Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Promotion of TH_3 (T=Si and Ge) group transfer within a tetrel bond by a cation-π interaction

Table S1 The particular value of intermolecular distance R(C···C, Å)=R_1+R_2 and energy barrier (ΔE, kcal/mol) in Be^{2+}···$PhSiH_3$···$C_3N_2H_4$ triad

R(C···C)	ΔE
4.6	9.40
4.7	9.62
4.8	9.86
4.9	10.09
5.0	10.34

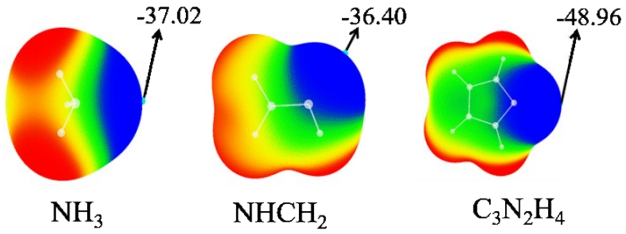

Figure S1 MEP maps of N-base monomers. Color ranges are: red, greater than 12; yellow, between 12 and zero; green, between zero and -12; blue, less than -12. All are in kcal/mol.

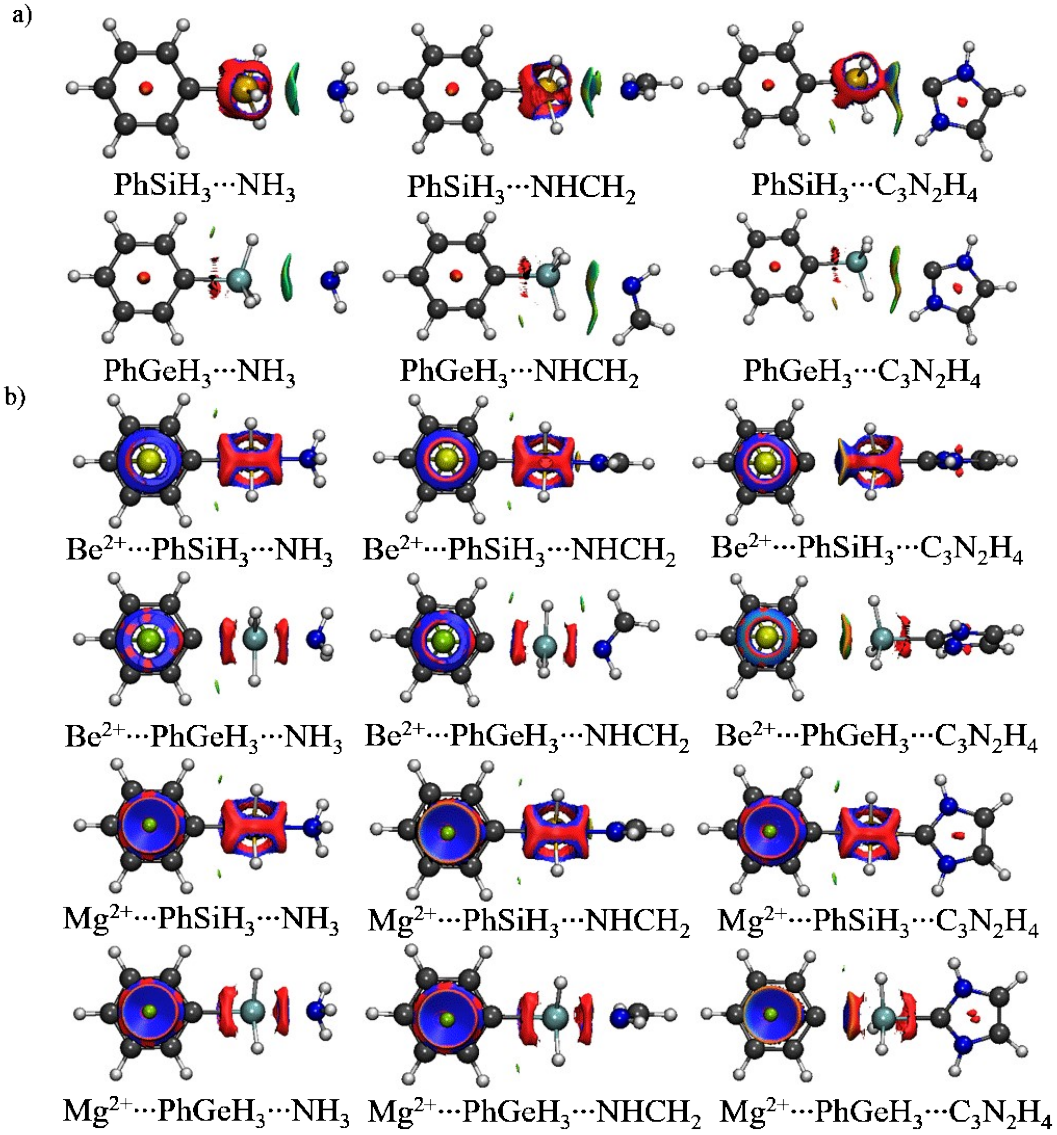

Figure S2 NCI isosurfaces (iso=0.4 a.u.) of a) binary and b) ternary systems. Blue, green, orange, and red areas represent strong attraction, weak attraction, weak repulsion, and strong repulsion, respectively. Diagrams are drawn by the Multiwfn [1] and the VMD programs [2].

[1] T. Lu, F. Chen, Multiwfn: a multifunctional wavefunction analyzer. *J. Comput. Chem*. 2012, **33**, 580-592.

[2] W. Humphrey, A. Dalke, K. Schulten, VMD: visual molecular dynamics. *J. Mol. Graph*. 1996, **14**, 33-38.

Cartesian coordinates of monomers and complexes

$PhSiH_3$

C	-1.64802100	1.20612500	0.00361200
C	-0.25419300	1.20370500	-0.01118900
C	0.46671200	0.00010300	-0.01524000
C	-0.25407400	-1.20363900	-0.01118400
C	-1.64783400	-1.20625200	0.00361500
C	-2.34658500	-0.00008300	0.01170600
H	-2.18756200	2.14453100	0.00451600
