100	-2.55901900
H	7.81755900	4.30929600	-3.08611500
H	8.01099600	5.00928900	-1.46138000
C	5.51767300	4.33646400	-0.46167800
H	6.21133800	4.62809000	0.34116600
H	4.79564700	3.63329200	-0.02536600
H	4.96244600	5.23365600	-0.77798400
C	5.83980800	-2.75642500	0.06037100
C	6.15675800	-3.00363100	1.41208300
C	5.78266500	-4.23148800	1.96815200
H	6.02478300	-4.43645300	3.01371900
C	5.11186700	-5.19125100	1.22048100
H	4.83453600	-6.14610100	1.67304800
C	4.77559700	-4.91955600	-0.09992100
H	4.22657700	-5.66580400	-0.67966000
C	5.11913200	-3.70442700	-0.69819200
C	6.84471700	-1.97175400	2.28133200
H	7.17512200	-1.14729800	1.63332100
C	8.07502000	-2.52467400	2.99784700
H	8.58794400	-1.71997100	3.54639600
H	8.79669500	-2.96500400	2.29243200
H	7.81087500	-3.30396500	3.73014900
C	5.84728500	-1.37863900	3.27749800
H	6.31238200	-0.56878700	3.85901500
H	5.48161400	-2.14552400	3.98007700
H	4.97715100	-0.94912100	2.76137700
C	4.72376800	-3.44414400	-2.13924200
H	4.97011000	-2.39551600	-2.36048800
C	5.52216200	-4.31377600	-3.11085700
H	5.23990900	-4.09383100	-4.15235900
H	5.33635400	-5.38480700	-2.93130600
H	6.60402200	-4.14076500	-3.01548600
C	3.22165400	-3.62292300	-2.35170900
H	2.63825000	-2.96942700	-1.68667100
H	2.90341500	-4.65923000	-2.15983500
H	2.94871500	-3.38588400	-3.39098200

Cartesian coordinates of the optimized geometry of **S1** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.02926200	-2.24328200	-0.05047100
Ga	0.53335400	0.13770900	-0.22100500
Cl	0.26300900	-0.93873600	2.08245600
N	2.33903500	0.88093700	-0.04984800
N	-0.36669400	1.85189300	-0.00179500
C	2.60623400	2.11432500	0.37465300
C	1.61711500	3.08180000	0.60611000
H	1.96933100	4.04622900	0.96791500
C	0.23329900	2.96933400	0.40892700
C	4.03468500	2.50051100	0.63314900
H	4.52238600	1.75339500	1.27685900
H	4.09447900	3.48544100	1.11054100
H	4.61025800	2.52777000	-0.30386300
C	-0.61152200	4.17957500	0.68683000
H	-1.41921100	3.92883000	1.39053400
H	-1.10148800	4.53313300	-0.23232400
H	-0.00731000	4.99400900	1.10270700
C	3.38992500	-0.04603900	-0.30060400
C	4.13745100	0.03187800	-1.47993500
C	5.13574400	-0.90454000	-1.73596900
H	5.71555700	-0.83798700	-2.65964900
C	5.38500700	-1.93079400	-0.82509300
H	6.16361300	-2.66874100	-1.03074500
C	4.62669900	-2.01922400	0.34086600
H	4.80505300	-2.82942300	1.05152800
C	3.62944700	-1.08297400	0.60662500
C	-1.77897100	1.82666800	-0.19949000
C	-2.33128000	2.29505700	-1.39434800
C	-3.71057000	2.25327000	-1.58589700
H	-4.13826800	2.62023400	-2.52198500
C	-4.53923500	1.73666900	-0.59172500
H	-5.61971700	1.69534300	-0.74583200
C	-3.98412200	1.24924600	0.58998300
H	-4.62522300	0.81498000	1.35910500
C	-2.60676700	1.28604900	0.78793700
C	-2.02035700	-1.95712000	-0.09698000
C	-2.67181200	-1.65484700	-1.30191800
C	-4.06285100	-1.65678000	-1.39203600
H	-4.54712800	-1.40760000	-2.33999400
C	-4.83541400	-1.96138900	-0.27183600
H	-5.92635600	-1.96204300	-0.33940000
C	-4.20536800	-2.25644300	0.93691300
H	-4.80319700	-2.49277000	1.82183000
C	-2.81340700	-2.25624700	1.02035400
H	3.01387600	-1.15266700	1.50651100
H	3.92025300	0.82629500	-2.19805600
H	-2.15584000	0.87989400	1.69581200
H	-1.66982200	2.68814400	-2.17024800
H	-2.33443400	-2.48517100	1.97746000
H	-2.08551200	-1.40042200	-2.19183100

Cartesian coordinates of the optimized geometry of **S2** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.63803600	0.71310200	-1.00513400
Ga	-1.20281100	-0.30596800	0.38169400
Cl	-1.70059600	-0.70284700	2.53004700
Si	2.22607800	0.78836700	1.87956800
N	-1.37730700	-2.10535200	-0.42810700
N	-2.92522400	0.31338700	-0.36380400
N	2.11730200	0.88357900	0.08607200
C	-2.51402700	-2.62035200	-0.87845800
C	-3.69833000	-1.87584400	-1.00802900
H	-4.56975400	-2.42420700	-1.36243300
C	-3.87736400	-0.49506500	-0.81596100
C	-2.53508400	-4.06367400	-1.29447400
H	-2.30384600	-4.71585800	-0.43895900

H	-1.75917600	-4.25480400	-2.05127200
H	-3.51166200	-4.34686400	-1.70387600
C	-5.22332200	0.08499800	-1.15196400
H	-5.56116700	0.76347800	-0.35483100
H	-5.96675700	-0.70850000	-1.29308300
H	-5.17495300	0.68111900	-2.07560900
C	-0.17774600	-2.85486300	-0.34388200
C	0.80896500	-2.69500200	-1.32494100
C	2.04025400	-3.33543800	-1.19298100
H	2.80421500	-3.19713400	-1.96177600
C	2.29347200	-4.14386900	-0.08605400
H	3.25842800	-4.64499100	0.01847100
C	1.31194500	-4.30337600	0.89249400
H	1.51057100	-4.92237500	1.77050900
C	0.08417200	-3.65740100	0.77222600
C	-3.09314500	1.71817000	-0.29864100
C	-3.07434400	2.49620000	-1.46300500
C	-3.16327600	3.88337400	-1.37868100
H	-3.14695000	4.48173900	-2.29280500
C	-3.25567900	4.50782800	-0.13494700
H	-3.31928300	5.59642500	-0.07127200
C	-3.25359200	3.73635400	1.02625500
H	-3.31502100	4.21813900	2.00494200
C	-3.17050000	2.34752000	0.95031500
C	3.32967000	1.12674700	-0.61656100
C	4.25223800	0.08809700	-0.80680400
C	5.44509600	0.31653500	-1.48790500
H	6.15287100	-0.50451100	-1.62808200
C	5.73447000	1.58254100	-1.99685000
H	6.66933900	1.76030600	-2.53310600
C	4.81814500	2.61784900	-1.81916500
H	5.03256100	3.61291400	-2.21701600
C	3.62654300	2.39428200	-1.13260300
C	3.92529600	1.43262000	2.35981400
H	4.08997900	2.45175800	1.97712800
H	4.73508700	0.79672500	1.97245100
H	4.00738100	1.46223600	3.45836200
C	2.03651900	-0.98488000	2.45129000
H	0.99786600	-1.33086100	2.34922900
H	2.30595200	-1.06485500	3.51697900
H	2.68999500	-1.65981700	1.87771100
C	0.92586700	1.90435200	2.64040600
H	0.95511300	2.90600900	2.18402900
H	1.12401100	2.01402400	3.71921700
H	-0.08682100	1.48880400	2.53724400
H	-3.15728900	1.73080400	1.85215500
H	-2.96995100	2.00200500	-2.43179100
H	-0.67345700	-3.73621800	1.55471300
H	0.59949100	-2.06471100	-2.19405800
H	4.01043700	-0.90389900	-0.41730000
H	2.90695100	3.20261400	-0.98332600

Cartesian coordinates of the optimized geometry of **S3** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.00005700	1.52544800	0.00020900
C	-1.51702500	0.25177300	0.04508800
C	-1.48543900	-1.01511400	0.65681700
C	-2.62672600	-1.81184200	0.71852000
H	-2.58560300	-2.78872500	1.20734700
C	-3.82100100	-1.36602000	0.15064500
H	-4.71381200	-1.99526800	0.19102000
C	-3.87778000	-0.11253600	-0.45847600
H	-4.81442800	0.24201300	-0.89617200
C	-2.74095600	0.69246000	-0.49028700
H	-2.80532600	1.68825500	-0.94267400
H	-0.55495700	-1.38240400	1.09875300
C	1.51699000	0.25162800	-0.04520600
C	1.48517500	-1.01558300	-0.65626200

C	2.74115300	0.69260600	0.48944300
C	2.62643000	-1.81234300	-0.71796400
H	0.55451800	-1.38306500	-1.09764900
C	3.87797800	-0.11237900	0.45756500
H	2.80565300	1.68862700	0.94130200
C	3.82094500	-1.36619200	-0.15084800
H	2.58510800	-2.78949500	-1.20623200
H	4.81480800	0.24241700	0.89466600
H	4.71374200	-1.99545200	-0.19126200

Cartesian coordinates of the optimized geometry of **S4** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.33724700	-1.37831200	0.00038400
C	-1.33391900	-0.31579500	0.00014400
C	-1.44691800	1.08848400	0.00043400
C	-2.68972100	1.71532600	0.00028000
H	-2.75241100	2.80650200	0.00047300
C	-3.85673800	0.94876600	-0.00009100
H	-4.83283500	1.44074800	-0.00018500
C	-3.77702000	-0.44317700	-0.00035500
H	-4.68944700	-1.04473200	-0.00066600
C	-2.52904500	-1.06301100	-0.00024500
H	-2.47283000	-2.15654000	-0.00045600
H	-0.54660000	1.70625500	0.00071300
Si	2.04168300	0.41621600	-0.00009400
C	1.95133300	1.50295400	1.55132400
H	2.77591700	2.23557100	1.54479800
H	1.00381500	2.05672000	1.62865500
H	2.05565000	0.89298800	2.46267400
C	3.73091200	-0.43448300	-0.00004800
H	3.85419700	-1.07433800	-0.88827300
H	4.54714900	0.30679200	-0.00039800
H	3.85449700	-1.07385000	0.88848400
C	1.95039800	1.50141200	-1.55253900
H	1.00305700	2.05560400	-1.62913000
H	2.77533800	2.23365000	-1.54752500
H	2.05333200	0.89073000	-2.46355500

Cartesian coordinates of the optimized geometry of **S5** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.50319400	-1.19067500	-2.28738600
Ge	-0.24038200	-2.55619300	-0.43594400
Ga	3.35837300	1.23404500	0.31631700
Ga	-3.47855900	0.55286600	0.95679000
Cl	3.72738000	3.41068900	0.65220700
Cl	-4.19058900	0.85907100	3.04628900
N	3.23868700	0.42858200	2.10153400
N	5.07817400	0.43184600	-0.15700900
N	-3.46117800	2.34793200	0.17233100
N	-5.03752300	-0.07789500	-0.06256200
C	4.31838900	-0.02119600	2.73191900
C	5.58240600	-0.15309000	2.12106300
H	6.38920900	-0.46674400	2.78217500
C	5.92914200	-0.00562500	0.77290100
C	4.24057400	-0.41825000	4.17993300
H	3.93976900	-1.47297900	4.27537900
H	3.50263300	0.18472300	4.72520100
H	5.22566100	-0.30650200	4.65039400
C	7.34133900	-0.35034200	0.38572200
H	7.99555300	-0.30596200	1.26512600
H	7.71912400	0.33706200	-0.38408100
H	7.40623400	-1.36762900	-0.02898300
C	1.95981800	0.43176800	2.72164200
C	1.24001900	1.62996500	2.80166200
C	-0.02478700	1.64629000	3.38565700
H	-0.58257800	2.58333100	3.42635100
C	-0.58439100	0.47658400	3.89770600

H	-1.58934500	0.49383900	4.32393000
C	0.12604100	-0.71950400	3.80126800
H	-0.31188000	-1.65104500	4.16786100
C	1.16520900	-3.18107400	0.78119500
C	1.38434400	-0.74855400	3.20712700
C	5.40179800	0.44476900	-1.53410800
C	5.33666500	1.65179600	-2.24075600
C	5.55863000	1.66894800	-3.61618800
H	5.50563700	2.61711500	-4.15652700
C	5.84976900	0.48962900	-4.29992800
H	6.02164000	0.50636800	-5.37841300
C	5.91360900	-0.71447300	-3.59816900
H	6.12696600	-1.64651200	-4.12700100
C	5.68457400	-0.74025800	-2.22600300
C	-4.44678800	2.83853900	-0.56461900
C	-5.59065100	2.10228200	-0.92911800
H	-6.34913500	2.65306000	-1.48348000
C	-5.85545700	0.74227200	-0.72193400
C	-4.34046100	4.25148100	-1.06165100
H	-4.25516000	4.95838500	-0.22359000
H	-5.20735400	4.52322900	-1.67489900
H	-3.42441900	4.36597300	-1.66105500
C	-7.13819100	0.20276600	-1.29529200
H	-7.58221200	-0.55056900	-0.62963800
H	-6.96912900	-0.28567700	-2.26718400
H	-7.85565100	1.01777500	-1.45106700
C	-2.34331700	3.15387800	0.52680500
C	-2.41373500	3.98715700	1.64839700
C	-1.30972600	4.75515700	2.01433500
H	-1.37152700	5.40576900	2.89022300
C	-0.12685000	4.67994000	1.27913700
H	0.74879000	5.26390500	1.57132000
C	-0.05239200	3.83427900	0.17352800
H	0.88438600	3.76426900	-0.38305400
C	-1.15508500	3.07105200	-0.20573200
C	-5.24824900	-1.47680100	-0.02274700
C	-5.38844200	-2.11648100	1.21506400
C	-5.48127700	-3.50519300	1.27671400
H	-5.58632200	-3.99274500	2.24885100
C	-5.43872400	-4.27030900	0.11228900
H	-5.50664800	-5.35908400	0.16557500
C	-5.30270200	-3.63574200	-1.12259000
H	-5.25691900	-4.22595400	-2.04099800
C	-5.20322200	-2.24913700	-1.19165100
C	1.89352900	0.87202000	-0.94376200
H	1.04895100	0.56728500	-0.29790300
H	1.58578200	1.83312400	-1.37996600
C	2.15295800	-0.15872200	-2.05490900
H	2.95067200	-0.87375400	-1.80445300
H	2.49055100	0.32664500	-2.98413900
C	-1.80325000	-0.42817000	0.66652000
H	-1.40999100	0.03312500	-0.25436700
H	-1.09815600	-0.14374300	1.46012900
C	-1.85373200	-1.95135600	0.51486500
H	-2.71472300	-2.28896500	-0.08165000
H	-1.94763600	-2.44750500	1.49391200
C	0.43754200	-3.03506000	-3.07144500
H	0.08394000	-3.11264500	-4.11164600
H	1.46293300	-3.43965500	-3.04188300
C	-0.46291400	-3.75300800	-2.03726800
H	-0.21631000	-4.81661000	-1.89137400
H	-1.52368200	-3.70189200	-2.33651600
C	-0.88355400	0.02327400	-2.96048400
C	-0.53824200	1.26078800	-3.52047300
C	-1.51784600	2.17113700	-3.92154100
H	-1.22403600	3.13320000	-4.34922000
C	-2.86644400	1.85723800	-3.76627100
H	-3.63809200	2.57117100	-4.06468200
C	-3.22856700	0.62531700	-3.22101900

H	-4.28520500	0.38310500	-3.08933100
C	-2.24735200	-0.28026200	-2.82537800
C	2.50548200	-2.81155900	0.60010600
C	3.49958200	-3.23825500	1.48090400
H	4.53344300	-2.91714300	1.33045900
C	3.16702700	-4.04910200	2.56579700
H	3.94177100	-4.38341500	3.26058000
C	1.83820700	-4.42979700	2.76137800
H	1.57056000	-5.06392300	3.61058800
C	0.84997600	-3.99772500	1.87693300
H	-3.33508100	4.00786100	2.23441800
H	-1.10619800	2.40653700	-1.07094700
H	-5.40793600	-1.50916000	2.12343300
H	-5.05768500	-1.75677100	-2.15528800
H	0.51504400	1.53002100	-3.64013200
H	-2.55359200	-1.23154200	-2.38014400
H	-0.18749800	-4.29789000	2.05377800
H	2.78253400	-2.16005900	-0.23125400
H	1.91865500	-1.69219400	3.10275400
H	1.68483700	2.54894900	2.41271600
H	5.69064700	-1.68874700	-1.68405400
H	5.10966500	2.57188900	-1.69567500

