

Supplementary Information

Cooperative effects in weak interactions: enhancement of tetrel bonds by intramolecular hydrogen bonds

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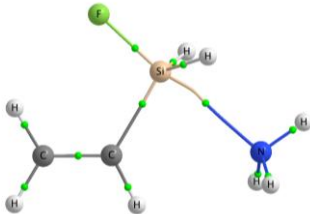
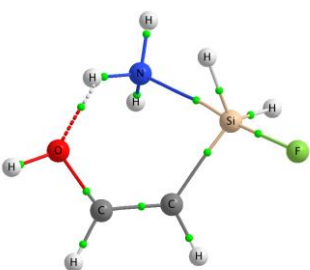
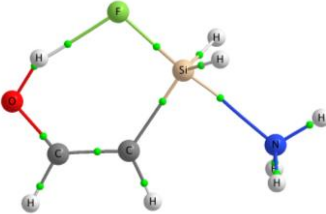
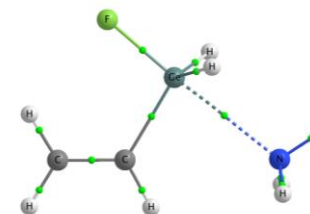
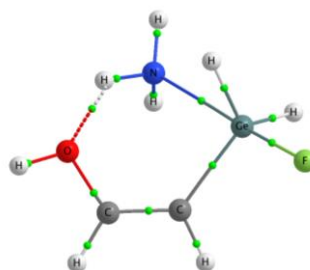
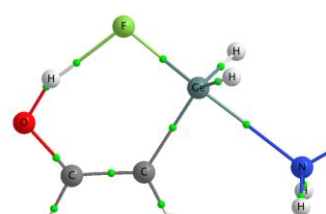
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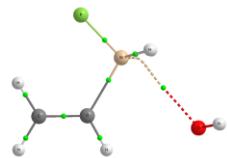
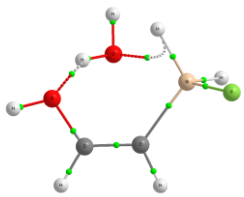
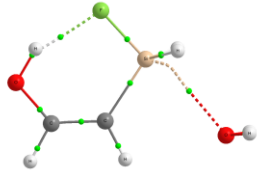
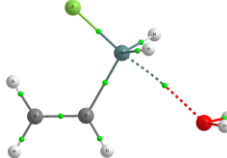
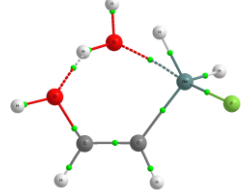
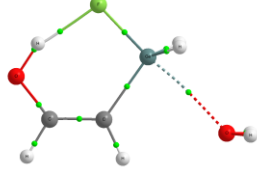
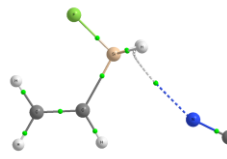
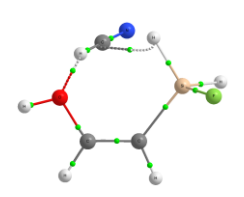
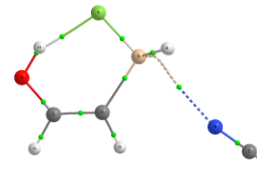
³ Irish Centre of High-End Computing, Grand Canal Quay, Dublin 2, Ireland & School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland; goar.sanchez@ichec.ie

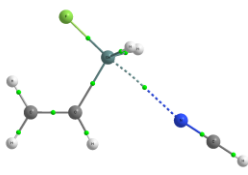
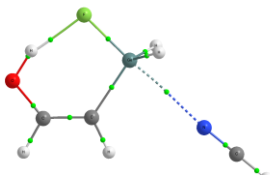
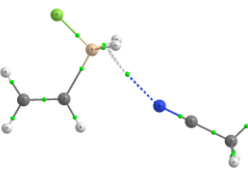
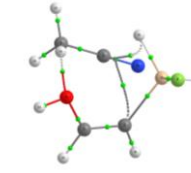
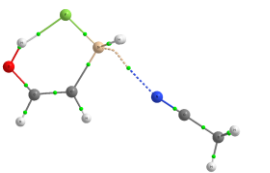
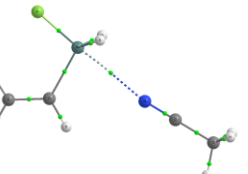
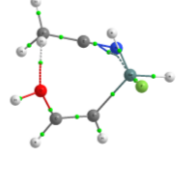
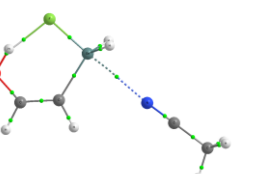
* Correspondence: goar.sanchez@ichec.ie; Tel.: +353 1 5241608 (ext. 47)

