

Novel derivatives of hypervalent germanium: synthesis, structure, and stability

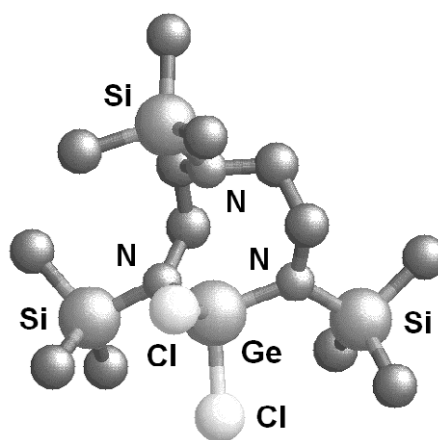
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Supporting information

Calculated Cartesian coordinates of transition states and stable compounds, electronic energies, numbers of imaginary frequencies.

Compound I

Atomic number	X	Y	Z
17	-0.48786626	-5.34406303	-0.04207685
32	1.66850488	-5.46620825	0.41882611
17	1.92665948	-7.67651896	0.43937837
14	3.04304579	-5.52509245	-2.50292326
14	3.06433096	-5.70739001	3.29729521
7	2.78839033	-4.82825843	-0.88141893
7	2.02737488	-4.85541822	2.11486689
6	2.75799695	-2.35191645	-0.45973816
1	2.45648547	-2.14775245	-1.49745712
1	3.42962599	-1.52458836	-0.15062674
6	3.56858539	-3.65670533	-0.45433281
1	3.98361903	-3.81771100	0.55416924
1	4.43591547	-3.52659679	-1.12133223
6	1.79470772	-2.37592058	1.82406628
1	2.87346878	-2.26255670	2.01869618
1	1.30598222	-1.50279385	2.29647079
6	1.29546609	-3.64395313	2.52765689
1	0.21636381	-3.75649555	2.33663356
1	1.40406115	-3.50931303	3.61431553
6	1.53843498	-6.52903980	-3.03625888
1	0.63102844	-5.91187234	-3.06486545
1	1.71843232	-6.91433553	-4.05123732
1	1.35021346	-7.38743650	-2.37998497
6	3.29079779	-4.11057197	-3.74307276
1	4.13610630	-3.45599986	-3.49051326
1	3.49595950	-4.53663047	-4.73644964
1	2.38704554	-3.49149863	-3.82741771
6	4.59429590	-6.60905694	-2.48943467
1	5.47493896	-6.04248029	-2.15463802
1	4.45970790	-7.45929301	-1.80690302
1	4.80994396	-7.00473322	-3.49255865
6	3.61306453	-4.44371278	4.60479119
1	4.03499068	-3.53450031	4.15507308
1	2.80693974	-4.14995879	5.29032904
1	4.40318399	-4.90737134	5.21460355
6	2.12747104	-7.09627319	4.17196604
1	1.83240359	-7.88175465	3.46425502
1	2.75009858	-7.55362006	4.95492453
1	1.21548032	-6.70734239	4.64672949
6	4.62412225	-6.36825214	2.45776218
1	5.24348402	-5.54690680	2.07058861
1	5.22342699	-6.91853103	3.19837898
1	4.40081268	-7.05387429	1.63155190
14	0.17596091	-1.43805686	-0.22922610
7	1.55144628	-2.41596070	0.37179068
6	-1.32527931	-1.70136174	0.88768678
1	-1.13296881	-1.41084695	1.92952838
1	-2.15369737	-1.07664608	0.52240024
1	-1.65810330	-2.74712771	0.87253614
6	0.63262445	0.40662568	-0.20944855
1	1.50422599	0.61058409	-0.84781496
1	-0.20304321	1.01602879	-0.58327891
1	0.86986172	0.75598706	0.80570557
6	-0.23337466	-1.95410489	-2.00080611
1	0.51365156	-1.60780145	-2.72799167
1	-0.32096362	-3.04544409	-2.07810719
1	-1.19834302	-1.51297706	-2.29056239

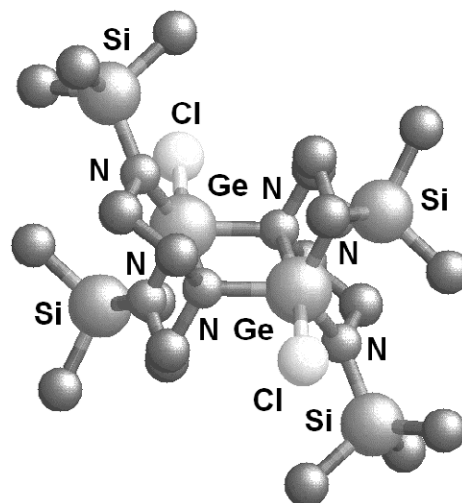


Energy = -4545.23612683 Hartree

Number of imaginary frequencies = 0.