Cartesian coordinates of the optimized geometry of Int-**1a** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.08637200	-0.97327800	0.70018200
Ga	-0.56751900	0.96339100	-0.67536900
Cl	-1.81187600	0.63207500	-2.49201200
N	-1.47703400	2.45111500	0.26464600
N	0.84917400	2.12730100	-1.43046300
C	-1.57370000	3.60560500	-0.40222700
C	-0.69553200	3.98425900	-1.42414800
H	-0.88975000	4.95250600	-1.88223300
C	0.51127000	3.36481500	-1.79093500
C	-2.68262900	4.56211000	-0.06514400
H	-3.61152600	4.19584100	-0.53131300
H	-2.47457000	5.56545400	-0.45512200
H	-2.87013800	4.61888300	1.01433500
C	1.46011300	4.17998600	-2.62417300
H	1.51363100	3.77576700	-3.64533600
H	2.48061300	4.14052700	-2.21867400
H	1.13194300	5.22432500	-2.67752000
C	-2.21598400	2.28421900	1.47803000
C	-1.61485000	2.66098000	2.70195600
C	-2.33514800	2.45925600	3.88211900
H	-1.88667500	2.73436100	4.83786100
C	-3.60974000	1.90256300	3.86460700
H	-4.14908200	1.74078300	4.80084200
C	-4.19392000	1.55996400	2.65303400
H	-5.19969300	1.13343700	2.63874600
C	-3.52027600	1.75615600	1.44317800
C	-0.23894100	3.30103900	2.74944400
H	0.33116300	2.88716900	1.90372700
C	-0.31151200	4.81704600	2.54410000
H	-0.68324600	5.08642500	1.54747100
H	0.68743500	5.26709600	2.65231800
H	-0.97379800	5.27906200	3.29372300
C	0.52579800	2.99650300	4.03514000
H	0.09413400	3.52449000	4.89984700
H	1.56803800	3.33779000	3.94321400
H	0.53708900	1.92149700	4.26547200
C	-4.20084200	1.39293800	0.14269700
H	-3.56735500	1.74641700	-0.68336800
C	-5.56898000	2.05879000	-0.00066700
H	-5.98750300	1.85226100	-0.99785500
H	-5.51309600	3.15094000	0.12658600
H	-6.28831900	1.67716100	0.74122300
C	-4.31255700	-0.11819400	-0.00665900

H	-4.98079700	-0.54878000	0.75615300
H	-3.33651200	-0.61449000	0.09045900
H	-4.70924100	-0.37425900	-0.99777500
C	2.17363800	1.67613100	-1.72106000
C	3.13976500	1.74490000	-0.69471200
C	4.46300600	1.42449300	-1.00445300
H	5.22408200	1.48883500	-0.22493800
C	4.82311000	1.02790600	-2.28733100
H	5.86475400	0.78822900	-2.51498700
C	3.85126300	0.91749900	-3.27391100
H	4.13519400	0.57792400	-4.27267100
C	2.51339100	1.23181700	-3.01604000
C	2.76550100	2.22155000	0.69385400
H	1.69464700	2.00114600	0.81827200
C	2.94080500	3.73576300	0.81970100
H	2.28726800	4.28572600	0.12741700
H	3.98250500	4.02580700	0.60833500
H	2.69907600	4.07073300	1.84009700
C	3.50367100	1.48606600	1.80463800
H	3.38492100	0.39847000	1.71199100
H	3.10778400	1.79043500	2.78486700
H	4.58104100	1.71605000	1.80747400
C	1.47801400	1.04421300	-4.10784100
H	0.54058000	1.51502700	-3.77610300
C	1.88559800	1.67398000	-5.43881800
H	1.05820100	1.60140300	-6.16104700
H	2.75266000	1.16249900	-5.88552400
H	2.15053700	2.73733100	-5.33443700
C	1.18030100	-0.44362700	-4.28619100
H	0.84501000	-0.89210900	-3.34291500
H	2.07515100	-0.99057300	-4.62458400
H	0.37972600	-0.59527500	-5.02608300
C	0.29266600	-2.87559800	0.33414100
C	1.55149400	-3.44168300	0.63892700
C	1.75881500	-4.82127900	0.49423600
H	2.74484900	-5.22636800	0.73617300
C	0.75102000	-5.65713700	0.03674400
H	0.92795300	-6.72913000	-0.07962700
C	-0.48255300	-5.10662300	-0.28186500
H	-1.29070900	-5.74137800	-0.65464000
C	-0.72809300	-3.73426000	-0.13668100
C	2.76159500	-2.68897000	1.08150500
C	3.17231400	-2.75073700	2.42642900
C	4.40054000	-2.19155600	2.78776000
H	4.70947800	-2.22817900	3.83700600
C	5.25282700	-1.61561900	1.84322200
C	4.83425000	-1.58902400	0.51216600
H	5.48869400	-1.15538800	-0.24799000
C	3.59599700	-2.09909600	0.11529400
C	2.32840100	-3.44589300	3.45790400
H	2.41766100	-4.54102600	3.36992800
H	1.25964200	-3.21477700	3.33889300
H	2.63533900	-3.16590900	4.47559000
C	6.56164300	-1.00476100	2.25086200
H	6.97866900	-1.49413100	3.14311100
H	6.43627800	0.06432300	2.49436400
H	7.30618600	-1.07011600	1.44381900
C	3.17303600	-2.03015200	-1.32142600
H	2.72712700	-2.97587000	-1.66233300
H	4.01749300	-1.77791500	-1.97505300
H	2.41208500	-1.24545500	-1.46255900
C	-2.10424600	-3.31937800	-0.54193800
C	-3.18719200	-3.53473100	0.33424400
C	-4.48683200	-3.37326100	-0.14475200
H	-5.32511200	-3.54784000	0.53684900
C	-4.74633200	-2.99894300	-1.46625200
C	-3.65978600	-2.77819700	-2.31090100
H	-3.83615500	-2.47736000	-3.34760000
C	-2.34237800	-2.94765300	-1.87596100

C	-2.95113000	-3.97181500	1.75014300
H	-3.89234800	-4.01078600	2.31581600
H	-2.26673000	-3.28269700	2.26434900
H	-2.48384400	-4.96838300	1.79116600
C	-6.15522600	-2.79767900	-1.94203100
H	-6.22382600	-2.85024200	-3.03800800
H	-6.53518200	-1.80808900	-1.63476700
H	-6.83619500	-3.55067600	-1.51777200
C	-1.20730100	-2.82336500	-2.84693900
H	-0.87504900	-3.81941500	-3.18483700
H	-0.33424100	-2.34275400	-2.38782100
H	-1.49805400	-2.23438500	-3.72602700
C	-0.85890900	-0.82595000	2.51524600
C	0.58049100	-0.39756100	2.46192300
H	-1.62879100	-0.07822600	2.72357500
H	-1.05663000	-1.79202400	2.99102100
H	0.77932200	0.67249100	2.54967100
H	1.33566700	-1.00589100	2.96414900

Cartesian coordinates of the optimized geometry of Int-**1b** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.95062900	0.40921600	0.23506200
Ga	1.25727100	0.01215300	-0.66332800
Cl	1.49328600	-0.14708800	-2.87226800
Si	-2.72863900	-1.63264800	-1.52269000
N	2.40160800	-1.48411000	-0.08260400
N	2.52815900	1.41558600	-0.17061800
N	-2.56817100	-0.33960800	-0.32907100
C	3.71838900	-1.34426500	-0.18420900
C	4.35359400	-0.12360900	-0.49122100
H	5.42602200	-0.18522900	-0.67220100
C	3.82030000	1.16619200	-0.41698800
C	4.62388400	-2.52445900	0.02804800
H	4.88666800	-2.96216500	-0.94733900
H	4.14734000	-3.30977800	0.62728600
H	5.55670400	-2.20717100	0.51139100
C	4.75240200	2.32408800	-0.63144100
H	4.51893000	2.78619000	-1.60411800
H	5.79918900	1.99851900	-0.64045400
H	4.61911700	3.10580400	0.12783500
C	1.81087000	-2.73742700	0.26233900
C	1.27546600	-2.88502000	1.56200500
C	0.67202300	-4.09852900	1.89739700
H	0.24922700	-4.23027400	2.89444500
C	0.60616900	-5.14441800	0.98266900
H	0.13222400	-6.08777700	1.26335800
C	1.13183100	-4.98091200	-0.29100000
H	1.06041000	-5.79937900	-1.01110700
C	1.73115000	-3.77976600	-0.68581400
C	1.41105200	-1.77370500	2.58414500
H	1.33539000	-0.82322700	2.03238200
C	2.78900300	-1.80972600	3.24798300
H	3.60079900	-1.69043100	2.51674700
H	2.94316500	-2.76589300	3.77278200
H	2.88495000	-0.99857500	3.98645200
C	0.30237600	-1.76570800	3.62772800
H	0.38145100	-0.86490800	4.25417500
H	0.36121100	-2.63463200	4.30206000
H	-0.68924700	-1.75585200	3.15422900
C	2.22853400	-3.64404900	-2.11332000
H	2.72161800	-2.66625300	-2.21444000
C	3.23584900	-4.73622100	-2.47693100
H	3.66135700	-4.54668500	-3.47443300
H	2.75900800	-5.72854900	-2.50921200
H	4.06491100	-4.79627400	-1.75666100
C	1.06185200	-3.64762700	-3.10176600
H	0.35178200	-2.83998300	-2.88607800
H	0.51718000	-4.60496800	-3.07140000

H	1.43107900	-3.49756500	-4.12780000
C	2.13055700	2.72132200	0.25037600
C	2.18315500	3.02335400	1.63215000
C	1.79208200	4.30001500	2.04317200
H	1.82142200	4.55601900	3.10335000
C	1.34316500	5.24683300	1.12775500
H	1.03093900	6.23523200	1.47274800
C	1.28130900	4.92689200	-0.22175500
H	0.91750900	5.66910300	-0.93624700
C	1.67741500	3.66876100	-0.68762900
C	2.63839200	1.99342700	2.65385500
H	2.33402200	1.00949500	2.26131200
C	4.16017900	1.95916000	2.82088500
H	4.54265900	2.95246500	3.10567600
H	4.67714500	1.64069000	1.90734100
H	4.43869800	1.24957300	3.61567300
C	1.98750100	2.17939400	4.02307100
H	2.39719800	3.05442200	4.55175200
H	2.18759600	1.30195700	4.65691800
H	0.89810600	2.30887000	3.95285400
C	1.58374300	3.35511600	-2.16632900
H	2.06139400	2.37967500	-2.33491700
C	2.32044700	4.38118800	-3.02580000
H	1.85011500	5.37578100	-2.97156000
H	2.30959600	4.07015400	-4.08172200
H	3.37066000	4.49507600	-2.71551100
C	0.12448200	3.21823300	-2.60129100
H	-0.40462200	4.18151600	-2.52311700
H	-0.41458200	2.49565700	-1.97101100
H	0.06236500	2.87101800	-3.64361200
C	-3.73175600	0.26284800	0.22357100
C	-4.29797600	-0.25068600	1.41874500
C	-5.47417000	0.32351900	1.91052900
H	-5.92464300	-0.07692900	2.82215100
C	-6.08182300	1.39401000	1.26537200
H	-7.00260500	1.82629100	1.66452100
C	-5.50393300	1.91639800	0.11460300
H	-5.97632900	2.76631200	-0.38536600
C	-4.33134500	1.37540300	-0.41990500
C	-3.67167600	-1.41483200	2.16866800
H	-2.64970200	-1.52837700	1.77442800
C	-4.41654700	-2.72778100	1.92112700
H	-5.46181600	-2.65643300	2.26303200
H	-3.93777600	-3.55366700	2.47145700
H	-4.43181100	-3.00015500	0.85858800
C	-3.58122600	-1.16568600	3.67469700
H	-3.10021300	-0.20576500	3.91121200
H	-2.99845500	-1.96440800	4.15954700
H	-4.57642700	-1.16112800	4.14651900
C	-3.74586100	1.98445100	-1.68154600
H	-2.78505700	1.48048300	-1.86214000
C	-3.46739500	3.48046000	-1.53609600
H	-3.01133800	3.87249100	-2.45841700
H	-2.77675900	3.68763700	-0.70745300
H	-4.39337400	4.05065900	-1.35940300
C	-4.64212600	1.73627000	-2.89569300
H	-5.61971300	2.23058400	-2.77597300
H	-4.83097400	0.66561300	-3.05308900
H	-4.17521500	2.13480800	-3.81036600
C	-4.55289000	-2.00910900	-1.77759800
H	-5.07064900	-1.17296200	-2.26822400
H	-5.08927300	-2.21805200	-0.84260000
H	-4.64344100	-2.89167000	-2.43161000
C	-1.83707500	-3.15242200	-0.87871700
H	-0.79576800	-2.92186900	-0.60942700
H	-1.81047800	-3.95858900	-1.62803900
H	-2.32577300	-3.54066900	0.02712000
C	-2.02007900	-1.12330000	-3.18521600
H	-2.61232200	-0.30297300	-3.61929400

H	-2.05604200	-1.97175000	-3.88812500
H	-0.97478400	-0.78530600	-3.12523200
C	-1.25075600	2.15870700	1.06396700
C	-1.02247000	1.05624400	2.08217700
H	-0.49893900	2.94684700	0.96897200
H	-2.27919400	2.52800800	1.00277900
H	-0.08861800	1.07553900	2.64821800
H	-1.88295900	0.76845600	2.69122400

Cartesian coordinates of the optimized geometry of Int-**2a** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-2.60024500	-0.88967200	-1.07368300
Ga	1.41632300	0.91261100	0.45264400
Cl	0.92249600	1.19962600	2.60534300
N	3.30967200	0.40853600	0.43663400
N	1.67046800	2.72391100	-0.26925000
C	4.27016000	1.33146900	0.39740000
C	4.03846700	2.69878400	0.18306200
H	4.92208100	3.33463900	0.21118100
C	2.84708500	3.33717800	-0.20280000
C	5.69909500	0.90363800	0.57754700
H	6.38899100	1.71461900	0.31745400
H	5.87386300	0.61821000	1.62522700
H	5.93140200	0.01823000	-0.03023900
C	2.94716100	4.79556300	-0.55091500
H	2.77125800	5.39251600	0.35788500
H	3.94837900	5.04191900	-0.92525800
H	2.19285600	5.09583400	-1.28908000
C	3.65496500	-0.97711700	0.47705600
C	3.94694300	-1.61836700	1.69909500
C	4.33026400	-2.96401000	1.66041200
H	4.56351900	-3.47636700	2.59692100
C	4.42676000	-3.65699000	0.46054200
H	4.74336700	-4.70272600	0.45480000
C	4.09756000	-3.01995100	-0.73134100
H	4.14971500	-3.57336000	-1.67115300
C	3.68840900	-1.68509400	-0.74536900
C	3.84746600	-0.91803500	3.04164100
H	3.59775600	0.13705500	2.85429100
C	5.16103400	-0.97531700	3.82347800
H	5.08354900	-0.37581400	4.74348200
H	5.40715200	-2.00605900	4.12393500
H	6.01378400	-0.59382100	3.24198500
C	2.70889800	-1.50295500	3.87868100
H	2.62491200	-0.96558800	4.83571500
H	1.74505700	-1.40544700	3.36318900
H	2.88355600	-2.56821700	4.10069700
C	3.31645300	-1.01215100	-2.05280500
H	2.70034200	-0.13848600	-1.79458200
C	4.54881200	-0.48357200	-2.78742200
H	5.09864200	0.25329900	-2.18429400
H	5.24157700	-1.30412800	-3.03440000
H	4.25702900	0.00819700	-3.72896700
C	2.47402200	-1.90924500	-2.95463400
H	1.60484500	-2.31786400	-2.41850600
H	2.10559100	-1.33848300	-3.82024300
H	3.05555400	-2.75601200	-3.35157500
C	0.52755700	3.36335700	-0.83998000
C	-0.30012200	4.19398900	-0.05832000
C	-1.42757700	4.75986400	-0.66371500
H	-2.07769000	5.40913500	-0.07187100
C	-1.73825900	4.50829600	-1.99319900
H	-2.62255900	4.96160900	-2.44753300
C	-0.92207100	3.67099800	-2.74628500
H	-1.17800000	3.46717500	-3.78743800
C	0.21634700	3.08441600	-2.19058100
C	-0.02537500	4.48264700	1.40433100
H	0.88483500	3.93538100	1.69052100