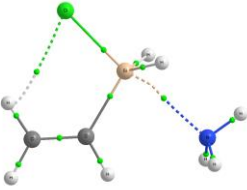
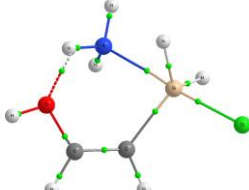
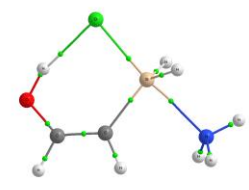
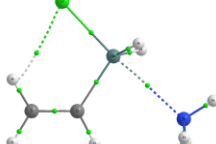
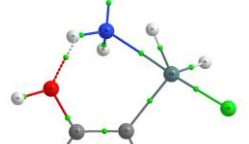
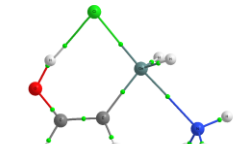
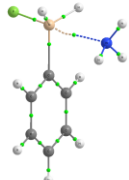
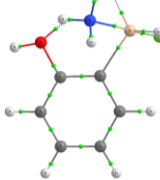
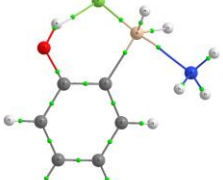
- Table S1: Molecular graphs and Cartesian coordinates for all the complexes studied at the MP2/aug-cc-pVTZ computational level
- Table S2. Molecular electrostatic potential maxima corresponding to the σ -hole on the tetrel atom, in kcal/mol, on the 0.001 a.u. electron density isosurface at the MP2/aug-cc-pVTZ computational level.
- Table S3: electron density, Laplacian, and total energy density, H at the bond critical point, in a.u. and intermolecular distance, in Å, at the MP2/aug-cc-pVTZ computational level.

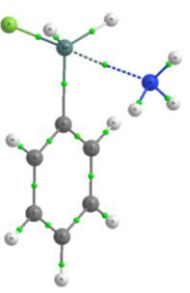
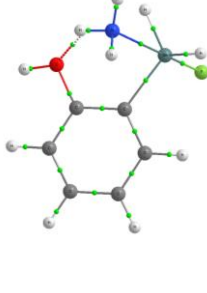
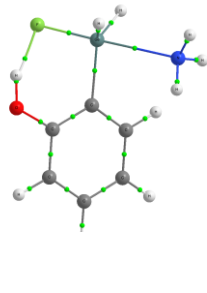
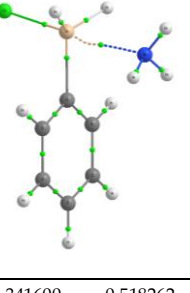
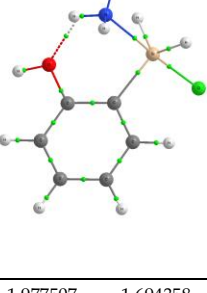
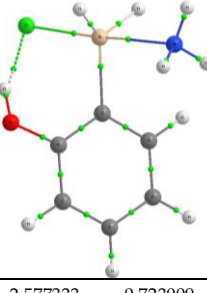
Table S1. Molecular graphs and Cartesian coordinates for all the complexes studied at the MP2/aug-cc-pVTZ computational level.

1T												
1SiF: NH ₃				1SiFOH _{rot} :NH ₃				1SiFOH:NH ₃				
												
C	1.107413	-0.757414	0.000000	C	-0.409368	-1.033608	-0.924454	C	-0.409368	-1.033608	-0.924454	
C	1.817105	0.381775	0.000000	C	-0.116385	-1.716378	0.185628	C	-0.116385	-1.716378	0.185628	
H	1.663940	-1.688472	0.000000	H	-0.551089	-1.665352	-1.794881	H	-0.551089	-1.665352	-1.794881	
H	2.900810	0.378457	0.000000	H	-0.053085	-2.798940	0.216509	H	-0.053085	-2.798940	0.216509	
H	1.325435	1.345784	0.000000	Si	-0.410071	0.817456	-1.212580	Si	-0.410071	0.817456	-1.212580	
Si	-0.763743	-0.728934	0.000000	H	0.363931	1.661262	-0.282070	H	0.363931	1.661262	-0.282070	
H	-1.428628	-1.168891	1.241968	H	-1.631705	1.387646	-1.816189	H	-1.631705	1.387646	-1.816189	
H	-1.428628	-1.168891	-1.241968	F	0.578234	0.856730	-2.538423	F	0.578234	0.856730	-2.538423	
F	-1.070557	0.884689	0.000000	O	0.125313	-1.094377	1.393805	O	0.125313	-1.094377	1.393805	
N	-0.476986	-3.230946	0.000000	H	0.419834	-1.754182	2.028928	H	0.419834	-1.754182	2.028928	
H	-1.403813	-3.641868	0.000000	N	-1.836325	0.876595	0.635796	N	-1.836325	0.876595	0.635796	
H	0.005560	-3.590450	0.815961	H	-2.066021	1.818912	0.929899	H	-2.066021	1.818912	0.929899	
H	0.005560	-3.590450	-0.815961	H	-1.362960	0.405620	1.400361	H	-1.362960	0.405620	1.400361	
H				H	-2.705165	0.386204	0.458505	H	-2.705165	0.386204	0.458505	
1GeF: NH ₃				1GeFOH _{rot} : NH ₃				1GeFOH: NH ₃				
												