Compound II

Atomic number	X	Y	Z
32	6.15548781	-5.77082584	-0.40874684
17	6.20284139	-7.75954691	-1.60386052
14	7.32423705	-8.08689147	1.67423314
14	8.13434753	-5.16923013	-2.99231734
7	6.84943169	-6.42704352	1.20594609
7	7.10019859	-4.69269155	-1.61659785
7	5.78142386	-3.96819060	0.66422725
6	6.16331774	-4.23567453	2.07040120
1	5.28654240	-4.61582299	2.61212688
1	6.48788267	-3.30913821	2.56625645
6	7.26163178	-5.30018429	2.06156102
1	8.21568029	-4.85421681	1.71952156
1	7.42462275	-5.63481185	3.09395349
6	6.62525288	-2.93571983	0.02797173
1	7.62299732	-2.97324455	0.49304425
1	6.20609225	-1.93103422	0.18828887
6	6.75913764	-3.26843727	-1.45332422
1	5.81900723	-3.00474878	-1.97201873
1	7.54710247	-2.63083676	-1.87610739
6	5.88849518	-9.31400997	1.55265318
1	5.04880269	-9.00595984	2.19137949
1	6.23237003	-10.29769002	1.90685472
1	5.52720557	-9.43300257	0.52474549
6	7.81579680	-8.03261437	3.51131282
1	8.72383432	-7.44351323	3.69866848
1	8.02635874	-9.06441416	3.83118786
1	7.01112046	-7.65163169	4.15602190
6	8.82601255	-8.74211478	0.72892302
1	9.66148978	-8.02951026	0.77032572
1	8.58874412	-8.93307752	-0.32444262
1	9.16608219	-9.68654246	1.17968661
6	9.12981612	-3.63479153	-3.51411725
1	9.70891384	-3.20688522	-2.68355218
1	8.50878992	-2.84205289	-3.95296831
1	9.84959239	-3.94613632	-4.28622462
6	7.13540560	-5.71890353	-4.50561585
1	6.54902885	-6.62128650	-4.29151308
1	7.81059397	-5.94011394	-5.34590143
1	6.44704347	-4.92622875	-4.83333133
6	9.39168831	-6.49048056	-2.50367582
1	9.97382494	-6.16994595	-1.62877824
1	10.09277187	-6.64723546	-3.33695613
1	8.91728308	-7.45055102	-2.72729827
32	3.80047863	-3.81301977	0.40986897
17	3.75194469	-1.82507272	1.60632342
14	2.63260919	-1.49633386	-1.67335183
14	1.82227424	-4.41552770	2.99398116
7	3.10835139	-3.15605408	-1.20533845
7	2.85581810	-4.89147369	1.61754162
7	4.17451737	-5.61535015	-0.66336950
6	3.79345675	-5.34778388	-2.06978258
1	4.67074224	-4.96845546	-2.61123779
1	3.46831758	-6.27416434	-2.56554550
6	2.69592194	-4.28248152	-2.06144549
1	1.74131204	-4.72787778	-1.72021941
1	2.53395004	-3.94740526	-3.09386368
6	3.33018406	-6.64771011	-0.02760295
1	2.33228933	-6.60906683	-0.49226916
1	3.74857445	-7.65257172	-0.18876092
6	3.19718579	-6.31560725	1.45382341
1	4.13786128	-6.57900399	1.97168813
1	2.40987557	-6.95359189	1.87720708
6	4.06425137	-0.26536678	-1.54275765
1	4.90810656	-0.57027800	-2.17751577
1	3.71911351	0.71745438	-1.89815013
1	4.41984316	-0.14612877	-0.51295455
6	2.15014196	-1.54866007	-3.51269986
1	1.24337688	-2.13801831	-3.70528788
1	1.94071388	-0.51663330	-3.83257794
1	2.95830075	-1.92862940	-4.15365612
6	1.12466383	-0.84851998	-0.73274490