C	0.20168700	5.97376500	1.65806300
H	0.48066500	6.14664700	2.70907400
H	0.99705100	6.38780600	1.02129200
H	-0.71189800	6.55671700	1.45957400
C	-1.15638100	3.95582500	2.28618500
H	-0.89782900	4.06757600	3.35024500
H	-2.09169700	4.50963400	2.10447400
H	-1.33850200	2.89020700	2.09733300
C	1.11012700	2.19542300	-3.03376600
H	1.62940700	1.51676800	-2.34086700
C	2.18995000	3.01140400	-3.74680200
H	2.82521600	3.55814000	-3.03586100
H	2.84381800	2.35371900	-4.34115600
H	1.73661000	3.74790200	-4.42947600
C	0.33443700	1.33430800	-4.02558700
H	-0.47630100	0.77450800	-3.53487400
H	-0.11163500	1.93613700	-4.83269200
H	1.00860900	0.60830300	-4.50443300
C	-3.06453100	-2.03667200	0.52438400
C	-2.56221700	-3.31973100	0.78551800
C	-3.04417100	-4.03751900	1.88779000
H	-2.64461500	-5.03489900	2.09201600
C	-4.03044100	-3.49795100	2.71174500
H	-4.40602600	-4.07402900	3.56097900
C	-4.54458700	-2.22847600	2.44872300
H	-5.32846900	-1.80657300	3.08391100
C	-4.06026200	-1.50164500	1.36018000
C	-1.52181400	-3.90184300	-0.10835200
C	-0.17047800	-3.89225900	0.28149000
C	0.78785100	-4.43256900	-0.58130000
H	1.83637100	-4.41232800	-0.27595600
C	0.44224700	-4.98106200	-1.81660600
C	-0.90629800	-4.98338900	-2.18219400
H	-1.20126400	-5.41530200	-3.14366200
C	-1.89593300	-4.45761100	-1.34993600
C	0.25437500	-3.32089900	1.60437000
H	-0.24165200	-2.36123600	1.81414700
H	-0.01221400	-3.99340200	2.43591000
H	1.34166800	-3.16539100	1.63208800
C	1.48516100	-5.55131800	-2.73433300
H	1.54244200	-4.98177300	-3.67610900
H	2.48102000	-5.53348100	-2.26956300
H	1.25592200	-6.59477400	-3.00240100
C	-3.33632700	-4.49081400	-1.77292900
H	-3.98381400	-4.86649200	-0.96660100
H	-3.69537300	-3.47873900	-2.02567200
H	-3.47379200	-5.12620600	-2.65883600
C	-4.52488500	-0.13686700	0.98226100
C	-4.11832400	0.98828900	1.73736500
C	-4.41493200	2.26163500	1.26045600
H	-4.08949300	3.12838400	1.84177700
C	-5.09418400	2.46739000	0.05201200
C	-5.51732800	1.35056700	-0.65898900
H	-6.08141600	1.48567700	-1.58655900
C	-5.26353200	0.04337800	-0.21002000
C	-3.35171600	0.82170300	3.01762800
H	-3.16918400	1.79386500	3.49461100
H	-3.88716800	0.18143300	3.73320900
H	-2.37364800	0.34531900	2.84365000
C	-5.33903500	3.85776300	-0.45478600
H	-6.08142400	3.86940200	-1.26515100
H	-5.69492800	4.52171700	0.34759900
H	-4.40578000	4.29183100	-0.84808000
C	-5.91707500	-1.10866800	-0.92759500
H	-6.95736900	-1.21546800	-0.57630700
H	-5.94791000	-0.93593700	-2.01243800
H	-5.41208300	-2.06452700	-0.74015900
C	0.06060800	-0.17065700	-0.47054100
H	0.17925500	-1.21331300	-0.13170800

H	0.26225000	-0.18251100	-1.55403700
C	-1.34441300	0.37412200	-0.16218900
H	-1.51167500	0.43307900	0.92099600
H	-1.47589900	1.38584300	-0.57780500

Cartesian coordinates of the optimized geometry of Int-**2b** at PBE0-D3BJ/def2-SVP level of theory:

Ge	2.18835900	-2.13852900	0.90930000
Ga	-1.76761500	0.05246100	-0.51891000
Cl	-1.34389000	-0.24965900	-2.69090700
Si	5.31481300	-2.23699900	0.98157300
N	-2.09350100	1.98068700	-0.38119300
C	-3.41974300	3.96463800	-0.91867300
H	-3.02284400	4.25927400	-1.90226100
H	-2.84570400	4.51877800	-0.16419800
H	-4.47367900	4.26311100	-0.87123300
N	-3.63673100	-0.48561700	-0.31031200
C	-3.27019400	2.47975600	-0.74913800
N	3.83173100	-1.36002800	0.49881800
C	-4.41194900	1.69348500	-0.99231900
H	-5.29248800	2.23695700	-1.33119000
C	-4.61127000	0.33577900	-0.69774500
C	-6.00992000	-0.20068100	-0.79511700
H	-6.04438900	-1.04193600	-1.50267900
H	-6.71179800	0.57477600	-1.12250000
H	-6.34238700	-0.59971700	0.17398000
C	-1.01328000	2.83580300	-0.00081100
C	-0.78937900	3.05378400	1.37862200
C	0.26039700	3.89474400	1.75509700
H	0.44259800	4.08652600	2.81345400
C	1.08937200	4.48195400	0.80460800
H	1.91102300	5.12941600	1.12010100
C	0.87869300	4.22785300	-0.54262800
H	1.54687200	4.66976400	-1.28525900
C	-0.16995200	3.40858300	-0.97522200
C	-1.67447200	2.40448200	2.42816000
H	-1.96269100	1.41808000	2.03042100
C	-0.95451400	2.16924700	3.75173400
H	-1.58912500	1.58124700	4.42961500
H	-0.72509500	3.11411300	4.26865000
H	-0.01114200	1.62213500	3.60986400
C	-2.96796400	3.18905800	2.65579600
H	-3.57625900	3.25665600	1.74380800
H	-2.74878600	4.21335400	2.99720900
H	-3.58426700	2.69958400	3.42669300
C	-0.33506700	3.15183600	-2.46025300
H	-1.22368500	2.51942100	-2.60024800
C	0.85930800	2.37099200	-3.00649600
H	1.03943300	1.45519600	-2.42876500
H	1.77853300	2.97536600	-2.97064100
H	0.68062200	2.07585600	-4.05166200
C	-0.53156700	4.44568100	-3.25180100
H	-0.73448500	4.21854800	-4.30979200
H	0.36985900	5.07801300	-3.21910500
H	-1.36689700	5.04997100	-2.86736800
C	-3.94879700	-1.77620800	0.21720900
C	-3.99015700	-2.90653800	-0.62520300
C	-4.29346500	-4.14745500	-0.05588200
H	-4.32898000	-5.03115500	-0.69776200
C	-4.54678600	-4.27878900	1.30348700
H	-4.78479400	-5.25758700	1.72645900
C	-4.48557600	-3.15881600	2.12398500
H	-4.67431300	-3.26500400	3.19529800
C	-4.18153700	-1.89787000	1.60460200
C	-3.69187700	-2.82473700	-2.10833000
H	-3.54052200	-1.76672300	-2.36583600
C	-2.38662200	-3.55228500	-2.43302500
H	-2.47292600	-4.63367700	-2.23865100

H	-1.55416100	-3.16143800	-1.83077200
H	-2.11988800	-3.41153000	-3.49127300
C	-4.84228700	-3.35671200	-2.96226800
H	-5.00873800	-4.43356900	-2.80026500
H	-4.62139200	-3.21430800	-4.03131300
H	-5.78966300	-2.84070300	-2.74254800
C	-4.10759900	-0.70651100	2.54041000
H	-3.78555700	0.16104100	1.94568300
C	-3.06744900	-0.92835500	3.63705200
H	-3.32347900	-1.79342800	4.26826200
H	-3.00729500	-0.04885200	4.29538300
H	-2.06896300	-1.10856900	3.21240200
C	-5.47255900	-0.36705100	3.13967200
H	-5.85315200	-1.19203900	3.76272100
H	-6.22134700	-0.16677100	2.35916200
H	-5.40445500	0.52908700	3.77640000
C	-0.42812900	-0.79542100	0.64205000
H	-0.37072100	-0.24551400	1.59669800
H	-0.81731400	-1.79820000	0.89697000
C	0.94705900	-0.87948000	-0.02237400
H	1.39597700	0.11672100	-0.16587600
H	0.85326900	-1.30367200	-1.04073000
C	3.95879900	-0.12304000	-0.19065000
C	4.09255400	1.07087200	0.55940500
C	4.22423900	2.28518400	-0.11626200
H	4.32124900	3.21025500	0.45487300
C	4.24175400	2.33683800	-1.50579100
H	4.35544900	3.29468600	-2.01918700
C	4.10743300	1.16311500	-2.23482300
H	4.11060300	1.20591800	-3.32697800
C	3.95546300	-0.07511300	-1.60330800
C	4.06488400	1.03124400	2.07526900
H	4.48039300	0.05774900	2.37552600
C	4.91604000	2.11301100	2.73186200
H	5.94112100	2.12176100	2.33086800
H	4.97508100	1.94317700	3.81800400
H	4.48928300	3.11811900	2.58653600
C	2.62973500	1.08630000	2.59799000
H	2.03006400	0.23640100	2.23822600
H	2.12344900	2.00031400	2.25233400
H	2.60871300	1.06841500	3.69939100
C	3.81876300	-1.32370000	-2.45202600
H	3.58111600	-2.15301200	-1.76868800
C	2.68604500	-1.22049000	-3.47316100
H	2.56764200	-2.17399300	-4.01158300
H	2.89051200	-0.44409900	-4.22744500
H	1.72200000	-0.97491600	-3.00452900
C	5.14187900	-1.66101600	-3.14180700
H	5.06526200	-2.60800700	-3.69957000
H	5.96386300	-1.75724400	-2.41707500
H	5.42509000	-0.87243100	-3.85735200
C	5.45313200	-3.83631300	0.00380200
H	4.56918400	-4.46853200	0.18516000
H	6.34483600	-4.40624900	0.31117000
H	5.52295700	-3.65127600	-1.07825700
C	5.22545800	-2.68031500	2.80692500
H	4.33976100	-3.30035000	3.01609500
H	5.17092200	-1.78449300	3.44450200
H	6.11864600	-3.25405600	3.10282100
C	6.79257000	-1.12957500	0.65153800
H	6.84469500	-0.82926000	-0.40578300
H	7.72340100	-1.66104600	0.90586800
H	6.74795000	-0.20952300	1.25361900

Cartesian coordinates of the optimized geometry of Int-**3b** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.05806000	-0.53743700	2.08257500
Ga	-4.99813100	-0.10827300	-0.64654300

Cl	-6.32977400	-1.24337900	0.73770600
Si	0.84160500	-2.86521200	3.00580500
N	-5.41236300	-0.84625000	-2.42064000
C	-6.90635500	-1.16330600	-4.33205100
H	-7.24807700	-2.18232500	-4.10083100
H	-6.05146800	-1.27042800	-5.01503600
H	-7.71457100	-0.62817100	-4.84351700
C	-2.40140100	3.01843900	1.70475800
H	-3.36846400	3.08243600	2.22503600
H	-2.37944400	2.07305200	1.14831300
H	-2.37197900	3.82823400	0.96280700
C	-1.29514400	2.18595100	4.44005400
H	-0.57681800	2.42325100	5.23727800
H	-1.24610600	1.09905500	4.26190100
H	-2.30770800	2.41910600	4.80731800
Ge	0.54505400	1.03504000	0.95201600
Ga	4.97509100	-0.05992600	-0.49639200
Cl	6.08759900	0.99813300	1.11591500
Si	-0.94499000	3.17151900	2.86990700
N	-5.93480400	1.59739300	-0.91991700
C	-6.50050900	-0.44937500	-3.07428400
N	-0.72799600	-2.35826900	2.31294900
C	-7.29843300	0.63523300	-2.67045800
H	-8.19969500	0.80062700	-3.25796100
N	0.50378400	2.61371300	2.02086000
C	-6.99170500	1.63435800	-1.73655200
N	5.70867800	0.71041700	-2.15846500
C	-7.89949600	2.83121400	-1.69660100
H	-8.32315400	2.95145400	-0.68898500
H	-8.71658000	2.72913400	-2.41976900
H	-7.34575200	3.75686600	-1.90847900
N	5.90840600	-1.78081900	-0.65487700
C	-4.59624500	-1.87400600	-2.98365600
C	-3.41879900	-1.49822900	-3.66479800
C	-2.67822100	-2.49183400	-4.31013300
H	-1.77156300	-2.21824300	-4.85305600
C	-3.07656100	-3.82308500	-4.26939100
H	-2.49079100	-4.58606100	-4.78740400
C	-4.19867300	-4.18431800	-3.53478400
H	-4.48087300	-5.23765300	-3.46610900
C	-4.96980600	-3.22884300	-2.86583900
C	-2.97500300	-0.04914300	-3.71965300
H	-3.39493200	0.44804100	-2.83211400
C	-1.46019800	0.10327200	-3.64270600
H	-1.18621400	1.16278000	-3.53527400
H	-0.96050900	-0.26928700	-4.54997800
H	-1.04406200	-0.43582500	-2.77866400
C	-3.54656300	0.66611400	-4.94415000
H	-4.64632500	0.67113500	-4.93525600
H	-3.21601300	0.17569600	-5.87372100
H	-3.20963100	1.71412800	-4.97575700
C	-6.12311800	-3.67805900	-1.99004400
H	-6.67674200	-2.78371400	-1.66802400
C	-5.57328600	-4.33768200	-0.72481500
H	-4.87761800	-3.67633400	-0.19202000
H	-5.03505600	-5.26791900	-0.96793700
H	-6.38851900	-4.58345700	-0.02748700
C	-7.09613100	-4.61342100	-2.70591500
H	-7.95255000	-4.84092600	-2.05301300
H	-6.62226000	-5.57286200	-2.96701300
H	-7.48959300	-4.17788400	-3.63732000
C	-5.57403100	2.80515600	-0.24251000
C	-6.10963400	3.10603800	1.02675000
C	-5.81436700	4.35088800	1.59219100
H	-6.22632900	4.60019200	2.57307900
C	-5.01775000	5.27678400	0.92997500
H	-4.80966000	6.24795700	1.38493600
C	-4.46776600	4.95100200	-0.30377700
H	-3.82034200	5.67054200	-0.81166000

C	-0.72629200	4.97773200	3.33712100
H	-1.62232500	5.33006700	3.87324800
H	-0.59389000	5.60282800	2.44119100
H	0.14943100	5.13704400	3.98366100
C	-4.71952400	3.71415300	-0.90316900
C	-6.96884200	2.12133200	1.79398600
H	-7.19977800	1.27993300	1.12482400
C	-6.18752300	1.54494600	2.97524300
H	-5.92740200	2.33038300	3.70362900
H	-5.25533800	1.07040200	2.63937400
H	-6.77808500	0.77405100	3.49268500
C	-8.29193100	2.72700100	2.25927800
H	-8.14075900	3.52511500	3.00325500
H	-8.91798800	1.95394700	2.73047200
H	-8.86326900	3.15898800	1.42319300
C	-4.08588600	3.39127000	-2.24354100
H	-4.34010800	2.34849600	-2.48241700
C	-2.56225500	3.49412000	-2.18350400
H	-2.23273300	4.51573000	-1.93826600
H	-2.12004700	3.23451600	-3.15752400
H	-2.13595300	2.81908400	-1.42695100
C	-4.65279500	4.26472100	-3.36297100
H	-4.44379300	5.33127000	-3.18248200
H	-5.74253500	4.14796300	-3.45611300
H	-4.20435200	3.99480400	-4.33184000
C	-3.10023400	-0.16216500	-0.10611100
H	-2.61774400	-0.94397600	-0.71491900
H	-2.60964600	0.77867400	-0.39809700
C	-2.92173600	-0.46005400	1.38322200
H	-3.39280600	-1.42151200	1.63393900
H	-3.43323900	0.29505500	2.00046700
C	-1.76131300	-3.32945700	2.20456400
C	-1.74128700	-4.26930700	1.14836300
C	-2.70406200	-5.28105100	1.11797500
H	-2.68234800	-6.01304400	0.30627200
C	-3.69310400	-5.36496600	2.08906700
H	-4.44071000	-6.16045600	2.04942400
C	-3.74147700	-4.40793000	3.09538500
H	-4.53816500	-4.45601100	3.84124700
C	-2.79700800	-3.38095400	3.17338800
C	-0.71550200	-4.19089100	0.03620000
H	-0.03738800	-3.36305800	0.28319500
C	0.11342500	-5.46906000	-0.07843300
H	0.60962800	-5.72152600	0.87006600
H	0.89312200	-5.35588700	-0.84634700
H	-0.51201600	-6.32929400	-0.36545000
C	-1.37875000	-3.85370500	-1.29666300
H	-1.96570300	-2.92556000	-1.23684500
H	-2.06757200	-4.64897400	-1.61850100
H	-0.62622400	-3.72479000	-2.09066000
C	-2.91868300	-2.36169000	4.29250200
H	-2.28115600	-1.49949200	4.03151300
C	-4.34413800	-1.83410800	4.45441100
H	-4.35501300	-0.96953300	5.13651400
H	-5.01124000	-2.59605900	4.88760400
H	-4.77887200	-1.52257800	3.49338300
C	-2.38232900	-2.90660000	5.61566200
H	-2.47348200	-2.15382700	6.41460000
H	-1.32330100	-3.18859000	5.53511700
H	-2.94452800	-3.80194400	5.92606000
C	1.36498500	-1.63116200	4.32403800
H	1.52650500	-0.62608700	3.90683500
H	2.31129900	-1.95970800	4.78411900
H	0.60639100	-1.54585600	5.11761200
C	2.13948500	-2.92394200	1.65986500
H	2.01733500	-2.08020000	0.96841600
H	2.07909400	-3.85008700	1.07410100
H	3.15370500	-2.87069800	2.07932800
C	0.66110800	-4.57132900	3.76645200

