

Table S1 Change of T-X bond length (Δr , Å) and frequency shift of its stretch vibration ($\Delta \nu$, cm^{-1}) in the TH_3X complexes

	Δr			$\Delta \nu$		
	T=C	T=Si	T=Ge	T=C	T=Si	T=Ge
X=CH ₃	---	0.015	0.016	---	-22.3	-21.2
X=H	---	0.016	0.019	---	-83.4	-77.3
X=NH ₂	0.001	0.027	0.027	-5.5	-68.1	-69.7
X=OH	0.003	0.036	0.041	-8.7	-80.8	-74.5
X=I	0.007	0.128	0.115	-10.7	-67.5	-56.4
X=Br	0.008	0.104	0.096	-15.3	-79.9	-62.7
X=Cl	0.008	0.089	0.085	-20.9	-104.1	-79.3
X=F	0.006	0.044	0.051	-25.4	-101.6	-89.4
X=CN	0.001	0.061	0.063	-3.5	-83.0	-67.5
X=NO ₂	0.001	0.068	0.073	-3.1	-39.0	-49.3

Table S2 Deformation energy (DE, kcal/mol) in the TH_3X complexes

T=C	DE	T=Si	DE	T=Ge	DE
X=CH ₃	---	X=CH ₃	1.7	X=CH ₃	1.2
X=H	---	X=H	1.7	X=H	1.2
X=NH ₂	0.5	X=NH ₂	3.8	X=NH ₂	2.4
X=OH	0.5	X=OH	5.5	X=OH	3.8
X=I	0.5	X=I	9.3	X=I	6.2
X=Br	0.5	X=Br	8.7	X=Br	5.8
X=Cl	0.5	X=Cl	8.2	X=Cl	5.6
X=F	0.5	X=F	6.9	X=F	5.1
X=CN	0.5	X=CN	6.7	X=CN	4.2
X=NO ₂	0.5	X=NO ₂	9.4	X=NO ₂	6.9

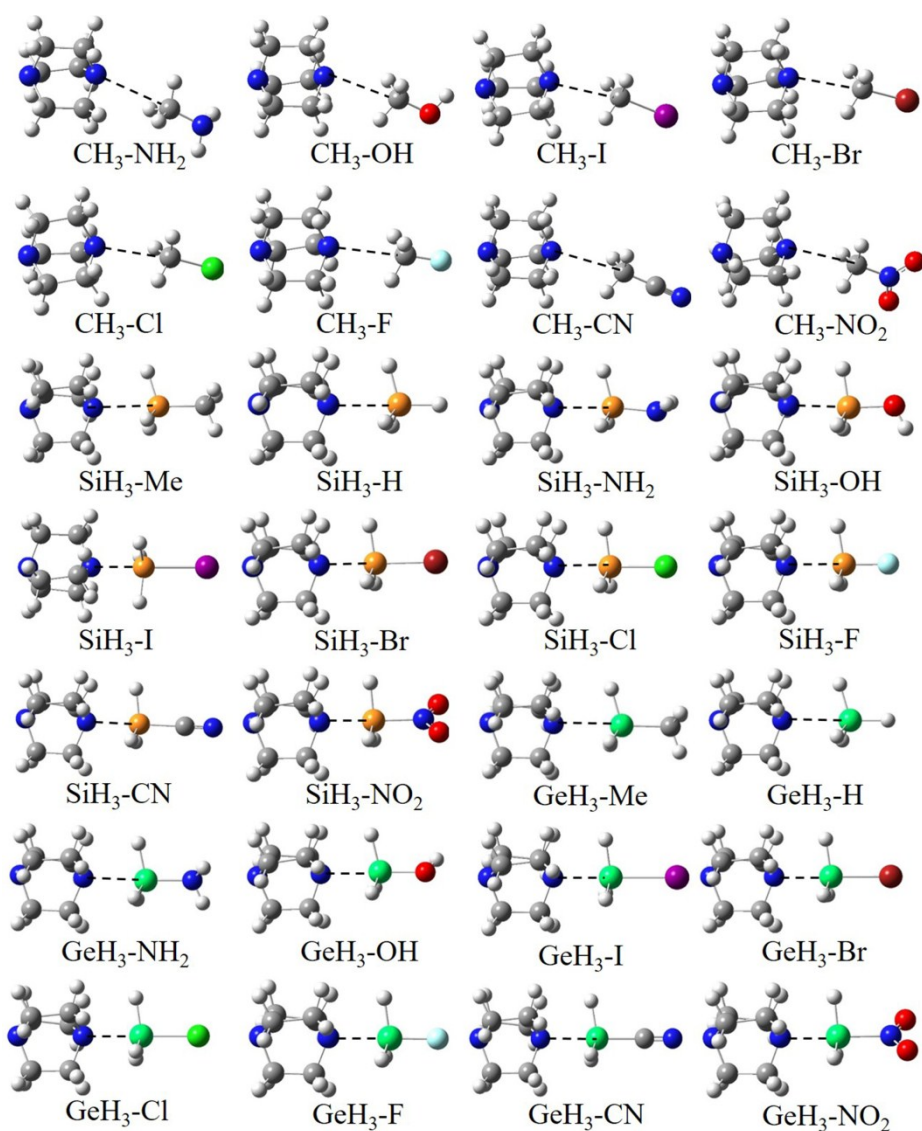


Fig. S1 Optimized structures of complexes between DABCO and TH_3X ($\text{T}=\text{C}, \text{Si}, \text{Ge}$; $\text{X} = -\text{Me}, -\text{H}, -\text{OH}, -\text{NH}_2, -\text{F}, -\text{Cl}, -\text{Br}, -\text{I}, -\text{CN}, -\text{NO}_2$).