H	0.27472300	2.15010300	-0.02500700
H	0.27484000	-2.15006800	-0.02500700
H	-2.18728200	-2.14471200	0.00451500
H	-3.42882300	-0.00018000	0.02068500
Si	2.34332300	0.00002500	0.00684000
H	2.86039600	-0.01681600	1.39589000
H	2.84632200	-1.20419600	-0.69412600
H	2.84483200	1.22124900	-0.66514500

$PhGeH_3$

C	-2.22457800	1.20628100	-0.00000900
C	-0.82978500	1.20118500	0.00001600
C	-0.11485300	-0.00242700	0.00001000
C	-0.83422600	-1.20457800	0.00001600
C	-2.22767500	-1.20499800	-0.00000500
C	-2.92509300	0.00220100	-0.00001100
H	-2.76162900	2.14602100	-0.00001000
H	-0.29640400	2.14478500	0.00004100
H	-0.30825800	-2.15285000	0.00003000
H	-2.76785300	-2.14299600	-0.00000200
H	-4.00732000	0.00348800	-0.00002700
Ge	1.81596300	0.00014200	-0.00000400
H	2.33888400	-0.71522500	1.23236400
H	2.33890100	-0.71416400	-1.23299800
H	2.29010700	1.44041900	0.00061100

Be^{2+}-$PhSiH_3$

C	1.62847500	-1.22734700	-0.13281800
C	0.20744300	-1.22078300	-0.09247700
C	-0.54099600	0.00024300	-0.07085800
C	0.20776200	1.22097100	-0.09248600
C	1.62881900	1.22723000	-0.13277900
C	2.34088900	-0.00017200	-0.15096800
H	2.16993400	-2.16525300	-0.06611300
H	-0.31212000	-2.16902700	0.00272000
H	-0.31152600	2.16937100	0.00266900

H	2.17067300	2.16489500	-0.06591800
H	3.42427300	-0.00037600	-0.09810300
Si	-2.51393300	0.00002000	-0.02302300
H	-2.82930000	-1.24361000	0.69449000
H	-2.82977500	1.24339300	0.69477000
H	-2.84319700	0.00007800	-1.45507800
Be	0.93043800	-0.00015300	1.16179900