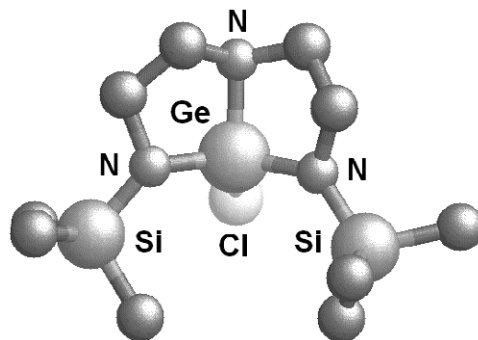
1	0.29168320	-1.56367149	-0.78037696
1	1.35699890	-0.66113855	0.32239557
1	0.78344886	0.09664573	-1.18103842
6	0.82652791	-5.95005659	3.51499276
1	0.24665640	-6.37674493	2.68433139
1	1.44734123	-6.74360926	3.95264461
1	0.10736231	-5.63911231	4.28783723
6	2.82202113	-3.86704823	4.50718851
1	3.41002447	-2.96588347	4.29241530
1	2.14715535	-3.64374390	5.34718375
1	3.50873459	-4.66081978	4.83562246
6	0.56494098	-3.09367613	2.50691333
1	-0.01648994	-3.41265377	1.63097879
1	-0.13678091	-2.93870212	3.33998726
1	1.03929808	-2.13307115	2.27836373

Energy = -7352.29516409 Hartree

Number of imaginary frequencies = 0.

Compound III

Atomic number	X	Y	Z
32	4.47703905	-5.10430001	-0.55842888
17	6.39233637	-6.11049508	-0.95310369
14	3.78859572	-6.75005275	2.25517804
14	3.09916960	-6.60724899	-3.12589898
7	4.02473673	-5.33396481	1.21962343
7	3.33364750	-5.25206494	-2.00844954
7	4.43167575	-3.23508750	-0.51404458
6	4.27642945	-2.90751965	0.91481935
1	5.27846124	-2.82086035	1.36231553
1	3.77098343	-1.93715293	1.03162056
6	3.49777834	-4.01877973	1.65780929
1	2.41401180	-3.92294163	1.45752727
1	3.63814456	-3.89965156	2.74318148
6	3.27302416	-2.87988973	-1.35668863
1	2.31804982	-2.93199340	-0.79725511
1	3.38085301	-1.85364199	-1.74482107
6	3.20731751	-3.86696308	-2.52938010
1	4.01000352	-3.62371860	-3.24996377
1	2.24417044	-3.74528179	-3.04773721
6	4.75058731	-8.22060899	1.57086395
1	5.82482793	-8.00568305	1.50849498
1	4.61181896	-9.07806625	2.24615930
1	4.40444120	-8.52737241	0.57595702
6	4.42838399	-6.34522964	3.99344309
1	3.82898690	-5.57454442	4.49724107
1	4.39076818	-7.24739253	4.62182765
1	5.47147190	-6.00241360	3.95732472
6	1.94558787	-7.18123761	2.37500925
1	1.36256734	-6.33338407	2.76264990
1	1.53597486	-7.44731682	1.39047649
1	1.78312210	-8.03292029	3.05144680
6	1.35894098	-6.46459652	-3.86229064
1	0.59656147	-6.41623696	-3.07292750
1	1.25063217	-5.57621865	-4.49993696
1	1.14337908	-7.34259213	-4.48868746
6	4.36511253	-6.58612636	-4.53426638
1	5.38764294	-6.66496329	-4.14031348
1	4.19717700	-7.42788365	-5.22196029
1	4.29778907	-5.65958120	-5.12198799
6	3.25165157	-8.21381151	-2.14697100
1	2.55494095	-8.23611731	-1.29787735
1	3.01229766	-9.06640601	-2.79794797
1	4.27370909	-8.36248822	-1.77273080

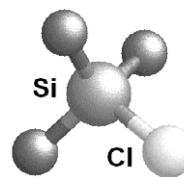


Energy = -3676.13029045 Hartree

Number of imaginary frequencies = 0.

Compound Me3SiCl

Atomic number	X	Y	Z
14	3.91380628	-4.36760851	0.27480125
17	5.65062880	-5.58268420	0.28916323
6	2.91876034	-4.81162815	1.81008110
1	3.50186619	-4.62292210	2.72089861
1	1.99926080	-4.20977482	1.85899728
1	2.63522734	-5.87213703	1.79775564
6	4.49438634	-2.57698448	0.31060239
1	5.11786428	-2.35161515	-0.56444531
1	3.63234766	-1.89365072	0.30437249
1	5.08537041	-2.37650024	1.21379155
6	2.97517030	-4.76765535	-1.30747525
1	3.59071805	-4.55351773	-2.19091098
1	2.69197724	-5.82795406	-1.33549134
1	2.05761563	-4.16436657	-1.37254061

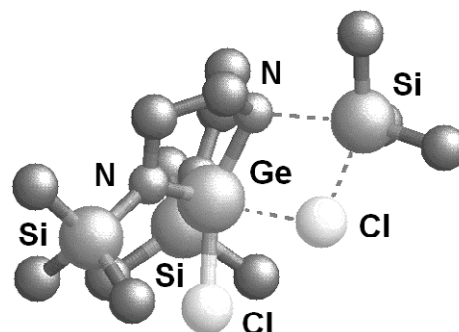


Energy = -869.09762433 Hartree

Number of imaginary frequencies = 0.