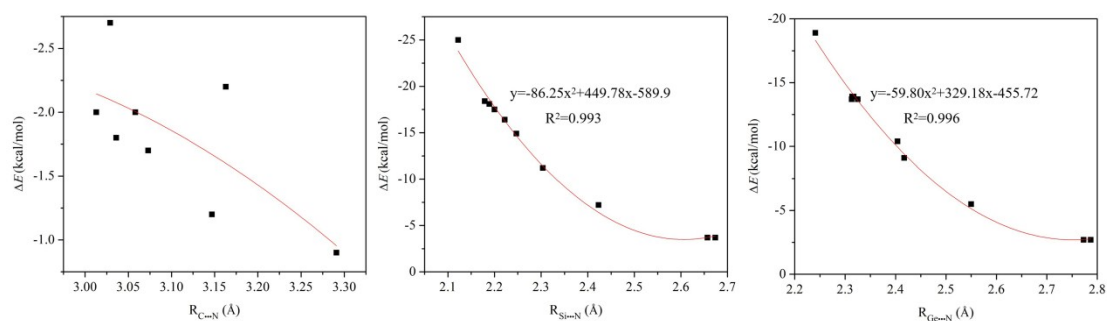


Fig. S2 Relationship between the interaction energy (ΔE) and the binding distance (R) in the complexes

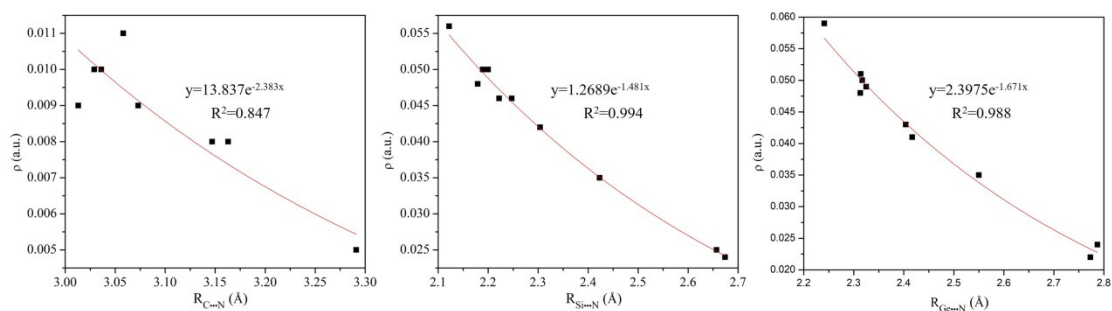


Fig. S3 Relationship between the electron density (ρ) and the binding distance (R) in the complexes

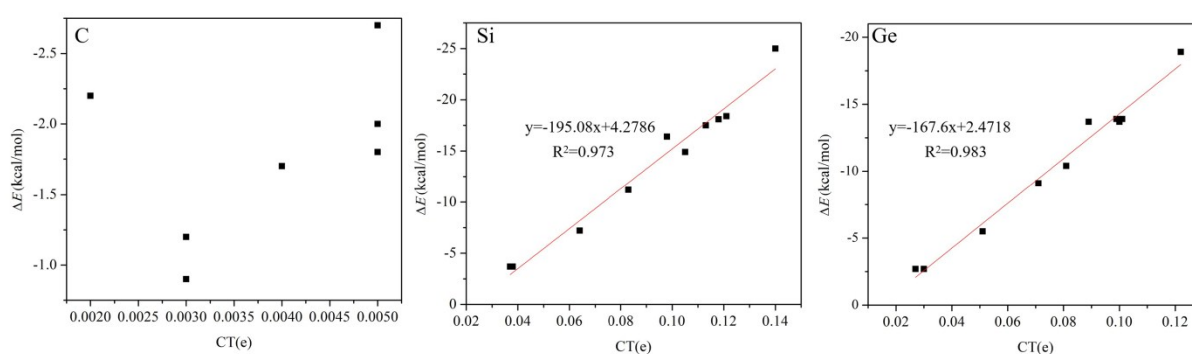


Fig. S4 Relationship between the interaction energy (ΔE) and the charge transfer (CT) in the complexes

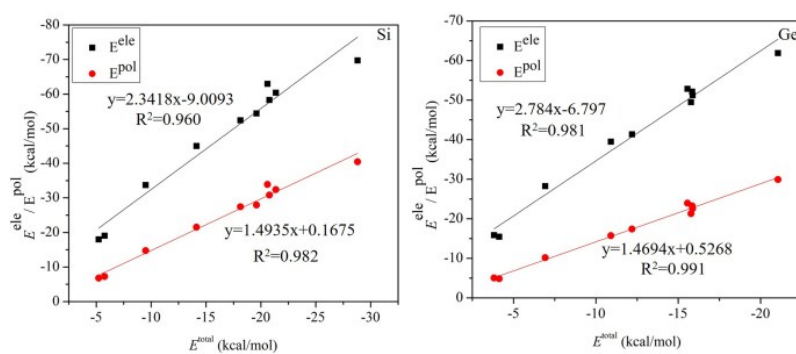


Fig. S5 Relationship between the total interaction energy (E^{total}) and the electrostatic/polarization energy (E^{ele}/E^{pol}) in the SiH_3X and GeH_3X complexes

Cartesian coordinates of complexes

DABCO-CH₃NH₂

C	-0.34817100	-0.53728800	1.24899200
C	-1.73193000	0.15117900	1.47665200
H	-0.38310200	-1.60701000	1.51650500
H	0.44272200	-0.06193800	1.85374700
H	-2.41317800	-0.49459000	2.05584900
H	-1.62072600	1.10304500	2.02292800
C	-0.93243800	-1.22799600	-0.96742500
H	-0.69893800	-1.06055000	-2.03247000
H	-0.77733600	-2.29828700	-0.75038800
C	-2.39040500	-0.78139000	-0.62768300
H	-2.97700400	-0.58982600	-1.54188000
H	-2.91880100	-1.55167700	-0.04096700
C	-1.53685100	1.45259000	-0.52306600
H	-1.95932200	1.58521900	-1.53325400
H	-1.62232700	2.41464000	0.00954700
C	-0.05412200	0.96629000	-0.58830500
H	0.35578500	1.05606000	-1.60873000
H	0.59038700	1.55223700	0.08850400
N	0.04080100	-0.44872700	-0.17369300
N	-2.37251600	0.45645300	0.18005900
C	3.31394300	-0.12145100	-0.06653900
H	2.87676800	0.49624600	-0.86391700
H	2.79844400	0.12697500	0.87951200
H	3.08639300	-1.16868700	-0.30808500
N	4.77528000	0.07097300	-0.05323400
H	4.99928800	1.03680800	0.18645600
H	5.19583300	-0.50116300	0.67896500