Be^{2+}-$PhGeH_3$

C	-2.21677800	1.22703900	-0.13354200
C	-0.79577600	1.21952000	-0.09220700
C	-0.04802700	-0.00002300	-0.06842200
C	-0.79580900	-1.21954500	-0.09220400
C	-2.21681000	-1.22702400	-0.13353600
C	-2.92896300	0.00001600	-0.15094700
H	-2.75855200	2.16466200	-0.06722200
H	-0.27669400	2.16786100	0.00343400
H	-0.27675800	-2.16790200	0.00342700
H	-2.75861500	-2.16463000	-0.06721300
H	-4.01227900	0.00003100	-0.09845000
H	2.28438900	-1.27686100	0.72456800
H	2.30797500	-0.00032600	-1.47992000
H	2.28432000	1.27720500	0.72398800
Be	-1.51785700	0.00001900	1.16091200
Ge	1.97783200	0.00000000	-0.01128500

Mg^{2+}-$PhSiH_3$

C	1.47357200	-1.22050800	-0.49542000
C	0.06953600	-1.21434200	-0.32370500
C	-0.66912100	0.00029300	-0.23027000
C	0.06977400	1.21478000	-0.32322000
C	1.47382700	1.22069700	-0.49486400
C	2.17912800	0.00005300	-0.57895300
H	2.00620400	-2.16128600	-0.58188600
H	-0.45303600	-2.16504600	-0.28292300
H	-0.45263700	2.16555100	-0.28211000
H	2.00668000	2.16137700	-0.58101900
H	3.25281800	-0.00005500	-0.72883100
Si	-2.61322200	0.00003400	-0.06422700
H	-3.03662300	-1.24552200	-0.71843700
H	-2.85094600	-0.00670700	1.39382600
H	-3.03605300	1.25179300	-0.70688600
Mg	0.96403300	-0.00053500	1.50550300

Mg^{2+}-$PhGeH_3$

C	-2.01531700	1.22035900	-0.51329000
C	-0.61849300	1.21361900	-0.28954400

C	0.11639800	-0.00001800	-0.17550600
C	-0.61864800	-1.21368200	-0.28966900
C	-2.01539100	-1.22020400	-0.51345800
C	-2.71676900	0.00016300	-0.62463600
H	-2.54518500	2.16126200	-0.61320000
H	-0.09924400	2.16440500	-0.21896800
H	-0.09946600	-2.16450200	-0.21904400
H	-2.54550800	-2.16094200	-0.61371600
H	-3.78468100	0.00006900	-0.81091700
H	2.42499000	-1.26332400	0.72886100
H	2.56386400	-0.00874600	-1.47104600
H	2.42533900	1.27182800	0.71436500
Ge	2.11560200	0.00001300	-0.03397800
Mg	-1.56917100	-0.00015800	1.50229800

$PhSiH_3\cdots NH_3$

C	2.47196700	-1.20451900	0.00442800
C	1.07778500	-1.20168800	-0.01268400
C	0.35195800	-0.00087700	-0.01771700
C	1.07545200	1.20136200	-0.01267900
C	2.46959300	1.20691100	0.00442200
C	3.17045800	0.00186800	0.01412900
H	3.01198200	-2.14298000	0.00596000
H	0.54993300	-2.14916500	-0.02830700
H	0.54584900	2.14788000	-0.02828000
H	3.00777900	2.14642200	0.00593700
H	4.25282900	0.00293400	0.02518800
Si	-1.53421800	-0.00296300	0.00507500
H	-2.00200500	0.00630300	1.40950900
H	-1.99184500	1.21879700	-0.69229100
H	-1.98839400	-1.23485200	-0.67625300
N	-4.64686700	0.00094800	-0.00064100
H	-5.02737300	-0.81996100	0.45444500
H	-5.05508500	0.03672600	-0.92685300
H	-4.99983500	0.80440400	0.50499200

$PhSiH_3\cdots NHCH_2$

C	2.87358300	-1.20626700	-0.12570100
C	1.48910500	-1.20147100	0.03936100
C	0.76939900	0.00029200	0.12101800
C	1.48999300	1.20150300	0.03891500
C	2.87447400	1.20520900	-0.12615400
C	3.56874900	-0.00080100	-0.20971000
H	3.40920500	-2.14545000	-0.18406900
H	0.96460300	-2.14825000	0.11147100
H	0.96616200	2.14867100	0.11069700