H	-0.02488400	-4.58079000	4.62535100
H	1.65010400	-4.91409200	4.11146800
H	0.28240400	-5.29986900	3.03489600
C	1.63381800	3.47503000	2.03620900
C	1.77346300	4.46269900	1.02760000
C	2.83951300	5.36071900	1.09619600
H	2.94598400	6.12781600	0.32579500
C	3.77273400	5.29504500	2.12553800
H	4.60268700	6.00456700	2.16182600
C	3.65267700	4.30767200	3.09367700
H	4.39620500	4.24386600	3.89228700
C	2.59598100	3.39186500	3.07059300
C	0.79905000	4.52333300	-0.13250100
H	-0.13266000	4.04854000	0.20968400
C	1.32346600	3.69804500	-1.30818300
H	2.29722800	4.07325900	-1.65811700
H	0.62066300	3.71823600	-2.15666800
H	1.46572100	2.64180000	-1.02842800
C	0.46081500	5.94332800	-0.57500500
H	0.12410900	6.56201100	0.27091100
H	-0.34325400	5.92630000	-1.32744700
H	1.32220200	6.44949200	-1.03890100
C	2.49513800	2.35038000	4.16606100
H	1.66971300	1.67870500	3.88228000
C	2.14111100	2.99411500	5.50748000
H	2.95821700	3.64569800	5.85701400
H	1.97159000	2.22603000	6.27907000
H	1.23596900	3.61419600	5.43719200
C	3.77105500	1.51868500	4.29687900
H	4.60575000	2.12290800	4.68706300
H	4.09565000	1.10753100	3.33166300
H	3.61584500	0.68292500	4.99746700
C	2.50051800	0.57645100	0.99201700
H	3.02349000	1.50125900	1.27801700
H	2.69631200	-0.14054300	1.80422600
C	3.01113800	0.06338300	-0.35311500
H	2.71642900	0.75692600	-1.15960500
H	2.56151300	-0.90606500	-0.62545300
C	7.50732800	1.02361400	-3.78764300
H	6.76434400	1.28760400	-4.55282800
H	8.30502800	0.42562400	-4.24335900
H	7.94136400	1.96961200	-3.43205600
C	6.87186000	0.28866800	-2.64203200
C	7.55792000	-0.83648600	-2.14935700
H	8.53437000	-1.02256700	-2.59324400
C	7.08070100	-1.83777000	-1.29349400
C	7.94377000	-3.05593500	-1.11945000
H	8.25960800	-3.14280000	-0.06914100
H	8.83508600	-3.00139800	-1.75482200
H	7.39018300	-3.97657800	-1.35154400
C	5.02731700	1.79851500	-2.78381400
C	3.94574700	1.50668600	-3.64435900
C	3.30686100	2.56465600	-4.29500400
H	2.47433000	2.35650600	-4.96939800
C	3.71302400	3.87955600	-4.09528000
H	3.20477200	4.69492000	-4.61527400
C	4.74733200	4.15334100	-3.21038400
H	5.04132200	5.19016100	-3.03036800
C	5.41721500	3.12999300	-2.53085300
C	3.50224100	0.07616800	-3.88266700
H	3.76836300	-0.49400800	-2.97987800
C	1.99448500	-0.05193900	-4.06502800
H	1.44787300	0.44042200	-3.24771400
H	1.69886900	-1.11137600	-4.07473500
H	1.65260200	0.38722200	-5.01533700
C	4.25874200	-0.56021100	-5.04908900
H	4.08968800	0.00413900	-5.98005100
H	3.91947700	-1.59516200	-5.21359300
H	5.34185700	-0.59200700	-4.86296700

C	6.48626800	3.49151800	-1.51819000
H	6.95059300	2.55970200	-1.16291500
C	7.57945100	4.38613100	-2.10284800
H	7.18610800	5.37697200	-2.37996500
H	8.04117900	3.95518100	-3.00430000
H	8.37516500	4.54804000	-1.35966500
C	5.84358800	4.15926700	-0.30352300
H	6.59306700	4.34381900	0.48109400
H	5.05894500	3.53184200	0.13786000
H	5.39004700	5.12477800	-0.57791500
C	5.40494200	-2.97988900	-0.06157700
C	5.74886300	-3.33498400	1.25850200
C	5.31294400	-4.57224100	1.74456000
H	5.57593400	-4.86564300	2.76369100
C	4.55378600	-5.43199800	0.96022600
H	4.23132300	-6.39732500	1.35744400
C	4.18543900	-5.04762300	-0.32412300
H	3.56772400	-5.71544200	-0.92922100
C	4.58963900	-3.81883800	-0.85179400
C	6.52973600	-2.40443300	2.16478500
H	6.90943400	-1.57445200	1.55094100
C	7.72434600	-3.08544600	2.82959500
H	8.31122300	-2.34956600	3.40014500
H	8.39470300	-3.55320800	2.09201100
H	7.41063800	-3.87104100	3.53514300
C	5.60070000	-1.78667100	3.21128900
H	6.14403900	-1.05775500	3.83106000
H	5.17830100	-2.55941500	3.87467600
H	4.76792400	-1.24921700	2.73717700
C	4.17947400	-3.42222800	-2.25728600
H	4.40452900	-2.35135500	-2.36584700
C	4.99908300	-4.16403300	-3.31366800
H	4.69393100	-3.86118500	-4.32752300
H	4.85813900	-5.25363800	-3.22917500
H	6.07380500	-3.95435200	-3.21410300
C	2.68270800	-3.60333700	-2.49596800
H	2.08550500	-3.07921600	-1.73486700
H	2.39015200	-4.66465100	-2.48099400
H	2.40203700	-3.20677200	-3.48356000

Cartesian coordinates of the optimized geometry of Int-4 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.52255800	-1.33529800	-1.08120700
Ga	0.56099400	0.30122800	0.35295000
Cl	0.51524700	0.18759700	2.58230300
N	2.38835500	0.84394500	-0.06849900
N	-0.23524200	2.05034700	-0.04672400
C	2.76243000	2.11568300	-0.20075900
C	1.87059100	3.19757400	-0.22055900
H	2.32189600	4.18336900	-0.32020900
C	0.46293200	3.16388400	-0.20539200
C	4.22733700	2.40977700	-0.35594400
H	4.78952100	2.03501800	0.51254500
H	4.40762600	3.48558500	-0.46200200
H	4.63333900	1.89019900	-1.23696000
C	-0.27597100	4.45849700	-0.39122400
H	-1.06194500	4.56457400	0.37093600
H	-0.78166900	4.47809400	-1.36840300
H	0.40618400	5.31490900	-0.33431800
C	3.32780200	-0.21822900	-0.10516300
C	3.58261800	-0.88249900	-1.30983100
C	4.43278200	-1.98644500	-1.33130700
H	4.62594800	-2.50198700	-2.27515500
C	5.02761500	-2.43731100	-0.15339100
H	5.68837600	-3.30684200	-0.17105000
C	4.76728400	-1.78032300	1.04897600
H	5.22037100	-2.13669800	1.97703100
C	3.91795600	-0.67619000	1.07834700

C	-1.64799600	2.00145600	-0.17348100
C	-2.23840900	1.98086100	-1.44247400
C	-3.61200000	1.79247100	-1.56779300
H	-4.06491000	1.76316000	-2.56159800
C	-4.40219600	1.61274500	-0.43315600
H	-5.47554000	1.43962600	-0.53430800
C	-3.81357900	1.63078200	0.82914800
H	-4.42459600	1.47023100	1.71978400
C	-2.44050400	1.82245100	0.96405700
C	-2.28005300	-1.70512000	-0.21697200
C	-2.52601100	-1.64119800	1.16337500
C	-3.80461300	-1.85627100	1.67670600
H	-3.96977100	-1.80558500	2.75643200
C	-4.87058400	-2.12590700	0.81894800
H	-5.87294400	-2.29273900	1.22193200
C	-4.65000900	-2.17733500	-0.55599100
H	-5.47990800	-2.38276500	-1.23760700
C	-3.36722100	-1.96721700	-1.06335100
H	3.67485500	-0.17440800	2.01735500
H	3.09296600	-0.53075900	-2.22090000
H	-1.95970700	1.79846300	1.94416100
H	-1.60424400	2.08216200	-2.32624700
H	-3.21197000	-2.00720400	-2.14687800
H	-1.71255200	-1.40360700	1.85558600
C	0.68334100	-2.56869400	0.38892100
C	0.46256300	-3.14523900	-0.89211000
H	1.67682000	-2.19755800	0.65238400
H	0.02504500	-2.79867200	1.22868300
H	1.29960900	-3.23118400	-1.58997900
H	-0.31936100	-3.90228600	-1.00409400

Cartesian coordinates of the optimized geometry of Int-5 at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.30219100	-1.60622600	0.26645900
Ga	-0.56674900	0.47232900	-0.52402900
Cl	-0.40565400	0.85839600	-2.70022000
N	-2.38380400	0.88065700	0.04760700
N	0.25406300	2.03092700	0.31012700
C	-2.75000700	2.08880600	0.47555200
C	-1.84458000	3.12941500	0.73309700
H	-2.28561800	4.07363800	1.04884900
C	-0.43740600	3.08635100	0.71661300
C	-4.20940700	2.37029700	0.70327100
H	-4.82543200	1.89924300	-0.07589800
H	-4.39411800	3.45139000	0.70993900
H	-4.54555000	1.96348400	1.66891700
C	0.31462100	4.29188900	1.20075300
H	0.96126600	4.68730900	0.40324400
H	0.98088700	4.01637300	2.03210800
H	-0.36822700	5.08153700	1.53450900
C	-3.28604000	-0.20873700	-0.03813300
C	-3.86216000	-0.75856600	1.11359400
C	-4.67268600	-1.88648200	1.02035700
H	-5.11222100	-2.31151800	1.92576700
C	-4.90461200	-2.48526300	-0.21796400
H	-5.53292200	-3.37589100	-0.28741700
C	-4.31890200	-1.94872900	-1.36363200
H	-4.48689200	-2.41685700	-2.33622300
C	-3.51169800	-0.81638200	-1.27910600
C	1.67458600	1.98484300	0.34759700
C	2.31777100	1.36103900	1.42128100
C	3.70262700	1.21576800	1.41452800
H	4.19663500	0.70712500	2.24504100
C	4.45123800	1.69194600	0.34016600
H	5.53562900	1.56347000	0.33037200
C	3.80967200	2.30864000	-0.73301300
H	4.39056000	2.66823900	-1.58562600
C	2.42378000	2.44911600	-0.73817500

C	2.20196000	-1.91364700	0.00857500
C	2.83718200	-1.31583800	-1.08918000
C	4.21111400	-1.45306800	-1.27926400
H	4.68916700	-0.97557000	-2.13826800
C	4.97258200	-2.19160000	-0.37499300
H	6.05022600	-2.29891100	-0.52225200
C	4.35218400	-2.79269200	0.72045800
H	4.94371200	-3.37242600	1.43413400
C	2.97843100	-2.65204600	0.91109700
H	-3.03896800	-0.39444500	-2.16947900
H	-3.64629500	-0.30983700	2.08581900
H	1.90422100	2.89026500	-1.59127900
H	1.71662400	0.96846100	2.24443200
H	2.50937200	-3.11812400	1.78230100
H	2.25499400	-0.72688600	-1.80513700
C	-0.80837200	-3.19292400	0.56989600
C	-0.46716600	-2.46947600	1.85635100
H	-1.84946100	-3.15584100	0.23110000
H	-0.32709400	-4.16112400	0.39517800
H	-1.28634600	-1.95710100	2.37122900
H	0.22098900	-2.96875400	2.54807200

Cartesian coordinates of the optimized geometry of Int-6 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.57531500	2.90963600	-0.48431200
Ga	0.60917500	-0.43311000	0.16624600
Cl	0.14224100	0.75254300	-1.75888500
N	2.48048900	-0.86486700	-0.10628200
N	-0.06595400	-2.22137400	-0.14938400
C	2.87722400	-1.96160700	-0.74597600
C	2.00356900	-2.99857400	-1.11332000
H	2.45102300	-3.81915200	-1.67191000
C	0.64402100	-3.14786100	-0.79336800
C	4.32965700	-2.10262400	-1.09637400
H	4.67205700	-1.22635100	-1.66709000
H	4.50999800	-3.01046100	-1.68323100
H	4.94572800	-2.14008700	-0.18556200
C	-0.02573200	-4.42585000	-1.21385000
H	-1.05187300	-4.23529900	-1.55857900
H	-0.09520700	-5.13273100	-0.37348300
H	0.54590500	-4.90948100	-2.01527600
C	3.39956800	0.15024400	0.28077000
C	4.09642500	0.04668200	1.48840200
C	4.94311800	1.07540400	1.89440900
H	5.48329900	0.98950300	2.84017200
C	5.09075800	2.21549100	1.10505700
H	5.74873700	3.02474600	1.42930600
C	4.38637600	2.32374400	-0.09297200
H	4.48596400	3.21947800	-0.71015300
C	3.54096500	1.29688400	-0.50778800
C	-1.39813700	-2.45518300	0.28710900
C	-1.67170400	-3.41286300	1.27046800
C	-2.97311700	-3.58417700	1.73382700
H	-3.17798800	-4.33353600	2.50222600
C	-4.00592100	-2.78975700	1.23609300
H	-5.02439900	-2.91755800	1.60951400
C	-3.73018800	-1.82053700	0.27355300
H	-4.52137600	-1.17294700	-0.10794200
C	-2.43226100	-1.65085400	-0.20287000
C	-2.44313400	2.18410600	-0.25144600
C	-3.09519000	2.19310500	0.99134000
C	-4.44560600	1.85975800	1.11141600
H	-4.92714200	1.87894600	2.09306500
C	-5.17911100	1.50039000	-0.01795900
H	-6.23796600	1.24319700	0.07135400
C	-4.55073200	1.47526200	-1.26473800
H	-5.11790500	1.19679300	-2.15759700
C	-3.20460400	1.82132900	-1.37457500

C	0.22226800	2.19357200	1.24149700
C	0.01423400	0.72786500	1.61635800
H	1.29721000	2.44074700	1.20772700
H	-0.20246100	2.86385700	2.01672500
H	0.54177400	0.45141700	2.54672500
H	-1.05311500	0.50382900	1.77627300
H	-2.73294100	1.81079400	-2.36306600
H	-2.54331600	2.47106700	1.89549200
H	2.96591600	1.38061600	-1.43230400
H	3.95704000	-0.84162200	2.10900300
H	-0.85333200	-4.00628900	1.68445400
H	-2.21631500	-0.88467300	-0.95114800