DABCO-CH₃OH

C	0.24398600	0.58029600	1.17696900
C	1.76784500	0.91852100	1.12555100
H	-0.37064000	1.48195800	1.01437500
H	-0.04185300	0.14594200	2.15002000
H	1.94019100	2.00715400	1.16372000
H	2.30817800	0.45950500	1.97046400
C	0.11673000	0.26398500	-1.19145800
H	-0.03098400	-0.50167100	-1.97213000
H	-0.65756800	1.03827200	-1.32551100
C	1.55285300	0.87410300	-1.25835300
H	2.06622000	0.59452300	-2.19360600
H	1.52254300	1.97532200	-1.20419600
C	2.28718800	-1.07961900	-0.08581200

H	2.62646000	-1.45262200	-1.06689000
H	2.99207900	-1.44687500	0.67885900
C	0.82484400	-1.53620400	0.21955200
H	0.49008300	-2.31634800	-0.48487700
H	0.73630200	-1.94118200	1.24190100
N	-0.10208000	-0.38936800	0.11613700
N	2.36652800	0.39580700	-0.12070000
C	-3.23806600	-0.13144700	0.05502800
H	-2.70437000	0.78195900	0.34398800
H	-2.84408000	-0.47733300	-0.91427500
H	-3.04501600	-0.90407200	0.81628900
O	-4.63112500	0.21880300	-0.02187100
H	-5.12196400	-0.57783700	-0.26008000

DABCO-CH₃I

C	-2.20532900	-0.05970700	1.35609600
C	-3.57080800	-0.81256900	1.26052800
H	-1.39764800	-0.73532300	1.68674300
H	-2.25760500	0.78043900	2.06907200
H	-3.43225200	-1.90407800	1.33691600
H	-4.25906400	-0.50075900	2.06377300
C	-1.89940700	-0.59241100	-0.95632700
H	-1.50545600	-0.21129400	-1.91423300
H	-1.22833100	-1.39683200	-0.61000400
C	-3.36775400	-1.10216300	-1.10700000
H	-3.80026400	-0.79422800	-2.07360700
H	-3.41994700	-2.20200000	-1.04637700
C	-4.27777700	0.92851600	-0.22315800
H	-4.86828700	1.13984600	-1.13027500
H	-4.82006100	1.34911100	0.64025800
C	-2.83610100	1.52097300	-0.32984000
H	-2.61082000	1.84764600	-1.35914000
H	-2.70555900	2.38892500	0.33813300
N	-1.83383400	0.49844600	0.03873000
N	-4.21802500	-0.53658300	-0.03887600
C	1.23687900	0.40049100	0.00146300
H	0.75854900	-0.25217300	0.73744800
H	0.85507600	0.20718800	-1.00527200
H	1.11639200	1.45313100	0.27432300
I	3.34830300	-0.04908400	-0.00032600

DABCO-CH₃Br

C	1.56113900	0.06618900	1.34870800
C	3.07915400	0.43351700	1.36588700

H	0.93489300	0.94547000	1.57839600
H	1.32628600	-0.72013000	2.08612200
H	3.24803500	1.42633500	1.81519700
H	3.66178200	-0.30398600	1.94286900
C	1.31956000	0.69662800	-0.94661300
H	1.13117900	0.29538000	-1.95717700
H	0.54045000	1.44721200	-0.72894800
C	2.75052000	1.31246900	-0.83662800
H	3.21742700	1.42506300	-1.82928200
H	2.72230700	2.30664900	-0.36003400
C	3.54529500	-0.92735200	-0.54816400
H	3.84062600	-0.88343400	-1.60991900
H	4.28536400	-1.54771400	-0.01560500
C	2.10006500	-1.49732100	-0.38491900
H	1.73358300	-1.94559500	-1.32381000
H	2.06024200	-2.27196000	0.39943300
N	1.16701300	-0.42025400	0.00941300
N	3.61783700	0.44724000	-0.01015600
C	-1.86711000	-0.30709000	0.00720600
H	-1.39878500	0.37500500	0.72312600
H	-1.48739400	-0.13560500	-1.00437100
H	-1.72171700	-1.34871000	0.30832600
Br	-3.78628500	0.05956800	-0.00148500

DABCO-CH₃Cl

C	0.76136700	0.19551500	1.33231800
C	2.20082100	0.79528900	1.23979900
H	0.02337100	0.96606000	1.61444900
H	0.70970100	-0.61398900	2.08000100
H	2.17754700	1.89761200	1.26683500
H	2.83520900	0.44869100	2.07256400
C	0.56190700	0.65543700	-1.00806500
H	0.14951800	0.27600600	-1.95879700
H	-0.02614300	1.54118900	-0.71230400
C	2.07936400	0.99997800	-1.14219900
H	2.49678600	0.60574900	-2.08377500
H	2.24742800	2.08971300	-1.12600300
C	2.74868700	-1.07466100	-0.15154800
H	3.33197100	-1.38704000	-1.03380000
H	3.22496500	-1.51166200	0.74211500
C	1.25463000	-1.51553200	-0.27012300
H	1.01754800	-1.86171400	-1.29036100
H	1.01825200	-2.33454500	0.42991600
N	0.35962200	-0.37741900	0.02996300

N	2.84161300	0.39523200	-0.03011600
C	-2.69419900	-0.22162800	0.00152500
H	-2.24242900	0.37315000	0.80172600
H	-2.29358200	0.07328800	-0.97350200
H	-2.53294500	-1.28964400	0.17850700
Cl	-4.47184200	0.09388600	-0.00098500

DABCO-CH₃F

C	0.29046800	0.20279400	1.34367100
C	1.84310200	0.37151900	1.35529900
H	-0.21730300	1.16190300	1.54360600
H	-0.04362500	-0.52329700	2.10423500
H	2.13887600	1.34637400	1.77754400
H	2.32652100	-0.41851100	1.95404300
C	0.13000500	0.78614300	-0.97232600
H	-0.10341700	0.37768000	-1.97040800
H	-0.55054900	1.63453900	-0.78534000
C	1.62644400	1.22161700	-0.87224100
H	2.10489900	1.24858900	-1.86544300
H	1.72207700	2.22392400	-0.42212100
C	2.13093100	-1.09172500	-0.51757800
H	2.42576200	-1.11562800	-1.58010900
H	2.78852000	-1.78535700	0.03253200
C	0.62599300	-1.46963800	-0.33835100
H	0.20414600	-1.89904000	-1.26278300
H	0.49087100	-2.20696500	0.47102700
N	-0.16313600	-0.27112200	0.01857200
N	2.37805000	0.27748100	-0.01909800
C	-3.17192500	-0.10493900	0.00758000
H	-2.72477100	0.62587700	0.69316300
H	-2.79105800	0.03864800	-1.01116300
H	-2.97175000	-1.12678900	0.35234100
F	-4.57263400	0.09765700	-0.00708400