H	3.41080500	2.14396500	-0.18488500
H	4.64388100	-0.00121600	-0.33531500
Si	-1.10883700	0.00109400	0.29856000
H	-1.48914400	1.23091000	1.02585400
H	-1.70862100	-0.00081300	-1.05700200
H	-1.48997000	-1.22623300	1.02966400
C	-4.69286700	-0.00083600	-0.74577400
N	-4.11007300	0.00047800	0.38984200
H	-4.79719100	-0.00331200	1.14438100
H	-5.77392300	-0.00543200	-0.88135600
H	-4.07620300	0.00271300	-1.63990100

$PhSiH_3 \cdots NHC$

C	1.99664400	-0.11750000	-0.00005900
C	2.88440000	-1.20520300	0.00016000
C	2.55018900	1.17097400	-0.00026500
C	4.26536800	-1.01683300	0.00018200
H	2.49511600	-2.21841000	0.00031500
C	3.93129700	1.37070400	-0.00024400
H	1.89315200	2.03425900	-0.00044700
C	4.79195600	0.27485700	-0.00002000
H	4.92962500	-1.87211200	0.00035400
H	4.33449600	2.37581900	-0.00040600
H	5.86405800	0.42479500	-0.00000500
H	-0.42833000	0.99420600	-0.00059700
H	-0.21056300	-1.14422600	-1.22425600
H	-0.21070700	-1.14325200	1.22471900
C	-4.57531300	1.06718400	0.00013300
C	-5.08695900	-0.19649600	0.00024700
H	-5.06600300	2.02334300	0.00017300
H	-6.10441200	-0.54294400	0.00041200
N	-3.99100500	-1.03485500	0.00014100
N	-3.20594200	0.90779400	-0.00011200
C	-2.79046900	-0.38901000	-0.00007900
H	-4.04595300	-2.03882700	0.00020000
H	-2.53818700	1.66167200	-0.00026500
Si	0.11883300	-0.38692600	-0.00005200

$PhGeH_3 \cdots NH_3$

C	2.84012500	-1.19386100	0.00101500
C	1.44639100	-1.20064600	0.00007900
C	0.71592200	-0.00492600	-0.00047700
C	1.42672200	1.20130700	-0.00002800
C	2.82180800	1.21687600	0.00090100
C	3.53065000	0.01748600	0.00143900
H	3.38618800	-2.12867200	0.00142300

H	0.92687300	-2.15293400	-0.00022000
H	0.88719100	2.14185100	-0.00044500
H	3.35289500	2.16022800	0.00122600
H	4.61300600	0.02568300	0.00217800
N	-4.44577500	0.02799700	0.00238600
H	-4.82512600	-0.91042200	-0.03167700
H	-4.83657600	0.52835100	-0.78666800
H	-4.82028600	0.46278200	0.83690400
Ge	-1.22406600	-0.01530000	-0.00161800
H	-1.70638200	-0.74202500	1.23850300
H	-1.67163800	1.43169500	-0.00066500
H	-1.70530400	-0.74033600	-1.24307400

$PhGeH_3\cdots NHCH_2$

C	-3.27658400	-0.97242200	-0.01469100
C	-1.89425000	-1.15054800	-0.01045500
C	-1.02229800	-0.05378000	0.00144600
C	-1.57977600	1.23046300	0.00906200
C	-2.96232500	1.41764700	0.00492300
C	-3.81323200	0.31451700	-0.00695500
H	-3.93336900	-1.83305700	-0.02394500
H	-1.49564600	-2.15942900	-0.01650300
H	-0.92855500	2.09756300	0.01835000
H	-3.37334900	2.41918700	0.01099400
H	-4.88637900	0.45561700	-0.01018500
Ge	0.90212700	-0.30197000	0.00781000
H	1.29978700	-1.06472700	-1.23957900
H	1.50834900	1.08743000	0.02020500
H	1.28946000	-1.08385400	1.24640600
C	4.48146800	0.88089200	-0.02721700
N	3.99558800	-0.29884400	0.01079300
H	4.74501700	-0.99147200	0.01993500
H	5.54723000	1.10650000	-0.04701500
H	3.79224500	1.72056700	-0.04081200