Cartesian coordinates of the optimized geometry of Int-7 at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.34147100	-0.79150800	-1.14604000
Ga	-0.90027100	0.71014600	0.24102500
Cl	-0.53346700	0.34305400	2.39450100
Si	1.20399300	-3.28059100	0.62101900
N	-2.82611400	0.75400200	-0.02524300
N	-0.59863300	2.60906100	-0.05460800
N	1.61746200	-1.83993900	-0.30706400
C	-3.51863000	1.87021000	-0.23646500
C	-2.93247700	3.14079600	-0.35310000
H	-3.62076400	3.96523500	-0.53093900
C	-1.57261100	3.48779000	-0.26724100
C	-5.01184000	1.76931700	-0.35608500
H	-5.43444700	1.29140000	0.54049800
H	-5.29027400	1.13077500	-1.20763100
H	-5.46784300	2.75726200	-0.48683200
C	-1.20564900	4.93455000	-0.43041200
H	-0.76210400	5.32545700	0.49754400
H	-2.08207300	5.54004100	-0.68820800
H	-0.44022700	5.05077700	-1.21206400
C	-3.45895800	-0.51584700	0.07778700
C	-3.71450400	-1.26959100	-1.07181700
C	-4.26139200	-2.54539300	-0.96203800
H	-4.45281800	-3.13056200	-1.86443900
C	-4.54752400	-3.07979800	0.29352700
H	-4.96716600	-4.08458600	0.37839500
C	-4.28101400	-2.33380200	1.44030500
H	-4.48862600	-2.75282900	2.42753400
C	-3.73467800	-1.05608500	1.33785800
C	0.76118000	3.01145200	0.06574000
C	1.62652600	2.87994400	-1.02447800
C	2.97135700	3.21549900	-0.88942600
H	3.64501200	3.09683300	-1.74062800
C	3.45919400	3.67951200	0.33034500
H	4.51594900	3.93494800	0.43475300
C	2.60061200	3.79106400	1.42331500
H	2.98187800	4.13396300	2.38810900
C	1.25613800	3.44941700	1.29800400
C	2.89043400	-1.24197400	-0.13526500
C	3.97849600	-1.65241000	-0.91967600
C	5.23462200	-1.07135800	-0.75592000
H	6.07039400	-1.40560700	-1.37635000
C	5.42631300	-0.06654800	0.19174500
H	6.41142700	0.38857600	0.32003600
C	4.35077200	0.34960200	0.97623800
H	4.48692000	1.13479600	1.72341800
C	3.09532200	-0.23145300	0.81793100
C	2.15871200	-4.75603300	-0.05279200
H	3.24353300	-4.57418600	0.00738800
H	1.90361500	-4.93902900	-1.10854900
H	1.93898300	-5.67206800	0.51910800
C	-0.64404900	-3.56675100	0.44779000
H	-1.22371500	-2.74111900	0.89052900
H	-0.92481700	-4.48919300	0.98162300

H	-0.95515600	-3.67417900	-0.60229500
C	1.64979300	-3.02699700	2.42673900
H	2.72300900	-2.80846800	2.54191200
H	1.41898600	-3.92434100	3.02310500
H	1.08293800	-2.17683700	2.83759600
C	0.84561100	-0.43955100	-3.00439100
C	-0.20507800	-1.53018800	-2.87378900
H	0.53563600	0.50000500	-3.47506600
H	1.85739900	-0.74755200	-3.28981900
H	-1.21000900	-1.31382000	-3.25182900
H	0.11476700	-2.55809900	-3.07548300
H	2.25403300	0.08619000	1.43959300
H	3.81530800	-2.43548100	-1.66373600
H	-3.48999700	-0.47484200	2.22883700
H	-3.46451600	-0.85057900	-2.04883500
H	0.58115800	3.49739200	2.15488600
H	1.23891300	2.49570600	-1.96962000

Cartesian coordinates of the optimized geometry of Int-8 at PBE0-D3BJ/def2-SVP level of theory:

Ge	1.32835000	-2.18614100	0.12309800
Ga	-1.36216700	0.27611400	-0.17147100
Cl	-0.16310600	-0.32220500	1.66871100
Si	4.11275100	-1.12368300	1.23282100
N	-3.05274400	-0.67155000	0.07436500
N	-2.05854100	2.04138000	0.25846800
N	2.82746600	-1.04759300	0.01958100
C	-4.14570900	-0.12700200	0.59119100
C	-4.24303100	1.23599100	0.92192700
H	-5.19206000	1.55370200	1.35008200
C	-3.27881200	2.24132400	0.76361400
C	-5.33951000	-1.00224500	0.84013500
H	-5.06028600	-1.85388900	1.47853800
H	-5.70949100	-1.43056000	-0.10327200
H	-6.15075900	-0.44212900	1.31899500
C	-3.65279200	3.63031600	1.19713000
H	-2.95025800	3.99616000	1.96091900
H	-4.66999300	3.65583100	1.60383600
H	-3.58588900	4.33397000	0.35432200
C	-2.99227800	-2.05152900	-0.26494200
C	-3.43462500	-2.48670400	-1.51807400
C	-3.28504100	-3.82213300	-1.88369200
H	-3.62729100	-4.15519500	-2.86631700
C	-2.68470900	-4.72652900	-1.00776000
H	-2.55586900	-5.77045800	-1.30196300
C	-2.23693400	-4.29049500	0.23797300
H	-1.74789300	-4.98748200	0.92189100
C	-2.38947900	-2.95741400	0.61333400
C	-1.14241600	3.12825600	0.17067100
C	-1.12527200	3.94958600	-0.96017600
C	-0.24292200	5.02551900	-1.02762000
H	-0.23946400	5.66720300	-1.91175800
C	0.63640100	5.27886600	0.02465600
H	1.32790700	6.12261200	-0.02972900
C	0.64318500	4.43894300	1.13812700
H	1.34443000	4.61839800	1.95635400
C	-0.23914200	3.36332200	1.21259500
C	2.86564900	0.04470700	-0.87247700
C	3.29215800	-0.13213800	-2.19840500
C	3.29103200	0.93085700	-3.09792500
H	3.61593100	0.76592000	-4.12867400
C	2.88230800	2.20048600	-2.68881100
H	2.88023000	3.03431700	-3.39475000
C	2.47919100	2.39499300	-1.36802800
H	2.14882200	3.38019800	-1.03367600
C	2.46890400	1.33096700	-0.46969200
C	5.76243800	-0.89281300	0.36121400
H	5.78807400	0.06637300	-0.17917200

H	5.93569300	-1.69653100	-0.37164500
H	6.59485800	-0.89994800	1.08299300
C	4.06358100	-2.79168000	2.09157800
H	3.13431600	-2.93399700	2.66322700
H	4.91180600	-2.86188900	2.79230900
H	4.14383800	-3.61967100	1.37068900
C	3.90336800	0.23442400	2.52204500
H	4.04118200	1.23243500	2.07836700
H	4.63842900	0.12194100	3.33551100
H	2.89286800	0.19052600	2.95844400
C	-0.31879000	-0.23780500	-1.74245700
C	0.31973400	-1.61698600	-1.55009300
H	-0.98085600	-0.22668600	-2.62683800
H	0.44332500	0.53624100	-1.91193900
H	-0.45082100	-2.40278100	-1.64052200
H	1.04608100	-1.81684000	-2.36203700
H	2.11808800	1.47367000	0.55355000
H	3.61786800	-1.12746100	-2.50896700
H	-2.01237500	-2.59763400	1.57245800
H	-3.87646100	-1.76346100	-2.20742300
H	-0.23705600	2.69037600	2.07267400
H	-1.81482700	3.73857100	-1.78070700

Cartesian coordinates of the optimized geometry of Int-9 at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.00006700	0.90331700	0.00029300
C	-1.63743600	-0.11814800	0.04188200
C	-1.67399100	-1.37160300	0.66932200
C	-2.85676600	-2.10791900	0.71852000
H	-2.86932800	-3.08357800	1.21081400
C	-4.02140700	-1.59888300	0.14573500
H	-4.94910800	-2.17493000	0.18530500
C	-3.99772800	-0.35287700	-0.48029700
H	-4.90694600	0.04894800	-0.93448700
C	-2.81320600	0.37903700	-0.53617200
H	-2.80496000	1.34791800	-1.04300000
H	-0.76902800	-1.78011000	1.12842600
C	1.63751900	-0.11816100	-0.04161400
C	1.67349100	-1.37193400	-0.66847000
C	2.81373300	0.37917500	0.53538700
C	2.85613800	-2.10842500	-0.71807900
H	0.76817300	-1.78053500	-1.12677500
C	3.99811700	-0.35293400	0.47911100
H	2.80596200	1.34832700	1.04170300
C	4.02122300	-1.59925100	-0.14631600
H	2.86825600	-3.08432700	-1.20989600
H	4.90768500	0.04900400	0.93249400
H	4.94882400	-2.17543300	-0.18621700
C	-0.02755500	2.68890700	-0.76554500
C	0.02757400	2.68922300	0.76534500
H	0.87509200	3.01806600	-1.29132200
H	-0.94525300	3.06215300	-1.23427300
H	0.94530500	3.06258600	1.23391900
H	-0.87503800	3.01854200	1.29108000

Cartesian coordinates of the optimized geometry of Int-10 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.01929200	-0.77658100	-1.22025400
C	-1.86257800	-0.25148100	0.97556300
C	-1.25261200	1.01165500	0.90376600
C	-1.93683300	2.10718100	0.37003500
H	-1.44281200	3.08048400	0.32208600
C	-3.24176700	1.96001800	-0.08874900
H	-3.77826200	2.81503600	-0.50634700
C	-3.86463100	0.71288600	-0.00679800
H	-4.89205800	0.59243300	-0.35899600
C	-3.18085000	-0.38017100	0.51552000

H	-3.67124800	-1.35638900	0.56632500
H	-0.23581400	1.13895500	1.28301100
C	1.65895700	-0.12050500	-0.35371400
C	2.35458500	-0.76679000	0.68173000
C	2.19673700	1.07951600	-0.85082700
C	3.53200000	-0.23497900	1.20452700
H	1.97455700	-1.70743700	1.09107400
C	3.36602100	1.62653300	-0.32479800
H	1.68292600	1.59826300	-1.66791900
C	4.03603800	0.96682600	0.70518900
H	4.05944000	-0.75640000	2.00774500
H	3.76135400	2.56500700	-0.72224500
H	4.95660500	1.38753700	1.11786000
C	-1.06881500	-1.46202000	1.40469400
C	-0.53996500	-2.18045900	0.15622000
H	-0.22740900	-1.13103200	2.03299200
H	-1.69035700	-2.12857900	2.02718600
H	0.28480800	-2.87193100	0.40010500
H	-1.34213600	-2.78462800	-0.29890600

Cartesian coordinates of the optimized geometry of Int-**11** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.29018700	0.68280300	0.00071600
C	1.53328200	0.02110900	0.00028200
C	1.77623300	-1.35924600	0.00069500
C	3.07796900	-1.85954300	0.00037900
H	3.24593100	-2.93953300	0.00070300
C	4.16163100	-0.98344000	-0.00034500
H	5.18281500	-1.37216000	-0.00059100
C	3.93537500	0.39336200	-0.00074700
H	4.78074100	1.08627700	-0.00130600
C	2.63372200	0.88974800	-0.00045900
H	2.47798800	1.97260000	-0.00080300
H	0.93732700	-2.06232400	0.00129300
Si	-2.14687200	-0.77633600	-0.00017900
C	-2.11732600	-1.86114300	1.54042900
H	-2.98955900	-2.53528900	1.55356700
H	-1.20925300	-2.48271000	1.57807600
H	-2.14281600	-1.24816700	2.45429000
C	-3.68323900	0.31324900	-0.00117300
H	-3.71210800	0.95873900	-0.89259100
H	-4.59319400	-0.30860000	-0.00187300
H	-3.71350400	0.95879500	0.89015400
C	-2.11536800	-1.86077100	-1.54102000
H	-1.20706100	-2.48203900	-1.57790600
H	-2.98737600	-2.53519000	-1.55517200
H	-2.14012800	-1.24757500	-2.45474900
C	-0.48042400	2.48495100	-0.75662100
C	-0.48026400	2.48557400	0.75646400
H	-1.41836200	2.73873300	-1.26161500
H	0.39954600	2.89686500	-1.26345600
H	-1.41813600	2.73961400	1.26144500
H	0.39979800	2.89787200	1.26282000

Cartesian coordinates of the optimized geometry of Int-**12** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.96750500	-1.84116800	0.01734000
C	2.04378400	-0.16581400	0.04143300
C	3.32650100	-0.24629800	-0.52891400
C	4.17917600	0.85663500	-0.56363400
H	5.17286700	0.76984800	-1.01051700
C	3.75709100	2.07221400	-0.02823000
H	4.41934000	2.94146200	-0.05418800
C	2.48628800	2.17957500	0.54108900
H	2.15466800	3.13313200	0.96050800
C	1.64377400	1.07175200	0.57593700
H	0.65292100	1.17985200	1.02601200

H	3.66317600	-1.19696000	-0.95712300
Si	-2.93308000	0.51024700	-0.14929600
C	-4.18535500	-0.52304000	0.80164500
H	-5.09608800	0.05897700	1.01488500
H	-4.48265800	-1.41463700	0.22686100
H	-3.77127300	-0.86342200	1.76357700
C	-2.43014500	2.01014400	0.87395600
H	-1.67915800	2.61637400	0.34238600
H	-3.29932600	2.65540300	1.07871100
H	-2.00241600	1.71242500	1.84422800
C	-3.67121400	1.08027800	-1.78488000
H	-3.97124100	0.22176800	-2.40655200
H	-4.56420600	1.70461400	-1.62143500
H	-2.94577900	1.67646900	-2.36102600
C	-1.38819000	-0.53439000	-0.49756500
C	-0.73354200	-1.12127600	0.76960800
H	-0.68873200	0.12265700	-1.05186800
H	-1.66894000	-1.33736300	-1.20416400
H	-1.35823100	-1.92517700	1.18736200
H	-0.60098500	-0.36017700	1.55493100

Cartesian coordinates of the optimized geometry of TS-**1a** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.10360400	0.98571500	0.93855000
Ga	0.28483600	-0.95447900	-0.75662100
Cl	1.66919300	-1.34460500	-2.49675100
N	0.78899100	-2.56113100	0.35010200
N	-1.36042900	-1.84158600	-1.47581300
C	0.53426700	-3.77574500	-0.12844900
C	-0.34512300	-4.02085200	-1.19502300
H	-0.40594000	-5.05486900	-1.53069400
C	-1.30697200	-3.15336400	-1.72715900
C	1.19080300	-4.97665400	0.49514400
H	2.26385600	-4.98926400	0.25330400
H	0.73899500	-5.90476200	0.12626000
H	1.11828200	-4.94871200	1.59124300
C	-2.37624000	-3.79771900	-2.56947300
H	-1.98832400	-4.71739000	-3.02598000
H	-2.74760400	-3.12714500	-3.35360800
H	-3.23961700	-4.07202000	-1.94553600
C	1.59085900	-2.45088600	1.52476200
C	0.95312700	-2.26170800	2.77210500
C	1.74247800	-2.23170300	3.92576900
H	1.26517500	-2.09311100	4.89725000
C	3.12323200	-2.37852600	3.85885300
H	3.72192200	-2.35458200	4.77219400
C	3.73937900	-2.52802300	2.62337500
H	4.82719300	-2.61079700	2.57111600
C	2.99666600	-2.55676300	1.43886100
C	-0.55523500	-2.14499600	2.87679000
H	-0.90873700	-1.72400600	1.92239800
C	-1.20017000	-3.52393000	3.03251500
H	-0.99998200	-4.16784700	2.16427900
H	-2.29295900	-3.43478400	3.13379100
H	-0.81898300	-4.03537500	3.93092900
C	-0.99914200	-1.19751500	3.98667100
H	-0.77781300	-1.59886200	4.98812300
H	-2.08491400	-1.03279400	3.93604200
H	-0.51180900	-0.21640300	3.88273600
C	3.71860300	-2.63169400	0.10932300
H	2.97831500	-2.85232200	-0.67312700
C	4.79246900	-3.71679500	0.06698200
H	5.20411800	-3.79980200	-0.95042300
H	4.39777400	-4.70397100	0.35373000
H	5.63453100	-3.49076700	0.74018200
C	4.31304600	-1.26709300	-0.23464200
H	5.07475000	-0.96574500	0.50327200
H	3.54319500	-0.48418100	-0.26886800