DABCO-CH₃CN

C	0.58206300	0.23088900	1.30320500
C	2.10528900	0.57496400	1.33463300
H	-0.03348900	1.14088900	1.41005300
H	0.30726100	-0.46307500	2.11572700
H	2.27728400	1.60907900	1.67665200
H	2.65344000	-0.10202200	2.01091200
C	0.43198800	0.60045000	-1.05655900
H	0.27375100	0.08935500	-2.02165300
H	-0.33986400	1.38303400	-0.95544000

C	1.86886100	1.20567600	-0.96267000
H	2.37212100	1.20049500	-1.94379700
H	1.84124500	2.24709800	-0.60084100
C	2.61190300	-0.99869600	-0.39706200
H	2.94313300	-1.07853400	-1.44599000
H	3.32256500	-1.56571700	0.22694800
C	1.15236700	-1.52636500	-0.22184100
H	0.81077900	-2.07457500	-1.11598200
H	1.07237700	-2.20541800	0.64382000
N	0.22445500	-0.39860600	0.01359000
N	2.69071500	0.42637600	-0.01382800
C	-2.93559000	-0.25854300	0.00150500
H	-2.42021700	0.43331500	0.68082800
H	-2.52185200	-0.13196300	-1.00775500
H	-2.73527800	-1.28546600	0.33413000
C	-4.38234300	0.00922500	-0.00040800
N	-5.54809500	0.22621700	-0.00153800

DABCO-CH₃NO₂

C	1.02970000	-0.03940600	-1.32447300
C	2.56819300	-0.29377200	-1.40926400
H	0.46132700	-0.94954300	-1.58333900
H	0.71424500	0.76574300	-2.00984300
H	2.79088100	-1.24346800	-1.92337500
H	3.07703600	0.51666900	-1.95729600
C	0.91119800	-0.80775300	0.93972500
H	0.73735800	-0.47316300	1.97681700
H	0.17583800	-1.59808700	0.70923900
C	2.37420000	-1.31850800	0.74557400
H	2.88255500	-1.45867200	1.71393500
H	2.39324100	-2.28204000	0.20951100
C	3.00519800	0.98415500	0.56742000
H	3.33459400	0.89948300	1.61652600
H	3.68560600	1.68351500	0.05377200
C	1.52135800	1.46280000	0.47648300
H	1.15697000	1.83676400	1.44813000
H	1.40510700	2.27210700	-0.26405200
N	0.64897700	0.34592100	0.05201600
N	3.15212000	-0.34891200	-0.05317600
C	-2.37804800	0.24753400	0.01494000
H	-1.92130300	-0.35306100	-0.77813000
H	-2.00024300	-0.08209200	0.98935000
H	-2.22149800	1.31897000	-0.13317100
N	-3.84795300	-0.02170400	-0.00506900

O	-4.19781500	-1.21016500	-0.00037200
O	-4.61900000	0.94884600	-0.01049200

DABCO-SiH₃Me

N	0.07476900	0.00027500	0.00013000
C	0.59022000	1.38172000	-0.07997900
C	0.58991900	-0.62129400	1.23656000
C	0.58965200	-0.75997200	-1.15633100
N	2.66663400	-0.00028200	-0.00012000
H	0.09244100	1.88530400	-0.92629600
H	0.29163300	1.89837800	0.84770600
H	0.09228300	-0.13994100	2.09579400
H	0.29090600	-1.68290500	1.22015100
H	0.09163800	-1.74458100	-1.16908300
H	0.29086400	-0.21485200	-2.06751600
C	2.14208800	1.35866900	-0.25135300
H	2.63280400	2.05594000	0.44779800
H	2.43437700	1.64303100	-1.27598400
C	2.14184900	-0.46196800	1.30236300
H	2.63216900	-1.41628500	1.55665800
H	2.43440000	0.28308600	2.06096500
C	2.14152700	-0.89720500	-1.05121700
H	2.63197100	-0.64047400	-2.00482000
H	2.43367400	-1.92680800	-0.78526400
Si	-2.59960300	0.00007300	-0.00007700
H	-2.17589800	-1.42432500	0.14999400
H	-2.17597300	0.84230100	1.15843400
H	-2.17612200	0.58237800	-1.30869800
C	-4.50986400	-0.00009400	0.00009100
H	-4.90969300	1.02198200	-0.10828800
H	-4.90965300	-0.60505300	-0.83084400
H	-4.90953900	-0.41728700	0.93948900

DABCO-SiH₄

N	-0.39932900	0.00004600	-0.00000200
C	0.11639800	1.38243700	0.07353500
C	0.11632200	-0.75486200	1.16043100
C	0.11633100	-0.62749300	-1.23397100
N	2.19261300	-0.00004500	0.00000200
H	-0.38101300	1.97684000	-0.71187000
H	-0.18222700	1.79343800	1.05262900
H	-0.38109800	-0.37186300	2.06788900
H	-0.18235200	-1.80826700	1.02680700
H	-0.38113500	-1.60485000	-1.35602500

H	-0.18228200	0.01494300	-2.07944700
C	1.66817500	1.37822000	-0.09910200
H	2.15843700	1.99366400	0.67322000
H	1.96056900	1.77464100	-1.08570700
C	1.66810300	-0.60332400	1.24314900
H	2.15831100	-1.57992100	1.38999500
H	1.96050200	0.05287700	2.07977000
C	1.66810100	-0.77497700	-1.14404200
H	2.15835700	-0.41387600	-2.06320700
H	1.96044200	-1.82762800	-0.99405700
Si	-3.05671200	-0.00000100	-0.00000100
H	-2.66132700	-1.43679000	-0.02342600
H	-2.66148400	0.69814100	1.25604100
H	-2.66148200	0.73873600	-1.23260200
H	-4.56181800	-0.00009800	0.00000100