$PhGeH_3\cdots NHC$

C	-2.06692400	-0.06769700	-0.00001300
C	-2.99567400	-1.11706700	-0.00000500
C	-2.55756100	1.24347300	-0.00004100
C	-4.36701900	-0.86717800	-0.00002800
H	-2.65039900	-2.14555600	0.00002000
C	-3.92844400	1.50305800	-0.00006500
H	-1.86220800	2.07591500	-0.00004100
C	-4.83606300	0.44596900	-0.00005900
H	-5.06785700	-1.69250500	-0.00002100
H	-4.28672200	2.52475200	-0.00008600

H	-5.90041800	0.64290700	-0.00007600
H	0.48953200	0.95620900	0.00016200
H	0.19208900	-1.19760800	1.25057500
H	0.19217700	-1.19736000	-1.25068100
C	4.59435200	1.23679200	-0.00000500
C	5.26761000	0.05144600	0.00002300
H	4.95517700	2.24915800	-0.00003600
H	6.32176400	-0.15827300	0.00002200
N	4.29082800	-0.92325000	0.00005900
N	3.25778400	0.89841500	0.00001400
C	3.01345900	-0.44305400	0.00005400
H	4.47756800	-1.91104400	0.00008700
H	2.49705900	1.55825900	-0.00000100
Ge	-0.15438900	-0.42017100	0.00001200
	$Be^{2+}\cdots PhSiH_3\cdots NH_3$		
C	2.35492178	-1.22856602	-0.14902208
C	0.93401578	-1.21544802	-0.06722208
C	0.17636878	0.00016198	-0.01991808
C	0.93431378	1.21555198	-0.06715808
C	2.35521578	1.22833198	-0.14900708
C	3.06538278	-0.00019702	-0.18348408
H	2.90288678	-2.16267802	-0.09476808
H	0.41601578	-2.16286002	0.04410292
H	0.41649578	2.16305498	0.04425192
H	2.90341678	2.16230698	-0.09478708
H	4.14855178	-0.00031502	-0.15295308
Si	-1.97807069	0.00023450	0.00108080
H	-1.97359169	-1.28630450	0.72495780
H	-1.97349969	1.28471950	0.72856080
H	-1.92029869	0.00303550	-1.47280720
N	-4.04957108	-0.00021949	-0.04441572
H	-4.42557408	-0.81550149	-0.52784172
H	-4.42646408	0.81579051	-0.52588772
H	-4.46636608	-0.00165449	0.88604028
Be	1.64264900	-0.00007800	1.13758800
	$Be^{2+}\cdots PhSiH_3\cdots NHCH_2$		
C	2.72384249	-1.22869919	-0.23027781
C	1.31057649	-1.21552319	-0.06105981
C	0.55728449	0.00001081	0.03409219
C	1.31061749	1.21550081	-0.06125681
C	2.72388449	1.22860681	-0.23048081
C	3.43056049	-0.00006419	-0.30786981
H	3.27466149	-2.16241619	-0.20946881
H	0.79997849	-2.16250419	0.08362819