H	4.78191600	-1.29294500	-1.22878200
C	-2.58054600	-1.17722300	-1.79862900
C	-3.70347700	-1.38110300	-0.96780600
C	-4.93194200	-0.84018300	-1.35960400
H	-5.81043700	-0.99447100	-0.72795500
C	-5.05533200	-0.12625700	-2.54434200
H	-6.02697600	0.27007100	-2.84906900
C	-3.93094200	0.10374700	-3.33080700
H	-4.03046300	0.69232600	-4.24404500
C	-2.67569400	-0.39338000	-2.97047800
C	-3.61128500	-2.14824800	0.33907200
H	-2.61290000	-2.60600400	0.39239100
C	-4.64301100	-3.27053000	0.44787600
H	-4.59744100	-3.96224800	-0.40599100
H	-5.66979700	-2.87517400	0.49854100
H	-4.47267500	-3.85689600	1.36410600
C	-3.74496400	-1.19079900	1.51998200
H	-2.97830000	-0.40244300	1.50109600
H	-3.65902800	-1.73352400	2.47314600
H	-4.72467200	-0.69087000	1.50763200
C	-1.45941500	-0.12048700	-3.83490900
H	-0.59200300	-0.05288500	-3.16031500
C	-1.15407800	-1.26739800	-4.79887100
H	-0.28939700	-1.00886600	-5.42857600
H	-2.01393500	-1.46935600	-5.45843200
H	-0.89115600	-2.18907400	-4.26443900
C	-1.54841100	1.20126100	-4.59051400
H	-1.79138900	2.04134800	-3.92246500
H	-2.30632900	1.17074500	-5.38946400
H	-0.58424900	1.42115700	-5.07099900
C	0.23748500	2.80495200	0.08373200
C	-0.89363100	3.58336100	0.41759600
C	-0.97615400	4.93170300	0.05869000
H	-1.87203700	5.49883600	0.32658400
C	0.07062400	5.54002700	-0.62460000
H	0.01059300	6.59419200	-0.90577500
C	1.20132100	4.79305800	-0.93760200
H	2.03749000	5.26008500	-1.46541400
C	1.30511900	3.44051600	-0.58790900
C	-2.04871200	2.98320200	1.15176700
C	-2.06506300	2.96302600	2.56538100
C	-3.20445900	2.49575400	3.21829000
H	-3.21238600	2.47187300	4.31225600
C	-4.33984100	2.07848300	2.51564500
C	-4.30969700	2.12739300	1.12197700
H	-5.18612000	1.80651300	0.55177500
C	-3.18187600	2.56861900	0.42530400
C	-0.87632500	3.43968400	3.34304800
H	-0.59567900	4.46469600	3.05635100
H	-0.00004400	2.80162100	3.13560400
H	-1.07045100	3.41670600	4.42413100
C	-5.54502100	1.56934900	3.25049000
H	-5.34694700	0.57865900	3.69243000
H	-6.41239400	1.46819100	2.58291800
H	-5.82567500	2.24031700	4.07684400
C	-3.19584400	2.65137200	-1.07185800
H	-3.19594500	3.69959600	-1.41051900
H	-4.07740600	2.14978900	-1.48756400
H	-2.30240800	2.18292900	-1.50886600
C	2.58174300	2.76116700	-0.94618300
C	3.72912900	2.96677100	-0.15469000
C	4.93665200	2.39159400	-0.55431100
H	5.82524600	2.54175600	0.06738200
C	5.04276300	1.64365000	-1.73102000
C	3.90206200	1.48809300	-2.51774400
H	3.95998600	0.90839400	-3.44263600
C	2.67541800	2.04921300	-2.15335000
C	3.67449400	3.84807500	1.06126300
H	4.53120500	3.66495000	1.72624500

H	2.74671900	3.70142500	1.63088200
H	3.70055900	4.91170400	0.77227400
C	6.35808400	1.04466300	-2.13762000
H	6.24812000	0.39202900	-3.01504400
H	6.79375500	0.44597000	-1.32262000
H	7.09097500	1.82794700	-2.39151300
C	1.49221400	1.97026900	-3.06779000
H	1.29992200	2.95157500	-3.53259300
H	0.58092700	1.70222700	-2.51532900
H	1.64693500	1.22437600	-3.85665000
C	2.93419900	0.86213600	2.49383900
C	2.52983700	1.55205000	3.56157200
H	2.54524900	-0.13841900	2.29208000
H	3.68519900	1.24458400	1.79876900
H	1.77653100	1.14522200	4.24291400
H	2.92963200	2.54245200	3.79876300

Cartesian coordinates of the optimized geometry of TS-**1b** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.22356500	0.66972300	0.18030200
Ga	1.21030600	0.17720900	-0.58752300
Cl	1.75002400	0.17701400	-2.80072900
Si	-2.06413500	-1.99280100	-1.59952100
N	2.76097400	-0.93572800	-0.00126400
N	2.09437400	1.89540400	-0.07835900
N	-2.35219400	-0.71320800	-0.36860600
C	3.98837300	-0.43028300	-0.07885300
C	4.27244800	0.92063600	-0.35344000
H	5.32540400	1.15683700	-0.50302200
C	3.40194400	2.01659600	-0.30308900
C	5.18208500	-1.32145300	0.13158400
H	5.53381500	-1.70278700	-0.83897100
H	4.94324000	-2.18892900	0.75942200
H	6.00557700	-0.75610000	0.58579000
C	3.98775700	3.38363600	-0.51520300
H	3.73144600	3.71804500	-1.53356200
H	5.08012700	3.37264800	-0.41994400
H	3.56646500	4.12271200	0.17881500
C	2.55466300	-2.32074100	0.26752300
C	2.06253300	-2.69212600	1.54116100
C	1.81644600	-4.04398000	1.79028500
H	1.43464500	-4.35304300	2.76344800
C	2.04919900	-5.01095400	0.81787600
H	1.84944300	-6.06314200	1.03349300
C	2.52591000	-4.63101000	-0.42710400
H	2.69411300	-5.39126700	-1.19352500
C	2.78173200	-3.29011300	-0.73473800
C	1.82961900	-1.64925400	2.62078800
H	1.32823700	-0.79175000	2.13489300
C	3.14464300	-1.13464700	3.21171500
H	3.77813800	-0.64970400	2.45810400
H	3.71607000	-1.96194400	3.66180300
H	2.94592900	-0.39268600	4.00120200
C	0.91853700	-2.13808800	3.73949200
H	0.72064900	-1.32258300	4.44782500
H	1.38481300	-2.95337000	4.31439300
H	-0.04752600	-2.49813800	3.35463200
C	3.25028500	-2.95039400	-2.13801300
H	3.45557700	-1.87131500	-2.18327900
C	4.52488800	-3.70769700	-2.51573600
H	4.90586000	-3.35274300	-3.48574800
H	4.33803400	-4.78877700	-2.61469400
H	5.32259100	-3.58291200	-1.76867200
C	2.15021900	-3.22497800	-3.16444700
H	1.24882000	-2.63839700	-2.94857500
H	1.87914600	-4.29312700	-3.18330100
H	2.49129000	-2.94130000	-4.17180800
C	1.30703900	3.03356800	0.26469700

C	1.15996300	3.36567900	1.63488600
C	0.33744500	4.44537000	1.96656200
H	0.20882600	4.72371100	3.01315100
C	-0.33905700	5.17020400	0.98969600
H	-0.98772000	6.00111000	1.27673800
C	-0.18432900	4.83272000	-0.34629100
H	-0.71422800	5.40375900	-1.11257300
C	0.64492000	3.77499600	-0.73488600
C	1.85532500	2.56379700	2.72615700
H	1.73725300	1.50056000	2.45127100
C	3.35864200	2.84344500	2.82541700
H	3.54480900	3.92096000	2.96011900
H	3.91699300	2.49988200	1.94751000
H	3.77969300	2.31924600	3.69761700
C	1.24371800	2.77462400	4.10857700
H	1.50159500	3.76701300	4.51159100
H	1.64475000	2.03066200	4.81387700
H	0.14928400	2.69050500	4.10899300
C	0.79455600	3.45576000	-2.20812900
H	1.56802700	2.68275200	-2.31210300
C	1.24222100	4.67191400	-3.01817800
H	0.47444300	5.46174600	-3.03485500
H	1.43976200	4.38238200	-4.06180500
H	2.16232500	5.11509800	-2.60753200
C	-0.49186000	2.86532700	-2.78080000
H	-1.32052800	3.58937000	-2.74280800
H	-0.80701400	1.97133000	-2.21842800
H	-0.34569100	2.54805300	-3.82387200
C	-3.71885600	-0.51980100	0.01337200
C	-4.26618300	-1.26447400	1.09087700
C	-5.62328900	-1.11662000	1.39181400
H	-6.05342400	-1.69664800	2.21123600
C	-6.43616400	-0.24194800	0.68121400
H	-7.49444900	-0.14366500	0.93399300
C	-5.88447900	0.51610700	-0.34174900
H	-6.51612900	1.22033200	-0.88953400
C	-4.53647300	0.39642100	-0.69357600
C	-3.42870600	-2.20515800	1.94196900
H	-2.37572800	-1.91775900	1.78957700
C	-3.58138900	-3.67125600	1.53144400
H	-4.63127200	-3.99213900	1.62795500
H	-2.97058700	-4.31805300	2.18149900
H	-3.27171500	-3.85315000	0.49644900
C	-3.75606900	-2.08079100	3.43142500
H	-3.79914500	-1.03491800	3.76501100
H	-2.99955000	-2.60766200	4.03435400
H	-4.72693500	-2.54246100	3.67020000
C	-4.00881600	1.26760400	-1.81828800
H	-2.96262700	0.98111000	-1.99665400
C	-4.01860400	2.74412300	-1.42066100
H	-3.63966300	3.37087400	-2.24290600
H	-3.38490100	2.91937600	-0.53755100
H	-5.03765600	3.08667400	-1.18050300
C	-4.76223400	1.04029200	-3.12816800
H	-5.81558200	1.35346800	-3.05258600
H	-4.75193400	-0.02034400	-3.42033400
H	-4.30180400	1.62108600	-3.94274100
C	-3.70825500	-2.81337100	-2.01232000
H	-4.37142000	-2.09127800	-2.51224900
H	-4.25607400	-3.21322100	-1.14970100
H	-3.52083400	-3.63993400	-2.71735600
C	-0.82525200	-3.22356100	-0.92696000
H	0.12283200	-2.73179200	-0.66678000
H	-0.59720800	-3.99692600	-1.67630800
H	-1.19144400	-3.72280400	-0.01911700
C	-1.47330000	-1.24503600	-3.21266500
H	-2.24370400	-0.57812700	-3.63018300
H	-1.30611900	-2.05405500	-3.94313000
H	-0.53306900	-0.68180600	-3.12618900

C	-2.10554900	1.23917500	3.06252200
C	-1.36087500	0.39733100	3.78494500
H	-1.76749800	2.25227400	2.82564100
H	-3.10033700	0.96364300	2.69709400
H	-0.37562300	0.68309500	4.15735300
H	-1.70313200	-0.60900100	4.02847000

Cartesian coordinates of the optimized geometry of TS-**2a** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.40674900	0.65322900	-0.87019300
Ga	0.34980200	-0.98569500	0.55469400
Cl	-0.98059700	-1.09793200	2.35733600
N	0.22495000	-2.83094200	-0.14298100
N	2.09609400	-1.28747500	1.48172500
C	0.71824300	-3.83325100	0.57431700
C	1.62229500	-3.65549900	1.63499000
H	1.90423400	-4.56344500	2.16653000
C	2.33231400	-2.49907600	1.98999000
C	0.30488700	-5.24714400	0.27762600
H	-0.47126200	-5.54233800	1.00175300
H	1.15003900	-5.93725900	0.39779500
H	-0.11858700	-5.35429700	-0.72807300
C	3.42726700	-2.66736800	3.00677000
H	3.12364000	-2.20095500	3.95618900
H	4.35234800	-2.16429700	2.69486000
H	3.63540800	-3.72773500	3.19004200
C	-0.53304700	-3.04661700	-1.33335400
C	0.14430700	-3.03715900	-2.57386300
C	-0.61309800	-3.12426400	-3.74476900
H	-0.10796000	-3.11590800	-4.71290700
C	-1.99962800	-3.22347300	-3.69729800
H	-2.57653100	-3.27765400	-4.62360100
C	-2.64579500	-3.27365000	-2.46881200
H	-3.73308200	-3.37729300	-2.43459300
C	-1.93392000	-3.19838400	-1.26756800
C	1.66085700	-3.01915400	-2.64714600
H	2.02800100	-2.63292700	-1.68363800
C	2.20668500	-4.44217700	-2.79055600
H	1.87567100	-5.09112800	-1.96824900
H	3.30828300	-4.43762600	-2.79561400
H	1.86365200	-4.89752100	-3.73343900
C	2.21068500	-2.12464200	-3.75438500
H	1.93125300	-2.49278500	-4.75360500
H	3.31028300	-2.10992500	-3.71616700
H	1.85305400	-1.08886400	-3.66269600
C	-2.67387700	-3.34698700	0.04750500
H	-1.94294600	-3.23103900	0.86055500
C	-3.30015500	-4.73990700	0.15842000
H	-3.74831700	-4.87892500	1.15475400
H	-2.56506400	-5.54223400	-0.00089700
H	-4.10107500	-4.87590600	-0.58603800
C	-3.73347000	-2.27059000	0.25236300
H	-4.53208700	-2.33586500	-0.50427300
H	-3.29953800	-1.26374200	0.20315000
H	-4.19882000	-2.38198500	1.24284900
C	3.02015900	-0.23420700	1.76567400
C	4.07710200	0.00275900	0.85679300
C	5.01484700	0.99392300	1.16092100
H	5.84166500	1.17667300	0.47069500
C	4.92345000	1.73665400	2.33216800
H	5.66931000	2.50249000	2.55766200
C	3.87309000	1.50265800	3.21051000
H	3.79683400	2.09409000	4.12585800
C	2.90592500	0.52649700	2.95074200
C	4.26131200	-0.83502900	-0.39504300
H	3.32240000	-1.38429200	-0.55426900
C	5.35868100	-1.88381800	-0.20561400
H	5.13597800	-2.55934400	0.63273600

H	6.33186000	-1.40752200	-0.00518600
H	5.46444200	-2.50031200	-1.11249000
C	4.52743600	0.01662200	-1.63407700
H	3.73902200	0.76802500	-1.78497100
H	4.57176000	-0.61744800	-2.53181500
H	5.49034100	0.54681000	-1.56532200
C	1.77988500	0.32476500	3.94619900
H	1.22972900	-0.58242300	3.65860200
C	2.28968700	0.13688100	5.37514900
H	1.45532500	-0.12883500	6.04215000
H	2.74598800	1.05655500	5.77422700
H	3.04550600	-0.66055500	5.44372000
C	0.78051600	1.47968900	3.88249600
H	0.33484200	1.56907100	2.88242700
H	1.26110000	2.44009600	4.12993700
H	-0.04460500	1.31278100	4.59123200
C	-1.51641000	2.58994500	-0.23747100
C	-0.64581700	3.68521200	-0.45640000
C	-0.94474500	4.94643000	0.07508400
H	-0.24686700	5.76877500	-0.10598600
C	-2.10987100	5.16556200	0.80082800
H	-2.33225700	6.15686600	1.20354900
C	-2.99984200	4.11582900	0.98205700
H	-3.94252300	4.27481600	1.51242600
C	-2.71735200	2.84198800	0.47203000
C	0.60116800	3.62291200	-1.27402800
C	0.53585100	3.82293200	-2.66511800
C	1.71933100	3.80777300	-3.40850500
H	1.66356800	3.94906500	-4.49217400
C	2.96557800	3.61155400	-2.80835900
C	3.00884200	3.45917300	-1.42075100
H	3.97268200	3.32220200	-0.92144800
C	1.84784000	3.47122200	-0.64360100
C	-0.78851200	4.02387000	-3.34270300
H	-1.33959200	4.86842100	-2.90138300
H	-1.43272300	3.13797100	-3.22176200
H	-0.66264300	4.21284500	-4.41777200
C	4.22123100	3.53845200	-3.62784600
H	4.09064100	4.00860900	-4.61300900
H	4.51687200	2.48932300	-3.79900300
H	5.06353000	4.03229300	-3.12060300
C	1.93035300	3.32990700	0.84572300
H	1.67981900	4.27688800	1.35032300
H	2.93362200	3.02355200	1.16470300
H	1.21034500	2.58889900	1.21864900
C	-3.78935900	1.81414800	0.64863700
C	-4.64156800	1.50288900	-0.43000600
C	-5.71721600	0.63687200	-0.21877800
H	-6.37892500	0.40329800	-1.05852300
C	-5.97435500	0.07167900	1.03048900
C	-5.11726200	0.39439400	2.08451300
H	-5.29618700	-0.04087700	3.07230700
C	-4.03324100	1.25767600	1.92023200
C	-4.41359900	2.08429300	-1.79759700
H	-5.31103900	1.98147300	-2.42342800
H	-3.59444600	1.56339500	-2.32788500
H	-4.13363800	3.14673700	-1.75147600
C	-7.11014000	-0.88933600	1.22560600
H	-7.51544800	-0.83502500	2.24662300
H	-6.77407800	-1.92745300	1.06218400
H	-7.93043700	-0.69590100	0.51904000
C	-3.15043300	1.59172500	3.08643400
H	-3.37795300	0.94813800	3.94713700
H	-3.27189000	2.64073800	3.39925200
H	-2.09245500	1.44610200	2.83059000
C	0.06838400	0.56844700	-2.21190200
C	0.98281600	0.19892500	-1.07986400
H	-0.11516800	-0.26456000	-2.90128400
H	0.35732000	1.47986400	-2.73913600

H	1.64702700	-0.64363700	-1.31935000
H	1.56582000	1.03479800	-0.68081500

Cartesian coordinates of the optimized geometry of TS-**2b** at PBE0-D3BJ/def2-SVP level of theory:

Ge	-1.13913400	0.72744600	-0.27090000
Ga	1.18196800	0.11622100	-0.68944600
Cl	1.49198100	0.00316500	-2.91569200
Si	-2.61459000	-1.91186700	-1.35761900
N	2.49545600	-1.28071900	-0.15719300
N	2.33186500	1.63479500	-0.19179300
N	-2.55954300	-0.52238900	-0.26916800
C	3.78580800	-0.99530700	-0.31995800
C	4.28671700	0.29217300	-0.58894200
H	5.35256900	0.34269100	-0.80844200
C	3.63407200	1.52233000	-0.46290900
C	4.81334500	-2.09018900	-0.23616000
H	4.97584100	-2.50967000	-1.24094200
H	4.49313600	-2.91335600	0.41401300
H	5.77164600	-1.69190500	0.11941700
C	4.45435900	2.76011100	-0.68943700
H	4.40495100	2.99894700	-1.76466400
H	5.50802300	2.60037200	-0.42923000
H	4.06523900	3.62752300	-0.14279700
C	2.09582500	-2.61280400	0.17783600
C	1.76057400	-2.89082900	1.52239100
C	1.34903200	-4.18289100	1.85495600
H	1.08094800	-4.41227000	2.88755600
C	1.28140200	-5.18420400	0.89209300
H	0.95531100	-6.18948400	1.16866700
C	1.62836600	-4.89988800	-0.42064800
H	1.57148600	-5.68876200	-1.17431000
C	2.03810600	-3.61967900	-0.80955800
C	1.89776600	-1.82358500	2.58911700
H	1.66540200	-0.86755900	2.10073400
C	3.33546700	-1.72613900	3.10413500
H	4.04210100	-1.45842800	2.30680200
H	3.66117900	-2.68414800	3.53984200
H	3.41237900	-0.95449600	3.88646500
C	0.92645200	-1.99890600	3.75056900
H	0.91911500	-1.09607200	4.37940700
H	1.20950300	-2.84423300	4.39779200
H	-0.10017400	-2.17384100	3.39830600
C	2.38244500	-3.37733900	-2.26705100
H	2.75500300	-2.34761400	-2.36631500
C	3.46375700	-4.33626600	-2.76834200
H	3.77443800	-4.05975100	-3.78766100
H	3.09616000	-5.37376200	-2.80953500
H	4.35678900	-4.33288600	-2.12596900
C	1.13825200	-3.47559900	-3.14823000
H	0.36613400	-2.76766100	-2.82632000
H	0.70939300	-4.49053300	-3.12175800
H	1.38915700	-3.23656400	-4.19280500
C	1.78092400	2.86259200	0.28267100
C	1.86451800	3.14443700	1.66853900
C	1.25894600	4.31041600	2.14407600
H	1.30765500	4.54374900	3.20935800
C	0.57960600	5.17131200	1.28760200
H	0.09948400	6.06963700	1.68262100
C	0.52185600	4.88881400	-0.07104200
H	0.00354400	5.57662200	-0.74360000
C	1.12891300	3.74612200	-0.60325300
C	2.60892500	2.22986200	2.62961800
H	2.62999500	1.22790800	2.17052600
C	4.06460200	2.66677200	2.81369900
H	4.11389300	3.68830900	3.22351700
H	4.62577600	2.65581000	1.87135100
H	4.58033500	1.99386000	3.51659000

C	1.93487900	2.11265000	3.99620100
H	2.02650500	3.04426700	4.57589700
H	2.41988200	1.32058200	4.58735300
H	0.86597700	1.86965100	3.91160200
C	1.13830800	3.54065700	-2.10611900
H	1.61432200	2.57143700	-2.31251000
C	1.97590100	4.62626300	-2.78776600
H	1.51102700	5.61891000	-2.67492100
H	2.06559600	4.42027200	-3.86568900
H	2.98987300	4.68875200	-2.36672900
C	-0.26157500	3.49021500	-2.71289200
H	-0.79055100	4.45064400	-2.60212300
H	-0.87166000	2.70997600	-2.23554900
H	-0.19933800	3.26128100	-3.78746500
C	-3.76208000	-0.07043700	0.33688300
C	-4.18075700	-0.62647700	1.57253100
C	-5.38908900	-0.20845100	2.13784700
H	-5.71768300	-0.64985500	3.08268000
C	-6.17492700	0.76180900	1.52861200
H	-7.11526100	1.07884300	1.98588100
C	-5.74844100	1.32879100	0.33379200
H	-6.36166500	2.09781800	-0.14402000
C	-4.55744400	0.93012200	-0.27930500
C	-3.34497400	-1.65887100	2.30571100
H	-2.40306100	-1.75052200	1.74291300
C	-4.01114800	-3.03447200	2.32581400
H	-4.96974600	-3.00525400	2.86859300
H	-3.36495500	-3.77265900	2.82742000
H	-4.21621300	-3.40212900	1.31089000
C	-3.01699500	-1.20856200	3.72995300
H	-2.53482900	-0.21996600	3.74420200
H	-2.33854300	-1.92579600	4.21856500
H	-3.92415400	-1.14349900	4.35116600
C	-4.15846300	1.58857100	-1.58677000
H	-3.22617800	1.10985300	-1.92212700
C	-3.86817200	3.07752500	-1.39577500
H	-3.53462100	3.53368500	-2.34109900
H	-3.07628700	3.23419000	-0.64778600
H	-4.76562600	3.62049200	-1.05843600
C	-5.19761600	1.36640200	-2.68514600
H	-6.15978100	1.84184600	-2.43649100
H	-5.38926100	0.29539300	-2.84701600
H	-4.85105900	1.79694600	-3.63786800
C	-4.39851300	-2.47549600	-1.53296800
H	-5.01740300	-1.68661400	-1.98543100
H	-4.85802700	-2.73952100	-0.57011000
H	-4.44029600	-3.36022300	-2.18861300
C	-1.56882100	-3.30312700	-0.65591600
H	-0.56237300	-2.95194600	-0.38336100
H	-1.44734600	-4.12818100	-1.37435000
H	-2.02932100	-3.71163000	0.25624500
C	-2.00871000	-1.40029800	-3.06309600
H	-2.71807500	-0.68196300	-3.50487400
H	-1.95581800	-2.27291700	-3.73403300
H	-1.01443600	-0.92608600	-3.05806000
C	-1.32166000	1.66721200	1.50258200
C	-0.44603300	0.58173600	1.84518600
H	-0.91779900	2.68291500	1.47388800
H	-2.37977200	1.60000600	1.77915000
H	0.60132100	0.79283300	2.04807900
H	-0.84458400	-0.33730000	2.27089000

Cartesian coordinates of the optimized geometry of TS-**3a** at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.87788000	0.44070600	0.82779500
Ge	-1.11692100	1.11063600	-0.86171200
Ga	5.55669100	-0.82642900	0.19724300
Ga	-5.44487000	-0.85168900	-0.21802400

Cl	5.69320200	-2.46562900	1.70156800
Cl	-5.50186000	-2.32180600	-1.90288700
N	6.35574100	-1.58641100	-1.42268700
N	7.06127500	0.36184700	0.63320900
N	-6.23046400	-1.89180300	1.26275400
N	-7.05320400	0.24149100	-0.54439900
C	7.68152100	-1.64350900	-1.53721100
C	8.57430000	-0.98217300	-0.67421100
H	9.63047400	-1.17538800	-0.85551500
C	8.29547800	0.01567100	0.27479900
C	8.28031700	-2.44587600	-2.65683400
H	7.80018000	-2.20537900	-3.61585200
H	8.10833900	-3.51834800	-2.48381400
H	9.35924800	-2.27051300	-2.73647700
C	9.46722100	0.71058600	0.90761000
H	10.37572000	0.59117700	0.30546700
H	9.65034200	0.26628900	1.89902500
H	9.27035700	1.77859200	1.06912000
C	5.52218900	-2.15965300	-2.43482800
C	5.20745700	-3.53424100	-2.41487300
C	4.42350900	-4.04896600	-3.45337900
H	4.16867900	-5.11134200	-3.45015900
C	3.95317800	-3.23811500	-4.47742400
H	3.34083500	-3.66177900	-5.27652600
C	4.23107200	-1.87578100	-4.45777700
H	3.81890300	-1.23245500	-5.23672200
C	-0.34066100	0.86342100	-2.75973000
C	4.99951700	-1.31103300	-3.43667400
C	5.64061300	-4.45780000	-1.29311300
H	6.30267400	-3.89260900	-0.62081500
C	6.40320000	-5.68188400	-1.80031800
H	5.76078000	-6.33656400	-2.41013300
H	6.77051100	-6.28034000	-0.95251100
H	7.27042500	-5.40670000	-2.41969200
C	4.42824500	-4.88841700	-0.46696300
H	3.72379900	-5.47663500	-1.07644700
H	3.88914800	-4.02319800	-0.05794100
H	4.74408000	-5.50934400	0.38521500
C	5.24998000	0.18354200	-3.40897200
H	5.41821600	0.45174900	-2.35521900
C	6.51852300	0.56398400	-4.17298600
H	7.41437000	0.09928300	-3.73672900
H	6.66869600	1.65499600	-4.15559800
H	6.44906900	0.24960800	-5.22658100
C	4.05105600	0.99015200	-3.89740900
H	3.88883700	0.88005600	-4.98038300
H	4.21134200	2.06085900	-3.70690400
H	3.11761300	0.68899600	-3.39839600
C	6.80947900	1.54939800	1.38645600
C	6.82247300	1.53256400	2.79545100
C	6.54433600	2.72265700	3.47739500
H	6.55611600	2.72298700	4.57008900
C	6.24539100	3.89446200	2.79604600
H	6.03039500	4.81263400	3.34823000
C	6.21380200	3.89266700	1.40537300
H	5.96793100	4.81331000	0.87325000
C	6.49336300	2.73330900	0.67846600
C	7.09667600	0.27482200	3.59370000
H	7.31999200	-0.53528300	2.88402700
C	8.29284100	0.43452300	4.53185500
H	8.51395700	-0.51901700	5.03576200
H	8.09598700	1.18292900	5.31584900
H	9.19846000	0.75366200	3.99440900
C	5.84731100	-0.14304300	4.36740000
H	4.99002800	-0.26246500	3.69229600
H	5.57964600	0.60389200	5.13220300
H	6.00664400	-1.10771900	4.87248800
C	6.49672300	2.76378300	-0.83772500
H	6.27660300	1.74000800	-1.17585900

C	7.88002300	3.12661000	-1.38217000
H	8.64607300	2.40196800	-1.07466400
H	8.19086100	4.12112600	-1.02392100
H	7.86885100	3.14971700	-2.48292100
C	5.43267700	3.68560800	-1.42429000
H	5.39163500	3.56820400	-2.51733000
H	5.65220000	4.74654000	-1.22693500
H	4.43293200	3.46856100	-1.02136600
C	-7.54747400	-2.08005400	1.31598200
C	-8.47529400	-1.38849700	0.51710600
H	-9.51428400	-1.69109400	0.63546600
C	-8.26037700	-0.24827000	-0.27174600
C	-8.10676400	-3.07076300	2.29782600
H	-7.86129100	-4.09477600	1.98131600
H	-9.19649800	-2.97908900	2.37122400
H	-7.66212800	-2.93670000	3.29389100
C	-9.47036900	0.46803300	-0.79863000
H	-9.44794700	0.48575800	-1.89805900
H	-9.47794500	1.51802000	-0.47342100
H	-10.39557300	-0.01701800	-0.46713600
C	-5.38732300	-2.54195900	2.21600100
C	-4.99327700	-3.88393300	2.03216300
C	-4.20810200	-4.48443400	3.02261800
H	-3.89154600	-5.52205200	2.89323800
C	-3.81875200	-3.78911400	4.15889300
H	-3.20742200	-4.27886400	4.92029600
C	-4.18126300	-2.45438600	4.30661600
H	-3.83811900	-1.90119700	5.18185000
C	-4.95211000	-1.80347800	3.33963600
C	-5.35696800	-4.68554700	0.79682300
H	-6.05381000	-4.08669200	0.19219600
C	-6.03281100	-6.01404000	1.13932300
H	-6.37553100	-6.51396300	0.22040100
H	-6.90436900	-5.88451000	1.79888300
H	-5.33947700	-6.70305000	1.64708300
C	-4.12074200	-4.93050800	-0.06757100
H	-4.39323400	-5.49352000	-0.97306800
H	-3.36384300	-5.51324400	0.48151200
H	-3.66344500	-3.98938300	-0.40052900
C	-5.30915500	-0.33736800	3.50030300
H	-5.37389200	0.08500000	2.48484800
C	-6.67985400	-0.14913000	4.15231900
H	-7.48670300	-0.58717300	3.54823700
H	-6.90473900	0.92214800	4.27547900
H	-6.70589100	-0.61650000	5.14975100
C	-4.23708500	0.44637300	4.24850300
H	-3.23921200	0.29387500	3.81187900
H	-4.18364800	0.16306900	5.31121900
H	-4.46200100	1.52167400	4.21623700
C	-6.92498400	1.54610200	-1.11022100
C	-6.88100900	1.72620000	-2.50812800
C	-6.73769400	3.02516000	-3.00609400
H	-6.70313100	3.17765100	-4.08769600
C	-6.63354400	4.11988300	-2.15712200
H	-6.51981900	5.12586100	-2.56840800
C	-6.67504200	3.92705600	-0.78119500
H	-6.59570400	4.78875500	-0.11363200
C	-6.82350600	2.64960300	-0.23466200
C	-6.96319900	0.56543500	-3.47807700
H	-7.14086500	-0.35051100	-2.89574100
C	-8.10794900	0.72338600	-4.47825100
H	-7.95191000	1.58724600	-5.14375700
H	-9.07809100	0.86553200	-3.97765800
H	-8.18425900	-0.17202000	-5.11414700
C	-5.62982900	0.38047500	-4.19885000
H	-5.65507100	-0.51352300	-4.83967800
H	-4.81076000	0.24795600	-3.48023900
H	-5.39056300	1.25030000	-4.83163100
C	-6.89837300	2.48663900	1.27145100

H	-6.91750900	1.40808900	1.48579600
C	-8.18479400	3.08829500	1.83851400
H	-9.08024600	2.64346200	1.38026900
H	-8.22682000	4.17563700	1.66588200
H	-8.24532300	2.91855600	2.92505900
C	-5.66961400	3.07101100	1.96041100
H	-4.74765800	2.59476400	1.60073000
H	-5.72863900	2.92319700	3.04922200
H	-5.57928100	4.15404500	1.78241100
C	3.84624500	0.12055400	0.04156400
H	4.12486400	1.17848600	0.15654800
H	3.50133700	0.00316300	-0.99704600
C	2.77738100	-0.26939400	1.04710500
H	3.08637500	0.00352100	2.06762500
H	2.62284400	-1.35941200	1.06900600
C	-3.76403900	0.14498700	0.02603700
H	-4.03085000	1.21203800	-0.08648200
H	-3.44317000	0.03872000	1.07592100
C	-2.64170700	-0.22495000	-0.94162300
H	-2.99414000	-0.13823200	-1.98094800
H	-2.32340500	-1.26935400	-0.84019400
C	2.01183500	2.58854000	0.18892200
H	2.57808400	2.62537400	1.12337600
H	2.50559700	2.15002500	-0.68018500
C	0.86199700	3.28745000	0.02929300
H	0.38381000	3.38634200	-0.94030900
H	0.39643300	3.82797300	0.85020000
C	0.27456100	0.49347200	2.77258000
C	0.10148900	-0.78551900	3.36191600
C	-0.43107000	-0.91785300	4.65033200
H	-0.56006700	-1.92405200	5.05765300
C	-0.77174900	0.19739500	5.40265400
H	-1.18372800	0.08753300	6.40872000
C	-0.55713200	1.45709300	4.86145700
H	-0.78022700	2.35282400	5.44731600
C	-0.04257300	1.62126600	3.56656200
C	0.50037400	-2.07078200	2.70906500
C	-0.41405400	-2.75666900	1.88646200
C	-0.08310600	-4.02319500	1.40694100
H	-0.81214200	-4.54887500	0.78658700
C	1.13901700	-4.62883700	1.70993500
C	2.03448100	-3.93078200	2.52119900
H	3.00066300	-4.38021100	2.76748300
C	1.72436600	-2.67452300	3.05276800
C	-1.75837100	-2.16992300	1.60817000
H	-1.68536400	-1.11192100	1.33230700
H	-2.39551200	-2.22277400	2.50224000
H	-2.26685400	-2.70388300	0.79699900
C	1.45987400	-6.00069500	1.19225500
H	0.68123700	-6.72437800	1.48112100
H	2.42268700	-6.36302800	1.57760600
H	1.51399700	-6.01508100	0.09197300
C	2.68477900	-2.03317200	4.01135400
H	3.72166800	-2.23131100	3.70708300
H	2.54605700	-2.44106200	5.02688500
H	2.53817500	-0.94785900	4.08362700
C	0.21524800	3.03951800	3.18446400
C	-0.84383900	3.88138300	2.79160300
C	-0.57966700	5.22936000	2.53651200
H	-1.40330100	5.87394800	2.21462400
C	0.70810900	5.76244800	2.63852800
C	1.73801600	4.91392600	3.04908800
H	2.75311800	5.31035700	3.14775600
C	1.51104900	3.56559400	3.34380200
C	-2.21629300	3.33028500	2.56084900
H	-2.93843700	4.13571400	2.37331800
H	-2.56972000	2.72979200	3.40974600
H	-2.20877100	2.66791700	1.67678400
C	0.97620300	7.19220400	2.26900200