DABCO-SiH₃NH₂

N	-0.01196000	0.00080800	-0.01457600
C	0.51513700	1.24797200	-0.61210300
C	0.48743700	-0.09914600	1.37560300
C	0.51626700	-1.14662400	-0.78559100
N	2.58055500	-0.00100400	0.02148800
H	0.01984400	1.39467600	-1.58665900
H	0.22003400	2.07799900	0.05076700
H	-0.02905800	0.66597400	1.97938100
H	0.19412100	-1.09102200	1.75719400
H	0.00143000	-2.05794900	-0.43737000
H	0.24501500	-0.98226700	-1.84132600
C	2.06511400	1.14580700	-0.75501500
H	2.55848900	2.06301400	-0.39391200
H	2.35811700	0.99398700	-1.80704200
C	2.03523500	0.09256000	1.39175800
H	2.52368400	-0.67340500	2.01606200
H	2.30919600	1.08261200	1.79220400
C	2.06125000	-1.24046400	-0.59326500
H	2.57246700	-1.39389900	-1.55775400
H	2.32958500	-2.07881900	0.07066400
Si	-2.43489200	0.00036900	-0.03867700
H	-2.09613800	-1.28265300	0.64620600
H	-2.09702100	1.28241100	0.64829100
H	-2.06739800	0.00172700	-1.49410400
N	-4.22400300	-0.00062400	0.13053100
H	-4.72492400	0.82373900	-0.19640100
H	-4.72373800	-0.82618700	-0.19515500

DABCO-SiH₃OH

N	0.05731600	0.00885000	-0.00026600
C	-0.45915100	-0.78362600	-1.14345900
C	-0.46012200	-0.59024300	1.25465100
C	-0.47362500	1.38916300	-0.11210800
N	-2.53628200	-0.00921300	0.00037600
H	0.05409000	-0.43772600	-2.05603000
H	-0.17378100	-1.83318400	-0.96638300
H	0.06290800	-1.54759900	1.41533800
H	-0.18721100	0.09176800	2.07607900
H	0.03840400	2.01227000	0.63988400
H	-0.19951900	1.76227100	-1.11211000
C	-2.00504300	-0.61094400	-1.23998500
H	-2.50091600	-1.58198600	-1.40018500
H	-2.27896800	0.05251400	-2.07665000
C	-2.00330600	-0.77741200	1.14433000
H	-2.50822000	-0.43677900	2.06279000
H	-2.26471500	-1.83650700	0.98578400
C	-2.01811400	1.37095400	0.09642600
H	-2.52532000	1.99062500	-0.66076400
H	-2.28920800	1.76058300	1.09137900
Si	2.36096900	0.01057200	-0.00004200
H	2.06843900	0.77093100	1.25720100
H	2.07780900	-1.45174600	-0.00118400
H	2.06875700	0.77292700	-1.25608600
O	4.10076500	-0.11852800	0.00012200
H	4.56669600	0.72704200	0.00065000

DABCO-SiH₃I

N	-1.58933800	0.00000000	0.00000000
C	-2.11314400	-0.32135200	1.35635300
C	-2.11314200	1.33531200	-0.39987800
C	-2.11314300	-1.01396300	-0.95647200
N	-4.18051200	0.00000200	-0.00000100
H	-1.59228100	-1.22382100	1.71622400
H	-1.84144400	0.51923900	2.01466800
H	-1.59227800	2.09820400	0.20174700
H	-1.84144100	1.48513600	-1.45700900
H	-1.59227800	-0.87438300	-1.91796700
H	-1.84144300	-2.00437700	-0.55765900
C	-3.65486400	-0.52501000	1.27603500
H	-4.16042000	-0.00765900	2.10685600
H	-3.91623200	-1.59408900	1.33183300

C	-3.65486100	1.36758900	-0.18334700
H	-4.16041300	1.82842800	-1.04679700
H	-3.91622800	1.95045600	0.71460200
C	-3.65486200	-0.84257800	-1.09268900
H	-4.16041500	-1.82076700	-1.06006400
H	-3.91622800	-0.35636200	-2.04643900
Si	0.58936800	-0.00000200	0.00000000
H	0.42138400	0.45014000	-1.40825400
H	0.42138500	0.99451100	1.09396100
H	0.42138400	-1.44465700	0.31429200
I	3.19299700	0.00000000	0.00000000

DABCO-SiH₃Br

N	1.01451300	0.00003100	0.00018300
C	1.53889000	1.39289400	0.02529100
C	1.53899500	-0.71823700	1.19378100
C	1.53865500	-0.67462400	-1.21874600
N	3.60671200	-0.00004400	-0.00018400
H	1.01734000	1.96607800	-0.75874700
H	1.26858900	1.82207800	1.00329100
H	1.01767900	-0.32575000	2.08229300
H	1.26849600	-1.77975500	1.07651100
H	1.01716100	-1.64025800	-1.32298500
H	1.26809100	-0.04227300	-2.07936900
C	3.08044700	1.36610300	-0.19332200
H	3.58669200	2.04348500	0.51272300
H	3.34104700	1.68417600	-1.21576600
C	3.08060300	-0.51577200	1.27960000
H	3.58673500	-1.46599900	1.51311100
H	3.34146900	0.21061000	2.06623400
C	3.08025900	-0.85042200	-1.08660800
H	3.58625500	-0.57761800	-2.02638200
H	3.34100200	-1.89489900	-0.85090800
Si	-1.17415400	0.00008200	0.00000400
H	-0.98992100	-1.47341000	0.09563000
H	-0.99003100	0.81964100	1.22828400
H	-0.98999900	0.65404100	-1.32387500
Br	-3.53508900	-0.00002400	-0.00000200

DABCO-SiH₃Cl

N	0.32475900	0.00000900	0.00001100
C	0.84904400	-0.67474300	-1.21806900
C	0.84906900	1.39226500	0.02469700
C	0.84906500	-0.71750800	1.19339300

N	2.91751700	-0.00000900	-0.00001100
H	0.32810600	-1.64075300	-1.32172200
H	0.57793400	-0.04329700	-2.07917900
H	0.32813400	1.96504700	-0.76005900
H	0.57797500	1.82228600	1.00210400
H	0.32814300	-0.32427100	2.08181900
H	0.57795200	-1.77897300	1.07710100
C	2.39096500	-0.84984700	-1.08690500
H	2.89671600	-0.57593000	-2.02654200
H	2.65261100	-1.89433300	-0.85205400
C	2.39098700	1.36619700	-0.19254100
H	2.89675600	2.04298000	0.51449200
H	2.65263200	1.68504700	-1.21452000
C	2.39098700	-0.51636700	1.27942700
H	2.89674200	-1.46707600	1.51201700
H	2.65265000	0.20926200	2.06654800
Si	-1.87493900	0.00000500	-0.00000200
H	-1.67740700	0.82132000	1.22555900
H	-1.67740900	0.65071800	-1.32406000
H	-1.67740300	-1.47201900	0.09849500
Cl	-4.06480100	-0.00000300	0.00000100