H	0.80004249	2.16252081	0.08327519
H	3.27473849	2.16230781	-0.20982781
H	4.51351549	-0.00009019	-0.34279781
Si	-1.59405953	0.00008924	0.23320497
C	-4.42872895	-0.00032804	-0.66767116
N	-3.62292995	0.00024196	0.32618784
H	-4.08470895	0.00083796	1.23587384
H	-5.50336695	-0.00017504	-0.52946016
H	-4.02059395	-0.00097704	-1.67167016
H	-1.51783453	1.27761324	0.97033097
H	-1.65514953	-0.00089176	-1.24367103
H	-1.51789453	-1.27650376	0.97194397
Be	2.09072200	0.00007300	1.09683600
	$Be^{2+}\cdots PhSiH_3\cdots NHC$		
C	-1.91260748	-0.00104755	-0.11236599
C	-2.65642348	-1.17453855	0.25670101
C	-2.69342748	1.20201245	-0.21402399
C	-4.06709648	-1.17399055	0.46468801
H	-2.14325448	-2.13000055	0.28948401
C	-4.10461648	1.23794545	-0.01287899
H	-2.21121048	2.11341745	-0.55128499
C	-4.78887148	0.03774545	0.31053801
H	-4.60921048	-2.09620355	0.63962801
H	-4.67530248	2.14045245	-0.19936299
H	-5.87038248	0.03109145	0.36168701
C	4.94084910	-0.16286580	-0.48314427
C	4.80062010	0.22649620	0.82204773
H	5.82166210	-0.34699380	-1.07274627
H	5.53711210	0.44301220	1.57561573
N	3.45363410	0.30882520	1.04812573
N	3.67104810	-0.29521980	-0.97724727
C	2.73070010	-0.00900780	-0.04921427
H	3.03565110	0.57672320	1.92900973
H	3.45941510	-0.57302880	-1.92570927
Be	-3.48507100	-0.21541900	-1.07195000
Si	0.77534387	-0.02851309	-0.18263674
H	0.49010187	-1.44602209	-0.46723574
H	0.45974887	0.44789091	1.17766026
H	0.52453487	0.91131191	-1.28829774
	$Be^{2+}\cdots PhGeH_3\cdots NH_3$		
C	2.82445524	-1.22866482	-0.15183325
C	1.40342424	-1.21429882	-0.06724625
C	0.64518624	0.00033318	-0.01283025
C	1.40386624	1.21462518	-0.06730625

C	2.82493724	1.22844118	-0.15183525
C	3.53440124	-0.00023982	-0.18568725
H	3.37318124	-2.16239482	-0.09932425
H	0.88830624	-2.16309682	0.04466175
H	0.88900124	2.16357718	0.04446975
H	3.37400824	2.16197018	-0.09935225
H	4.61757224	-0.00045882	-0.15599125
N	-3.81160345	0.00010676	-0.05055224
H	-4.18815245	-0.81778024	-0.52651624
H	-4.18787245	0.80967776	-0.54073924
H	-4.23410745	0.00827976	0.87591976
Ge	-1.63075280	-0.00001994	0.00382349
H	-1.64078280	-1.30808094	0.75862349
H	-1.64024080	1.32077106	0.73612149
H	-1.58514080	-0.01370694	-1.50492351
Be	2.10115100	-0.00001000	1.13413700

$Be^{2+}\cdots PhGeH_3\cdots NHCH_2$

C	-3.19768976	-1.10630021	-0.14572314
C	-1.77869776	-1.18520121	-0.06670114
C	-0.94123376	-0.02268821	-0.01839914
C	-1.61859976	1.23781079	-0.07671914
C	-3.03657576	1.34584679	-0.15530414
C	-3.82531176	0.16663179	-0.18072714
H	-3.80708476	-2.00128521	-0.08878014
H	-1.32783376	-2.16640121	0.04299586
H	-1.03967076	2.15030179	0.02506086
H	-3.52298276	2.31355379	-0.10565014
H	-4.90592576	0.23766379	-0.14688014
Ge	1.33266587	-0.19545318	0.00457538
H	1.22734887	-0.85075018	-1.35156162
H	1.41563987	1.31010082	0.14026338
H	1.28316987	-1.08612118	1.22358338
C	4.27150189	0.71584639	-0.00640024
N	3.47118889	-0.27948761	-0.05491024
H	3.94410489	-1.17923461	-0.13822224
H	5.34730689	0.59125739	-0.05039324
H	3.86059889	1.71548439	0.08100076
Be	-2.39312600	0.07711700	1.13091300

$Be^{2+}\cdots PhGeH_3\cdots NHC$

C	-2.17094666	-0.02733248	-0.13221748
C	-2.91245066	-1.10472048	0.47122052
C	-2.96052066	1.14045452	-0.42924248
C	-4.31867966	-1.06105048	0.70693452
H	-2.40512866	-2.04202948	0.66992252