H	0.16514300	7.85525500	2.60552300
H	1.05259100	7.30240900	1.17390300
H	1.91883300	7.55440500	2.70367000
C	2.63525000	2.70550400	3.84793400
H	3.59917200	3.22792000	3.78740200
H	2.72229300	1.76638100	3.28289300
H	2.46275000	2.41140800	4.89585300
C	-0.14963400	2.03984600	-3.53582000
C	0.36957000	1.97068900	-4.83724300
H	0.47516400	2.89392900	-5.41258200
C	0.72612200	0.75483200	-5.40192200
H	1.14214200	0.71121200	-6.41182100
C	0.50133000	-0.40927000	-4.67892700
H	0.72467300	-1.38380700	-5.12199500
C	-0.06001500	-0.37476200	-3.39342900
C	-0.54165300	3.40706400	-3.07191300
C	0.44291500	4.41142000	-2.92098100
C	0.06803200	5.68171200	-2.47795300
H	0.84506600	6.43922300	-2.33471300
C	-1.25928900	6.00043300	-2.18617100
C	-2.22502500	5.01804200	-2.40139700
H	-3.27813800	5.24857900	-2.21161400
C	-1.89566000	3.73525100	-2.84885000
C	1.89888300	4.13216200	-3.17346100
H	2.17011500	3.10764500	-2.88692200
H	2.53340400	4.83207300	-2.61106300
H	2.15538500	4.23489300	-4.24025100
C	-1.62575100	7.34472600	-1.62768200
H	-0.98777100	8.14236700	-2.03665400
H	-1.50127000	7.35809200	-0.53109600
H	-2.67399500	7.59994100	-1.84063200
C	-3.00826900	2.75528800	-3.08120800
H	-3.31568300	2.27238300	-2.13819300
H	-2.72233900	1.96101400	-3.78223600
H	-3.90075500	3.26522900	-3.46904500
C	-0.42176700	-1.73089900	-2.86878100
C	0.49233400	-2.49627200	-2.12403200
C	0.19792500	-3.82652900	-1.82941900
H	0.93618800	-4.40867200	-1.27300200
C	-0.99534700	-4.42615800	-2.23739800
C	-1.90016900	-3.64805700	-2.95822500
H	-2.84895000	-4.08572000	-3.28162800
C	-1.62127100	-2.32208400	-3.30808800
C	1.80774300	-1.92149400	-1.71430500
H	2.20679300	-2.43253400	-0.82795800
H	1.70843900	-0.85187100	-1.49363700
H	2.54941200	-2.01836900	-2.52050500
C	-1.26966800	-5.86994800	-1.92904200
H	-2.24066000	-6.19094300	-2.33037800
H	-1.27761900	-6.06099300	-0.84392000
H	-0.49243400	-6.52137600	-2.36042300
C	-2.58545500	-1.59419300	-4.19911500
H	-2.40205400	-1.84821100	-5.25697200
H	-2.48679200	-0.50458900	-4.11442700
H	-3.61914800	-1.87366900	-3.95455300

Cartesian coordinates of the optimized geometry of TS-4 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.48611100	-1.36924900	-0.93408300
Ga	0.55896100	0.34097100	0.38019300
Cl	0.49998700	0.14958300	2.59742600
N	2.38561100	0.86670700	-0.03410100
N	-0.23385600	2.08696000	-0.01162100
C	2.76907600	2.13751900	-0.13974100
C	1.88195200	3.22457600	-0.13663900
H	2.33983100	4.21022200	-0.20356400
C	0.47394100	3.20022400	-0.13855300
C	4.23634100	2.42472800	-0.28185200

H	4.79559600	1.99027900	0.56039200
H	4.42822300	3.50297200	-0.32348700
H	4.63467500	1.95634900	-1.19445200
C	-0.24899000	4.50730700	-0.30215900
H	-1.10448200	4.56541800	0.38623200
H	-0.65357600	4.60414500	-1.32103400
H	0.42612500	5.35203600	-0.11976500
C	3.30894900	-0.20872600	-0.10583900
C	3.61937400	-0.78386900	-1.34275500
C	4.45560700	-1.89670700	-1.40427200
H	4.69243200	-2.34251300	-2.37333800
C	4.97938900	-2.44628200	-0.23458500
H	5.62854400	-3.32327600	-0.28411900
C	4.66231200	-1.87884600	0.99913100
H	5.05979300	-2.31234800	1.91978100
C	3.82776500	-0.76518800	1.06858400
C	-1.64266100	2.03906500	-0.17474500
C	-2.21545400	2.17438400	-1.44481300
C	-3.58602600	1.99830500	-1.61319800
H	-4.02436900	2.09589900	-2.60926800
C	-4.39143500	1.67013400	-0.52312100
H	-5.46249900	1.50850700	-0.66119000
C	-3.82020600	1.52461800	0.73887200
H	-4.44091600	1.24391400	1.59207600
C	-2.45101100	1.70703300	0.91753300
C	-2.27887300	-1.76271300	-0.21061200
C	-2.53325000	-1.83438700	1.16797400
C	-3.82893200	-2.01964300	1.64794100
H	-4.00512200	-2.07569200	2.72559200
C	-4.89808600	-2.12920000	0.75843800
H	-5.91390400	-2.27481100	1.13512400
C	-4.66440700	-2.04909900	-0.61291000
H	-5.49735200	-2.12855400	-1.31666800
C	-3.36594800	-1.86336300	-1.08924900
H	3.54241800	-0.33071500	2.02897500
H	3.18380100	-0.35682300	-2.24908200
H	-1.98642400	1.56514000	1.89573500
H	-1.57125800	2.38663100	-2.30116600
H	-3.19888500	-1.79064800	-2.16838600
H	-1.70871500	-1.72760500	1.87865100
C	0.64568300	-2.81021100	0.19561000
C	0.51616200	-3.10090000	-1.21184400
H	1.60806800	-2.46844400	0.58425800
H	-0.00211800	-3.31384000	0.91689500
H	1.38922100	-2.99779000	-1.86213500
H	-0.20106900	-3.86371200	-1.53072500

Cartesian coordinates of the optimized geometry of TS-5 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.25173500	-2.67903500	0.00679300
Ga	0.51704800	0.35875200	0.20752600
Cl	0.11034500	-0.13858700	2.34023000
N	2.40591300	0.84384000	0.16437500
N	-0.15104200	2.19384000	0.05988300
C	2.82878200	2.05784100	0.50699300
C	1.96585300	3.14932100	0.70043900
H	2.43739600	4.06944900	1.04265300
C	0.58884300	3.23601400	0.42571200
C	4.30024600	2.29065000	0.70596500
H	4.75948400	1.44648500	1.24033300
H	4.47139800	3.21571700	1.26956600
H	4.82045700	2.37920600	-0.25973100
C	-0.05557500	4.58735500	0.56527800
H	-1.06733200	4.49837600	0.98533600
H	-0.15377300	5.08283400	-0.41249500
H	0.55172600	5.23431400	1.21017500
C	3.29183900	-0.21258700	-0.16126200
C	4.06398700	-0.17135000	-1.32835100

C	4.86810200	-1.25442100	-1.67286300
H	5.46607100	-1.21407400	-2.58650300
C	4.89670200	-2.39311700	-0.86729100
H	5.52148600	-3.24511200	-1.14443700
C	4.11502700	-2.44254800	0.28545700
H	4.12026600	-3.33444600	0.91599100
C	3.31416400	-1.35949400	0.64141600
C	-1.50408900	2.31660300	-0.34278500
C	-1.85154500	3.01420800	-1.50577100
C	-3.17737100	3.05043300	-1.92964000
H	-3.43769600	3.59604500	-2.83993300
C	-4.16459400	2.37716900	-1.21042200
H	-5.20195200	2.39701900	-1.55189900
C	-3.81765100	1.66682400	-0.06243600
H	-4.57628500	1.11829100	0.49894600
C	-2.49578600	1.63514800	0.37403800
C	-2.20709000	-2.26567300	0.13045400
C	-2.76598500	-2.13847800	1.41334500
C	-4.12754600	-1.89466600	1.58965000
H	-4.53961200	-1.79217000	2.59712700
C	-4.96379700	-1.78821400	0.47803700
H	-6.03354300	-1.60571000	0.61191500
C	-4.43184000	-1.91466000	-0.80556300
H	-5.08364800	-1.82781100	-1.67897000
C	-3.06765400	-2.14708100	-0.97251400
H	2.69310900	-1.39152000	1.53977800
H	4.01106500	0.70886600	-1.97329000
H	-2.21755300	1.07442100	1.26967600
H	-1.06983400	3.50614100	-2.08886000
H	-2.66870300	-2.23651200	-1.98748300
H	-2.11525800	-2.21145400	2.29016700
C	0.05709200	-2.02951100	-1.84613200
C	-0.04128100	-0.54211500	-1.50565300
H	1.07628300	-2.30140000	-2.15779200
H	-0.64253300	-2.32186500	-2.64384800
H	0.60755200	0.07132800	-2.15916000
H	-1.07450900	-0.18229000	-1.62830400

Cartesian coordinates of the optimized geometry of TS-6 at PBE0-D3BJ/def2-SVP level of theory:

Ge	0.08131000	-1.20674000	1.06424300
Ga	0.84549100	0.67873800	-0.21943000
Cl	0.50678400	0.25133000	-2.38165900
Si	-1.25136200	-3.38567300	-0.78352000
N	2.77644700	0.89465800	0.04663900
N	0.40236800	2.57781100	-0.02066400
N	-1.43447400	-1.99835200	0.28518000
C	3.38356100	2.06525600	0.20723300
C	2.70024600	3.29075500	0.25096400
H	3.32343900	4.17507800	0.37109000
C	1.32202900	3.53067600	0.13226600
C	4.88036200	2.09435600	0.33182100
H	5.34316500	1.53193900	-0.49278600
H	5.20581500	1.60632000	1.26241000
H	5.25642300	3.12390700	0.32474400
C	0.87138800	4.96422700	0.16368400
H	0.30665600	5.20747400	-0.74883500
H	1.72688600	5.64372800	0.24915000
H	0.18721300	5.14249600	1.00604800
C	3.50366900	-0.32638500	0.03547800
C	3.94530400	-0.90018800	1.23213100
C	4.58860300	-2.13451900	1.21921700
H	4.92620300	-2.57803900	2.15885800
C	4.78232200	-2.81202300	0.01565100
H	5.27718700	-3.78569300	0.00825100
C	4.32834300	-2.24815200	-1.17507000
H	4.46382800	-2.77946400	-2.11991600
C	3.68942700	-1.00961700	-1.17006900

C	-0.96463900	2.93896700	-0.20378300
C	-1.79016900	3.20010600	0.89355200
C	-3.11934200	3.56566000	0.69792200
H	-3.75752800	3.76317700	1.56206400
C	-3.63474800	3.67193600	-0.59242300
H	-4.67770400	3.95938200	-0.74355000
C	-2.81848700	3.39274500	-1.68715800
H	-3.21853900	3.45953200	-2.70173100
C	-1.48934300	3.02078100	-1.49793100
C	-2.69801700	-1.37309700	0.35049100
C	-3.63634200	-1.75972600	1.32036900
C	-4.88887500	-1.15044500	1.38843200
H	-5.60376200	-1.46677400	2.15268500
C	-5.23093500	-0.14744300	0.48351500
H	-6.21375100	0.32752600	0.53207800
C	-4.30760100	0.24208300	-0.48798000
H	-4.56453000	1.02449100	-1.20468600
C	-3.05368900	-0.35775800	-0.55317600
C	-2.23232000	-4.84312200	-0.10613900
H	-3.29688500	-4.57769400	-0.00658900
H	-1.86241000	-5.13774800	0.88868800
H	-2.16438700	-5.71844500	-0.77223400
C	0.57534600	-3.82038700	-0.87257400
H	1.16090700	-2.99914500	-1.31519600
H	0.70332400	-4.70777500	-1.51415300
H	1.00734800	-4.05382600	0.11302700
C	-1.88253900	-2.97197100	-2.50332000
H	-2.94625000	-2.68843000	-2.47903500
H	-1.77645900	-3.83562400	-3.17955100
H	-1.31229000	-2.12729500	-2.92056800
C	-0.85192300	0.24288900	2.37437200
C	-0.31770600	-0.93289300	3.02174800
H	-0.31639600	1.18921500	2.48161400
H	-1.92436800	0.32183800	2.17712800
H	0.57167600	-0.85308400	3.65375900
H	-1.01438200	-1.72300100	3.31979500
H	-2.32669600	-0.05288600	-1.30987500
H	-3.36250900	-2.55386700	2.01924500
H	3.30470300	-0.57033700	-2.09240900
H	3.75964800	-0.37847700	2.17396900
H	-0.84520700	2.78060300	-2.34552600
H	-1.38273100	3.11740100	1.90267200

Cartesian coordinates of the optimized geometry of TS-7 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.02117500	-1.23141900	-0.81321500
C	-1.53204800	-0.02812900	0.12138000
C	-1.20668400	1.27659500	0.53107300
C	-2.17135100	2.28310700	0.56302700
H	-1.88770500	3.29051100	0.87861900
C	-3.48824400	2.00881200	0.20240000
H	-4.24478600	2.79635900	0.23115200
C	-3.83426200	0.71297900	-0.19624700
H	-4.86377900	0.48606300	-0.48527600
C	-2.87252300	-0.28628600	-0.23899800
H	-3.15902600	-1.29045000	-0.56791900
H	-0.17843100	1.50741100	0.82264700
C	1.57375800	-0.14957800	-0.25180100
C	2.37909500	-0.35411600	0.87670400
C	1.93307800	0.88876200	-1.12572700
C	3.49147500	0.44948000	1.13073700
H	2.14638500	-1.15365900	1.58777700
C	3.04040200	1.69903700	-0.87992500
H	1.32803200	1.07559800	-2.02058600
C	3.82378300	1.48001700	0.25285300
H	4.10260700	0.26942200	2.01922600
H	3.29453900	2.50384400	-1.57471100
H	4.69431700	2.11057400	0.45011300

C	-0.79868500	-1.41699400	1.41973300
C	-0.12511700	-2.52331200	0.79271500
H	-0.20335500	-0.72917300	2.02665200
H	-1.81930000	-1.55077300	1.78118300
H	0.90367300	-2.73030100	1.10194900
H	-0.71164000	-3.42228800	0.58451600

Cartesian coordinates of the optimized geometry of TS-8 at PBE0-D3BJ/def2-SVP level of theory:

Ge	-0.31758300	-0.97256500	-0.90623900
C	1.44101500	-0.27640900	-0.23710900
C	2.09558600	0.64385800	-1.07041900
C	3.34161600	1.17430900	-0.73522400
H	3.82933000	1.88919000	-1.40312400
C	3.96151100	0.79238100	0.45296000
H	4.93615500	1.20647900	0.72302900
C	3.33187800	-0.12490700	1.29445300
H	3.81432100	-0.43231800	2.22617200
C	2.08960300	-0.65423500	0.94733500
H	1.62645800	-1.37858700	1.62524900
H	1.62116900	0.95782600	-2.00694600
Si	-1.87640700	0.76678500	0.20881900
C	-1.15039400	2.18180800	-0.82116000
H	-1.74159000	3.09532900	-0.63823000
H	-0.10816000	2.38790800	-0.53411700
H	-1.17521800	1.95087200	-1.89621500
C	-3.60583900	0.36187900	-0.42022400
H	-4.09455600	-0.43083700	0.16688300
H	-4.23716200	1.26309300	-0.35319800
H	-3.57793800	0.04105700	-1.47210300
C	-2.00171900	1.52329900	1.94057600
H	-1.00017500	1.75926500	2.33505900
H	-2.56277700	2.46964000	1.87624100
H	-2.51248800	0.87336400	2.66689400
C	-1.20169500	-1.16490400	1.18955000
C	-0.69154200	-2.35827100	0.49464500
H	-2.26057500	-1.20028100	1.47792900
H	-0.56154900	-0.74770200	1.97425000
H	-1.43914500	-3.09739200	0.19160200
H	0.21616400	-2.81266700	0.90450200