DABCO-SiH₃F

N	0.08935100	-0.00028000	0.00038900
C	-0.43533400	-0.31629800	1.35513100
C	-0.43451900	1.33139400	-0.40335100
C	-0.43487600	-1.01542700	-0.95110400
N	-2.50442300	0.00027800	-0.00039000
H	0.08519500	-1.21736400	1.71889900
H	-0.16428300	0.52611500	2.01126600
H	0.08620600	2.09644000	0.19558800
H	-0.16267600	1.47845200	-1.46075300
H	0.08619700	-0.87975400	-1.91300800
H	-0.16388200	-2.00487900	-0.54961000
C	-1.97753800	-0.52007800	1.27758400
H	-2.48355700	0.00059300	2.10634900
H	-2.23999000	-1.58888800	1.33717800
C	-1.97675000	1.36690300	-0.18869700
H	-2.48223500	1.82445700	-1.05422800
H	-2.23922100	1.95321000	0.70692900
C	-1.97696100	-0.84641100	-1.08965900
H	-2.48302600	-1.82446400	-1.05330800
H	-2.23890200	-0.36371400	-2.04526200
Si	2.31130700	-0.00013600	0.00017600

H	2.08177300	0.45622500	-1.40188500
H	2.08214200	0.98654200	1.09590900
H	2.08247500	-1.44250000	0.30672000
F	4.01298500	0.00010600	-0.00029600

DABCO-SiH₃CN

N	0.21943500	-0.00000800	-0.00005800
C	0.74053700	-0.64089900	1.23518300
C	0.74065200	-0.74930600	-1.17266500
C	0.74057900	1.39017800	-0.06261800
N	2.81010900	0.00001600	0.00005700
H	0.22519900	-0.18689300	2.09784300
H	0.46241100	-1.70628100	1.19012700
H	0.22538500	-1.72343400	-1.21083400
H	0.46254500	-0.17763200	-2.07281100
H	0.22532100	1.91027600	-0.88717100
H	0.46240100	1.88386600	0.88253100
C	2.28489700	-0.44534700	1.30625800
H	2.78639400	-1.38543200	1.58642000
H	2.55332700	0.31903600	2.05341200
C	2.28501600	-0.90853700	-1.03877300
H	2.78655300	-0.68108800	-1.99296400
H	2.55349400	-1.93776500	-0.75036200
C	2.28495600	1.35391400	-0.26739100
H	2.78642200	2.06657400	0.40669900
H	2.55347100	1.61876300	-1.30292300
Si	-2.02794400	-0.00001600	0.00001300
H	-1.81864400	0.57769000	-1.35754700
H	-1.81866300	-1.46452900	0.17856000
H	-1.81861300	0.88686700	1.17903900
C	-3.96612100	0.00000800	0.00000100
N	-5.15795600	0.00001200	-0.00002300

DABCO-SiH₃NO₂

N	-0.57677500	-0.00968900	-0.00063600
C	-1.10840100	-0.80821600	-1.14296200
C	-1.10555100	-0.59426600	1.26584800
C	-1.09169400	1.38517800	-0.12406400
N	-3.16702000	0.00952900	0.00086200
H	-0.58269600	-0.48506200	-2.05611400
H	-0.84812000	-1.86058800	-0.94853300
H	-0.58815600	-1.55182500	1.43912700
H	-0.83287000	0.09810700	2.07786000
H	-0.56135000	2.00896600	0.61353400

H	-0.82205300	1.73927900	-1.13148300
C	-2.64701000	-0.59395900	-1.24189700
H	-3.16179000	-1.55242400	-1.41361100
H	-2.89955700	0.08167700	-2.07481300
C	-2.64702600	-0.77071800	1.14097100
H	-3.15162400	-0.43497000	2.06063600
H	-2.91191600	-1.82712900	0.97405600
C	-2.63144800	1.38151900	0.10269700
H	-3.13503000	2.01553800	-0.64400300
H	-2.88495000	1.76775900	1.10299200
Si	1.54482700	-0.02426300	-0.00082300
H	1.44444800	0.72242900	1.28415900
H	1.43149300	-1.50926800	-0.00660000
H	1.44493400	0.73277400	-1.27977700
N	3.49846600	-0.00665300	-0.00002700
O	4.15794800	-1.06959700	0.00043200
O	4.03402100	1.12520700	0.00071100

DABCO-GeH₃Me

N	0.56245800	-0.00011100	-0.00008000
C	1.07625400	-1.36864300	-0.19950900
C	1.07611800	0.85697100	-1.08552700
C	1.07598300	0.51147900	1.28490800
N	3.15301000	0.00012400	0.00010000
H	0.58011000	-2.03143700	0.53028100
H	0.77460100	-1.68901900	-1.21120500
H	0.58004600	0.55624600	-2.02442200
H	0.77424800	1.89325400	-0.85714500
H	0.57971200	1.47484600	1.49392600
H	0.77424100	-0.20452400	2.06814100
C	2.62879600	-1.38179100	-0.03106800
H	3.11834000	-1.92075100	-0.85919000
H	2.92358300	-1.86955600	0.91310600
C	2.62868600	0.71796700	-1.18110200
H	3.11804200	1.70471500	-1.23378100
H	2.92361000	0.14422600	-2.07559500
C	2.62852100	0.66406000	1.21235300
H	3.11794400	0.21641000	2.09325700
H	2.92322900	1.72564500	1.16273200
H	-1.75832300	1.45926200	0.17759700
H	-1.75853700	-0.57582600	-1.35273500
H	-1.75840900	-0.88362300	1.17488300
C	-4.18787300	0.00010000	0.00011500
H	-4.58004400	-1.02179100	-0.12469100

H	-4.57983200	0.40295600	0.94759100
H	-4.58000600	0.61921300	-0.82242000
Ge	-2.21061700	-0.00003800	-0.00004600