C	-4.36745866	1.21953552	-0.20747048
H	-2.49218866	1.97358352	-0.94077448
C	-5.04433066	0.10157052	0.34289752
H	-4.85745066	-1.93237548	1.06088552
H	-4.94320866	2.07345652	-0.54532248
H	-6.12461766	0.10694852	0.41378552
C	4.89634560	-0.34217122	-0.34228501
C	4.76610060	0.49333678	0.73420599
H	5.77225360	-0.74179522	-0.82169201
H	5.50765460	0.95352978	1.36261799
N	3.42121260	0.67653378	0.91054499
N	3.62366960	-0.62189222	-0.76232601
C	2.69628160	-0.00302022	-0.00234401
H	3.01031760	1.25128378	1.63385299
H	3.40193460	-1.21827022	-1.54771001
Ge	0.67894472	-0.04737883	-0.14695802
H	0.30391172	-1.48199683	0.12612598
H	0.27750672	0.92224117	0.93621098
H	0.38385872	0.41173117	-1.55114202
Be	-3.85343600	-0.40527100	-0.99160900

$Mg^{2+}\cdots PhSiH_3\cdots NH_3$

C	-2.11893208	1.22036136	-0.52386209
C	-0.72667408	1.20886136	-0.26398709
C	0.01846392	0.00000536	-0.12489409
C	-0.72667608	-1.20885864	-0.26397709
C	-2.11892908	-1.22035664	-0.52385709
C	-2.81812408	0.00000336	-0.64967509
H	-2.64896208	2.15952036	-0.63683909
H	-0.20927708	2.16016436	-0.17710909
H	-0.20929108	-2.16017064	-0.17709409
H	-2.64895808	-2.15951764	-0.63683209
H	-3.88146608	0.00000036	-0.85734409
Si	2.10108555	-0.00001919	-0.04076906
H	2.13937555	1.28525981	0.69228694
H	2.13939455	-1.28419619	0.69421894
H	2.14073855	-0.00121119	-1.51715206
N	4.22425953	0.00002383	-0.04652085
H	4.60479553	0.81466683	-0.52578685
H	4.60484853	-0.81529617	-0.52459085
H	4.63056753	0.00072583	0.88745215
Mg	-1.64385700	0.00000500	1.47897900

$Mg^{2+}\cdots PhSiH_3\cdots NHCH_2$

C	-2.44176958	1.22086072	-0.60019133
C	-1.06720858	1.20896872	-0.25898533

C	-0.33217258	-0.00004228	-0.07408133
C	-1.06741158	-1.20869828	-0.26048433
C	-2.44197358	-1.21992828	-0.60171333
C	-3.13263858	0.00062372	-0.76614533
H	-2.96470458	2.15991672	-0.74299133
H	-0.55536758	2.15974472	-0.13898233
H	-0.55572458	-2.15970628	-0.14165433
H	-2.96506458	-2.15871928	-0.74568533
H	-4.18255858	0.00087572	-1.03333533
C	4.63268728	0.00083711	-0.64112077
N	3.80997728	-0.00040989	0.33764723
H	4.25857228	-0.00146889	1.25360423
H	5.70561428	0.00074711	-0.48936877
H	4.23895728	0.00203511	-1.65115277
Si	1.73747030	-0.00036783	0.19226310
H	1.70038830	-1.27656683	0.94317810
H	1.90397330	0.00126317	-1.27888990
H	1.70034230	1.27423017	0.94589510
Mg	-2.07864500	-0.00082900	1.42870800
	$Mg^{2+}\cdots PhSiH_3\cdots NHC$		
C	1.44233401	-0.00042300	-0.08564608
C	2.18822101	-1.20750200	-0.24325408
C	2.18809301	1.20503000	-0.25594008
C	3.57533101	-1.22310500	-0.53299308
H	1.67121601	-2.15806000	-0.13883308
C	3.57516801	1.21776600	-0.54585008
H	1.67099201	2.15659100	-0.16166808
C	4.27225801	-0.00333700	-0.67428408
H	4.10525001	-2.16155000	-0.65201308
H	4.10492301	2.15497800	-0.67486608
H	5.33214401	-0.00444000	-0.89735408
Si	-0.77675688	-0.00035158	-0.02246957
H	-0.69880188	1.31775242	0.67037743
H	-0.66563488	-0.00425958	-1.50191457
H	-0.69761288	-1.31478558	0.67712043
Mg	3.09905300	0.00750900	1.46570800
C	-4.94964314	0.68407958	-0.03507426
C	-4.95019314	-0.68327142	-0.03957126
H	-5.76144214	1.38894758	-0.04782026
H	-5.76259214	-1.38735142	-0.05699726
N	-3.63162214	-1.06012842	-0.00917026
N	-3.63076414	1.05960558	-0.00220126
C	-2.79479014	-0.00064742	0.01154974
H	-3.31176814	-2.01803642	-0.00173126