Compound TS1

Atomic number	X	Y	Z
17	3.34586079	-7.16621478	-0.98761043
32	5.86981015	-7.49314695	-0.29828243
17	5.29891743	-9.66936896	-0.19668654
14	7.48229585	-8.76042834	-2.88773267
14	6.88427485	-8.47954935	2.69282062
7	6.86338012	-7.43454265	-1.86421117
7	6.61459258	-7.27523418	1.39332427
6	5.89452098	-5.18497755	-1.78501306
1	5.03681758	-5.41017252	-2.43377139
1	6.13175935	-4.11595671	-1.87752429
6	7.08534216	-6.03716697	-2.24661968
1	8.02753325	-5.64062958	-1.82124567
1	7.16639779	-5.92721400	-3.33745015
6	6.47562197	-4.93976082	0.57354672
1	7.45332758	-4.81199683	0.08015983
1	6.14508683	-3.94267110	0.90573048
6	6.65478549	-5.86024726	1.79101851
1	5.89045174	-5.63353647	2.55178706
1	7.62953918	-5.61203778	2.23866392
6	6.08652315	-9.64620500	-3.80392275
1	5.50842649	-8.93528911	-4.41063911
1	6.49717903	-10.41345035	-4.47707297
1	5.39698066	-10.13627260	-3.10529061
6	8.63139252	-7.97099758	-4.17825509
1	9.41109876	-7.34870197	-3.71797666
1	9.13574571	-8.77717323	-4.73176944
1	8.09192869	-7.36123993	-4.91591960
6	8.51418163	-9.98769635	-1.88837841
1	9.33934344	-9.47591240	-1.37420322
1	7.91248397	-10.51386540	-1.13791275
1	8.94903996	-10.74049584	-2.56241745
6	7.84496818	-7.58490956	4.06653147
1	8.81729294	-7.21048197	3.71712754
1	7.28683467	-6.74636107	4.50412973
1	8.04264920	-8.30489692	4.87469325
6	5.25520845	-9.08980914	3.43720160
1	4.64601821	-9.61574903	2.69144201
1	5.45262472	-9.78126938	4.26976513
1	4.66586821	-8.25052217	3.83343794
6	7.96042975	-9.92155137	2.12109210
1	8.87887215	-9.55509039	1.64276621
1	8.25193713	-10.51894902	2.99781873
1	7.44076625	-10.58079780	1.41712522
14	3.32137451	-5.00081610	-0.10628299
7	5.50833203	-5.51329565	-0.38746987
6	3.36786955	-5.13832722	1.78297350
1	4.10360164	-4.46693053	2.24209290
1	2.37497011	-4.86219509	2.16416540
1	3.57194415	-6.16578697	2.10923798
6	3.75343825	-3.25849481	-0.76935389
1	3.63700729	-3.20505303	-1.86058228
1	3.00259831	-2.57806674	-0.34032192
1	4.74719031	-2.87693849	-0.50745196
6	1.44508738	-4.97363263	-0.52823872
1	1.26987762	-4.97033503	-1.61350511
1	0.91879626	-5.84012281	-0.10663300
1	0.99130044	-4.05896298	-0.11450736

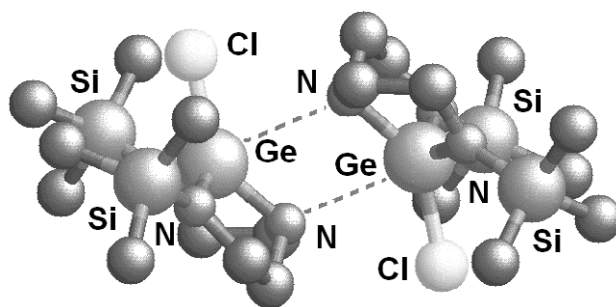


Energy = -4545.18993543 Hartree

Number of imaginary frequencies = 1.