DABCO-GeH₄

N	0.20975800	-0.00010500	0.00023700
C	0.72403500	-0.42856100	1.31549600
C	0.72365800	-0.92495300	-1.02861300
C	0.72360700	1.35331400	-0.28643700
N	2.80029600	0.00010900	-0.00023900
H	0.22950700	0.17942800	2.09258000
H	0.42126100	-1.47947500	1.46101900
H	0.22914200	-1.90190600	-0.89044600
H	0.42054500	-0.52551600	-2.01138400
H	0.22878500	1.72217300	-1.20140200
H	0.42083400	2.00469800	0.55099700
C	2.27682800	-0.26697700	1.35613700
H	2.76533600	-1.17602700	1.74449600
H	2.57327500	0.57893800	1.99859500
C	2.27648200	-1.04099000	-0.90954500
H	2.76464700	-0.92282000	-1.89116000
H	2.57304000	-2.02033900	-0.49828600
C	2.27637600	1.30815600	-0.44702200
H	2.76478300	2.09915900	0.14594300
H	2.57255200	1.44165400	-1.50090200
H	-2.14389300	0.44296900	-1.40237900
H	-2.14421200	-1.43603900	0.31767900
H	-2.14422500	0.99302600	1.08492200
H	-4.12739500	0.00005300	-0.00026600
Ge	-2.57750900	0.00000200	-0.00000300

DABCO-GeH₃NH₂

N	0.46219400	0.00107500	-0.00615300
C	0.98258600	1.23554500	-0.63007100
C	0.96750700	-0.07319600	1.38106500
C	0.98161500	-1.16009000	-0.75832100
N	3.05189900	-0.00120700	0.01250200
H	0.48680300	1.35957300	-1.60796400
H	0.68471700	2.07921600	0.01482000
H	0.46096400	0.70877300	1.97213900
H	0.66940700	-1.05479100	1.78594900
H	0.47494600	-2.06559700	-0.38286400
H	0.69542900	-1.02043900	-1.81415100
C	2.53354400	1.13808800	-0.77316100

H	3.02556600	2.05898700	-0.41945600
H	2.82668900	0.97813900	-1.82400700
C	2.51744100	0.10725100	1.38606600
H	3.00608000	-0.65688800	2.01258500
H	2.80127000	1.09879100	1.77597200
C	2.53007500	-1.24757200	-0.58606900
H	3.03081800	-1.40620100	-1.55528400
H	2.80994900	-2.07943100	0.08134200
H	-1.72456900	-1.30565700	0.70538500
H	-1.72639100	1.30983300	0.69912900
H	-1.70045400	-0.00352400	-1.51511200
N	-3.97593100	-0.00048800	0.14673800
H	-4.42974700	0.81787100	-0.26183400
H	-4.42940900	-0.81918400	-0.26158500
Ge	-2.08768200	0.00014700	-0.01855400

DABCO-GeH₃OH

N	-0.40132700	0.00704700	-0.00029500
C	-0.91385700	-0.78116900	-1.14486900
C	-0.91449400	-0.59443200	1.25220700
C	-0.92647600	1.38735000	-0.10809200
N	-2.99053900	-0.00882900	0.00039600
H	-0.40729600	-0.42543100	-2.05787200
H	-0.62024900	-1.83028200	-0.97588200
H	-0.39899200	-1.55767300	1.40453400
H	-0.63195900	0.08029500	2.07700000
H	-0.42099500	2.00513800	0.65329500
H	-0.64262800	1.76722800	-1.10334600
C	-2.46226900	-0.62010800	-1.23652800
H	-2.95410400	-1.59532100	-1.38376800
H	-2.74429600	0.03347400	-2.07831800
C	-2.46063100	-0.76987600	1.15053000
H	-2.96067000	-0.41542100	2.06649500
H	-2.73138400	-1.82828700	1.00317600
C	-2.47381500	1.37250300	0.08670300
H	-2.97572200	1.98355500	-0.68104000
H	-2.75341300	1.77187500	1.07547200
H	1.71599300	0.78680300	1.29684500
H	1.72799400	-1.49763300	0.00154700
H	1.71658500	0.78402300	-1.29871200
O	3.86596900	-0.12671800	0.00031400
H	4.30324200	0.73553400	-0.00067000
Ge	2.01570100	0.00821100	-0.00005300

DABCO-GeH₃I

N	-1.75810300	0.00000000	-0.00000100
C	-2.27676500	0.67108000	1.21910700
C	-2.27676100	0.72024200	-1.19072300
C	-2.27676200	-1.39131900	-0.02838500
N	-4.34547700	-0.00000200	-0.00000200
H	-1.76249500	0.23628300	2.09250900
H	-1.99643200	1.73475000	1.14829200
H	-1.76248900	1.69402900	-1.25088100
H	-1.99642800	0.12707800	-2.07647900
H	-1.76249200	-1.93031200	-0.84163100
H	-1.99642900	-1.86182700	0.92818600
C	-3.82157300	0.48017200	1.29458200
H	-4.32283700	1.42780800	1.54862600
H	-4.09145900	-0.26385200	2.06152200
C	-3.82156900	0.88106300	-1.06312900
H	-4.32283200	0.62724800	-2.01082500
H	-4.09145500	1.91726900	-0.80226600
C	-3.82156900	-1.36123400	-0.23145200
H	-4.32282600	-2.05506100	0.46220700
H	-4.09145300	-1.65342600	-1.25926300
H	0.34805000	-0.63017700	-1.38050500
H	0.34805000	1.51064200	0.14450400
H	0.34805000	-0.88046400	1.23600300
Ge	0.55537600	0.00000000	0.00000100
I	3.21129300	0.00000000	0.00000000

DABCO-GeH₃Br

N	1.26011200	0.00003700	-0.00004600
C	1.77897600	0.82204700	-1.12247800
C	1.77890400	0.56108200	1.27309000
C	1.77889300	-1.38306500	-0.15069100
N	3.84778700	-0.00004400	0.00006000
H	1.26421500	0.50386200	-2.04446600
H	1.49948300	1.86788500	-0.91517200
H	1.26416900	1.51865500	1.45852400
H	1.49935300	-0.14135400	2.07515600
H	1.26408900	-2.02242300	0.58584300
H	1.49940800	-1.72644500	-1.16007000
C	3.32364900	0.64174600	-1.22245800
H	3.82531600	1.61384900	-1.35362200
H	3.59309100	0.00163200	-2.07821800
C	3.32359300	0.73780700	1.16708200
H	3.82519600	0.36534100	2.07456400