H	-3.30993914	2.01712258	0.01168674
	$Mg^{2+}\cdots PhGeH_3\cdots NH_3$		
C	2.55765391	-1.22021568	-0.52307306
C	1.16535391	-1.20808868	-0.26357906
C	0.42182691	0.00009432	-0.12046306
C	1.16552891	1.20816132	-0.26362506
C	2.55782991	1.22006732	-0.52311706
C	3.25687591	-0.00012868	-0.64713206
H	3.08746191	-2.15942468	-0.63642206
H	0.64917891	-2.16018268	-0.17796906
H	0.64951191	2.16034432	-0.17806106
H	3.08777491	2.15919132	-0.63649906
H	4.32064391	-0.00020768	-0.85281906
N	-4.00946203	-0.00014801	-0.02818084
H	-4.39238203	-0.80811601	-0.51407284
H	-4.39280203	0.81688699	-0.49832384
H	-4.42105903	-0.00927301	0.90206816
Ge	-1.74973088	0.00007269	-0.02719011
H	-1.82530788	-1.31275731	0.72114489
H	-1.82550688	1.31224369	0.72226089
H	-1.83780488	0.00072469	-1.53513611
Mg	2.07532100	0.00000000	1.48246100
	$Mg^{2+}\cdots PhGeH_3\cdots NHCH_2$		
C	-2.80858233	1.22060714	-0.61828659
C	-1.43330733	1.20811714	-0.27955559
C	-0.69897333	0.00002314	-0.09262759
C	-1.43341333	-1.20779286	-0.28094359
C	-2.80869433	-1.21977986	-0.61968759
C	-3.49960933	0.00053914	-0.78165159
H	-3.33160733	2.15962814	-0.76077359
H	-0.92288633	2.15993814	-0.16160959
H	-0.92306433	-2.15978886	-0.16409259
H	-3.33180233	-2.15858886	-0.76325259
H	-4.55023233	0.00074014	-1.04617059
C	4.45765525	0.00079442	-0.73902067
N	3.67387925	-0.00030358	0.26997333
H	4.16895525	-0.00126758	1.16149433
H	5.53725525	0.00068142	-0.63815367
H	4.02611325	0.00184942	-1.73444767
H	1.46494708	-1.30894855	0.92323226
H	1.64762308	0.00141845	-1.34035774
H	1.46494408	1.30696345	0.92597026
Ge	1.46182908	-0.00019655	0.16207726
Mg	-2.43338200	-0.00076800	1.41169000

$Mg^{2+}\cdots PhGeH_3\cdots NHC$

C	1.72706640	0.01116954	0.02010179
C	2.51049240	1.22784854	0.00735879
C	2.45064940	-1.15279046	-0.44213121
C	3.88708340	1.28617954	-0.38431621
H	2.03489340	2.16489254	0.32541379
C	3.82641040	-1.13126546	-0.84140021
H	1.92537140	-2.11613246	-0.48425921
C	4.55093940	0.09356054	-0.79134621
H	4.43598740	2.23419754	-0.36898621
H	4.32819540	-2.04495546	-1.17845821
H	5.60533540	0.12219354	-1.08280321
C	-4.99027340	-0.74813454	-0.03787879
C	-5.03721340	0.62451946	-0.19307979
H	-5.78533140	-1.48773754	-0.00049279
H	-5.88066040	1.29848146	-0.31559779
N	-3.72447840	1.05331246	-0.16695379
N	-3.65166040	-1.06943254	0.07319721
C	-2.84630740	0.02572646	-0.00309479
H	-3.43865040	2.02434046	-0.26163479
H	-3.29490840	-2.01359454	0.19579721
Mg	3.48311300	-0.29712600	1.42815900
H	-0.62614840	-1.45300754	0.29475221
H	-0.51996940	0.63254646	-1.31786879
H	-0.61712740	1.01534446	1.25960521
Ge	-0.77560540	0.05878646	0.07649921