Compound TS2

Atomic number	X	Y	Z
32	6.76643049	-5.78454788	-0.14057437
17	6.10722115	-7.59208041	-1.28632277
14	7.92029855	-8.18240332	1.87102796
14	8.52105270	-5.24059258	-2.89721803
7	7.40792192	-6.53675082	1.43516618
7	7.75849185	-4.79131078	-1.35719668
7	6.10905367	-4.21620768	0.74009948
6	6.12680210	-4.56914475	2.16679339
1	5.18171390	-5.08162104	2.40608389
1	6.17735300	-3.65952959	2.78275504
6	7.29614094	-5.52008094	2.49917234
1	8.23600933	-4.94944579	2.60891808
1	7.09312906	-5.98797608	3.47464101
6	7.10017055	-3.18534123	0.37955438
1	8.02402028	-3.26147468	0.98592984
1	6.66803278	-2.18496351	0.54326155
6	7.46706181	-3.36445090	-1.09515492
1	6.63691796	-2.99058298	-1.72479041
1	8.34873266	-2.74512589	-1.31528478
6	6.41983646	-9.25896212	2.29354537
1	5.81422047	-8.79663212	3.08625441
1	6.73175888	-10.25372847	2.64433131
1	5.77990393	-9.39252810	1.41073773
6	9.03019980	-8.04959034	3.40560173
1	9.85338895	-7.33951705	3.24585052
1	9.47365363	-9.03431219	3.61484927
1	8.48225710	-7.74004091	4.30570945
6	8.93174775	-9.00019243	0.50314848
1	9.81234819	-8.39706974	0.24505872
1	8.34394879	-9.16701459	-0.40708380
1	9.28681437	-9.97867676	0.85968746
6	9.74646923	-3.86284658	-3.34517035
1	10.46396126	-3.67680666	-2.53391244
1	9.24514842	-2.91641404	-3.58941769
1	10.32040461	-4.16766851	-4.23280264
6	7.26454119	-5.38982496	-4.30876354
1	6.55399836	-6.20515980	-4.11846753
1	7.77676681	-5.59831175	-5.25988566
1	6.69341340	-4.45899321	-4.43579911
6	9.47388128	-6.85814929	-2.71191442
1	10.23154717	-6.78055201	-1.92067959
1	9.99133827	-7.08635758	-3.65533427
1	8.81295389	-7.70210383	-2.48033305
32	3.18435119	-3.79464062	0.14459093
17	3.84782617	-1.98329491	1.27784547
14	2.03628177	-1.41280214	-1.88409016
14	1.42642334	-4.32866595	2.90031364
7	2.54368398	-3.05736992	-1.43807702
7	2.19357036	-4.78434456	1.36448231
7	3.85709249	-5.36442904	-0.72196537
6	3.83649921	-5.02335861	-2.15228253
1	4.77761656	-4.50578341	-2.39581843
1	3.79285393	-5.93881084	-2.75980245
6	2.66010922	-4.08436941	-2.49201600
1	1.72391856	-4.66273790	-2.59278083
1	2.85711106	-3.62520830	-3.47263058
6	2.87281726	-6.40040770	-0.35439700
1	1.95079291	-6.33666619	-0.96461455
1	3.31371707	-7.39837538	-0.50805956
6	2.49946631	-6.21081653	1.11718097
1	3.33096108	-6.57087933	1.75313279
1	1.62300492	-6.83653673	1.34012998
6	3.53924369	-0.32998198	-2.28062901
1	4.15856644	-0.78883740	-3.06469337
1	3.22881715	0.66425034	-2.63431937
1	4.16485076	-0.19578592	-1.38776134
6	0.95446244	-1.54893851	-3.43835554
1	0.13423704	-2.26613150	-3.29627981
1	0.50685260	-0.56689180	-3.65149684
1	1.52103923	-1.84977880	-4.32983966
6	0.99951314	-0.60253659	-0.53081160



1	0.11661364	-1.20928385	-0.29063552
1	1.57241238	-0.44004017	0.38999725
1	0.64825442	0.37785598	-0.88590851
6	0.19773994	-5.70338706	3.34827097
1	-0.51580527	-5.89162408	2.53406759
1	0.69688077	-6.64944222	3.59832642
1	-0.38016318	-5.39495961	4.23205531
6	2.67859503	-4.17434309	4.31493249
1	3.39269751	-3.36290028	4.12085414
1	2.16352984	-3.95616078	5.26234022
1	3.24612420	-5.10587475	4.45217045
6	0.47739541	-2.71004341	2.70593071
1	-0.27217504	-2.78514566	1.90685005
1	-0.04943982	-2.48229514	3.64425303
1	1.14200164	-1.86674317	2.48246982

Energy = -7352.25087103 Hartree

Number of imaginary frequencies = 1.