H	3.59306400	1.79897000	1.04062100
C	3.32356300	-1.37963500	0.05549800
H	3.82520900	-1.97930500	-0.72077800
H	3.59295500	-1.80071700	1.03773600
H	-0.84201200	-0.79258200	1.29361900
H	-0.84212800	1.51668800	0.03943700
H	-0.84222100	-0.72405300	-1.33332600
Br	-3.48312700	-0.00001200	0.00003300
Ge	-1.05345300	0.00001800	-0.00004200

DABCO-GeH₃Cl

N	-0.68794700	-0.00000200	0.00000100
C	-1.20674100	0.91806700	1.04507500
C	-1.20674000	0.44602800	-1.31760600
C	-1.20674500	-1.36409700	0.27253200
N	-3.27600400	0.00000300	-0.00000100
H	-0.69310500	0.68148800	1.99188600
H	-0.92555600	1.94125300	0.74701500
H	-0.69310100	1.38427800	-1.58612900
H	-0.92555800	-0.32369300	-2.05468300
H	-0.69311000	-2.06577100	-0.40575600
H	-0.92556300	-1.61756500	1.30766800
C	-2.75186100	0.74954900	1.15953400
H	-3.25251800	1.73012300	1.20111800
H	-3.02303600	0.19027500	2.06968500
C	-2.75186000	0.62941500	-1.22889400
H	-3.25251800	0.17514200	-2.09888900
H	-3.02303100	1.69726700	-1.19962400
C	-2.75186500	-1.37895900	0.06935800
H	-3.25252400	-1.90525700	0.89776800
H	-3.02303900	-1.88753500	-0.87006300
H	1.41413300	-0.90365900	-1.21870400
H	1.41413100	1.50725600	-0.17323700
H	1.41413400	-0.60360300	1.39194300
Cl	3.90074200	0.00000200	-0.00000100
Ge	1.62906800	-0.00000200	0.00000100

DABCO-GeH₃F

N	-0.35807000	0.00000200	0.00000600
C	-0.87668000	-1.34746200	-0.34370800
C	-0.87669000	0.37607000	1.33879800
C	-0.87668100	0.97139800	-0.99507800
N	-2.94654700	-0.00000200	-0.00000700
H	-0.36321500	-1.68662600	-1.25881400

H	-0.59501800	-2.02347600	0.47987600
H	-0.36323400	-0.24685700	2.09007800
H	-0.59502600	1.42732000	1.51245600
H	-0.36322500	1.93348800	-0.83124400
H	-0.59500800	0.59616500	-1.99231400
C	-2.42195000	-1.27374200	-0.53280500
H	-2.92245300	-2.10601500	-0.01234000
H	-2.69384700	-1.32713200	-1.59958500
C	-2.42196100	0.17545100	1.36948800
H	-2.92246600	1.04232600	1.83002000
H	-2.69386700	-0.72171100	1.94911400
C	-2.42195300	1.09828800	-0.83669600
H	-2.92244900	1.06368400	-1.81770200
H	-2.69386100	2.04884000	-0.34954600
H	1.74308600	1.43452800	0.50146500
H	1.74308500	-1.15154700	0.99160900
H	1.74307600	-0.28299300	-1.49306700
F	3.78612400	0.00000500	-0.00000600
Ge	1.96647200	-0.00000200	0.00000200

DABCO-GeH₃CN

N	-0.62733100	0.00000100	-0.00000400
C	-1.14391500	0.86598800	1.08592400
C	-1.14392100	0.50745500	-1.29292900
C	-1.14391700	-1.37343700	0.20699400
N	-3.21479500	-0.00000200	0.00000700
H	-0.63682300	0.57943400	2.02284500
H	-0.85596800	1.90208500	0.84234600
H	-0.63683500	1.46213300	-1.51323100
H	-0.85596900	-0.22154000	-2.06842100
H	-0.63683700	-2.04156400	-0.50963500
H	-0.85596100	-1.68054200	1.22606500
C	-2.69163600	0.70363500	1.18840800
H	-3.18791900	1.68459100	1.26315800
H	-2.97032100	0.11281900	2.07619300
C	-2.69164400	0.67737000	-1.20356100
H	-3.18792800	0.25162100	-2.09046600
H	-2.97033800	1.74162000	-1.13579400
C	-2.69163900	-1.38100800	0.01517000
H	-3.18791500	-1.93621900	0.82733500
H	-2.97033600	-1.85444700	-0.94037900
H	1.52084400	-0.86187000	-1.24047500
H	1.52084400	1.50521400	-0.12617500
H	1.52084000	-0.64334100	1.36663100

C	3.77804400	-0.00000100	0.00000300
N	4.96983200	-0.00000300	0.00001600
Ge	1.77713900	0.00000100	-0.00000600

DABCO-GeH₃NO₂

N	-0.88430400	-0.00415200	-0.00047300
C	-1.40680500	-0.80290000	-1.14140700
C	-1.40501200	-0.59036300	1.26364700
C	-1.39774200	1.38668900	-0.12316500
N	-3.46965200	0.00587200	0.00071200
H	-0.88948000	-0.46871500	-2.05596200
H	-1.13256300	-1.85348100	-0.95354100
H	-0.89161100	-1.55191300	1.42966900
H	-1.12451100	0.09661300	2.07829300
H	-0.87721200	2.00895000	0.62341600
H	-1.11886200	1.74695700	-1.12644800
C	-2.94965100	-0.60950400	-1.23637800
H	-3.45587600	-1.57549800	-1.39114400
H	-3.21423800	0.05191000	-2.07705000
C	-2.94923000	-0.76093300	1.14991000
H	-3.44985600	-0.40948000	2.06598600
H	-3.22012100	-1.81821000	0.99827300
C	-2.94103900	1.38171600	0.08797500
H	-3.44169000	2.00209800	-0.67217600
H	-3.20568500	1.78036100	1.08058200
H	1.23076200	0.75954100	1.31872500
H	1.22357300	-1.54089500	-0.00619300
H	1.23158300	0.76989800	-1.31354000
N	3.39644300	-0.00243700	0.00021900
O	4.04306700	-1.07275500	0.00037600
O	3.94789000	1.12132100	0.00066500
Ge	1.35648700	-0.01280800	-0.00043500