C	1.137587	-0.725810	0.000000	C	-0.072184	-0.902637	-1.000469	C	0.441324	-1.315943	0.000000	
C	1.843091	0.412264	0.000000	C	-0.149225	-1.922415	-0.144321	C	1.543107	-0.537696	0.000000	
H	1.676384	-1.666027	0.000000	H	0.017129	-1.188062	-2.040998	H	0.648037	-2.377391	0.000000	
H	2.926446	0.406588	0.000000	H	-0.143977	-2.960051	-0.460575	H	2.534815	-0.976591	0.000000	
H	1.347378	1.374071	0.000000	Ge	0.071086	0.959657	-0.562366	Ge	-1.358963	-0.680711	0.000000	
Ge	-0.783304	-0.692843	0.000000	H	0.429578	1.307359	0.862149	H	-2.162365	-0.739053	1.282689	
H	-1.471834	-1.120749	1.278148	H	-0.867609	1.884472	-1.303070	H	-2.162365	-0.739053	-1.282689	
H	-1.471834	-1.120749	-1.278148	F	1.590764	1.328044	-1.404951	F	-0.994005	1.097578	0.000000	
F	-1.076447	1.051103	0.000000	O	-0.264331	-1.732034	1.214706	O	1.611287	0.802288	0.000000	
N	-0.479783	-3.336546	0.000000	H	-0.169598	-2.581271	1.657076	H	0.694645	1.151101	0.000000	
H	-1.401230	-3.759298	0.000000	N	-2.138399	0.498179	0.666110	N	-1.932111	-3.062485	0.000000	
H	0.005324	-3.695690	0.814446	H	-2.530156	1.229219	1.247898	H	-2.936358	-3.202051	0.000000	
H	0.005324	-3.695690	-0.814446	H	-1.892906	-0.282843	1.265244	H	-1.564239	-3.538169	0.816346	
H				H	-2.868732	0.183859	0.038566	H	-1.564239	-3.538169	-0.816346	
1SiF: H ₂ O				1SiFOH _{rot} : H ₂ O				1SiFOH: H ₂ O				

		
C 1.164324 -0.614442 0.000000 C 1.849890 0.538856 0.000000 H 1.714539 -1.548067 0.000000 H 2.933102 0.558435 0.000000 H 1.342285 1.495252 0.000000 Si -0.694108 -0.631331 0.000000 H -1.281684 -1.223956 1.217164 H -1.281684 -1.223956 -1.217164 F -1.154018 0.928213 0.000000 O -0.082657 -3.450646 0.000000 H -0.466730 -3.898473 0.760524 H -0.466730 -3.898473 -0.760524	C -0.341998 -1.041344 -1.012230 C -0.133271 -1.653117 0.156149 H -0.527004 -1.721638 -1.835935 H -0.147981 -2.730999 0.272647 Si -0.267314 0.777082 -1.394443 H 0.373129 1.569049 -0.331651 H -1.553967 1.330669 -1.841986 F 0.712306 0.884603 -2.690115 O 0.096241 -0.953395 1.320934 H 0.300778 -1.575393 2.026374 O -2.038492 0.840702 0.880040 H -2.054937 1.699934 1.312051 H -1.367185 0.335230 1.360494	C 0.404531 -1.227901 0.017035 C 1.546410 -0.517978 -0.070368 H 0.537566 -2.300790 0.039376 H 2.515381 -1.000766 -0.114036 Si -1.298927 -0.528139 0.098040 H -2.017445 -0.750527 1.366380 H -2.160864 -0.818744 -1.062577 F -1.068377 1.103709 0.038645 O 1.692800 0.824645 -0.116773 H 0.815292 1.236607 -0.076466 O -1.870564 -3.231157 0.207555 H -2.432859 -3.530652 -0.514166 H -2.343181 -3.488232 1.005867
1GeF:H ₂ O	1GeFOH _{rot} :H ₂ O	1GeFOH:H ₂ O
		
C 1.204582 -0.618342 0.000000 C 1.870219 0.543120 0.000000 H 1.757844 -1.549230 0.000000 H 2.952947 0.574280 0.000000 H 1.345772 1.489873 0.000000 Ge -0.709505 -0.654455 0.000000 H -1.342440 -1.197104 1.263846 H -1.342440 -1.197104 -1.263846 F -1.142808 1.045458 0.000000 O -0.131034 -3.423606 0.000000 H -0.440188 -3.924934 0.761206 H -0.440188 -3.924934 -0.761206	C 0.362749 -1.041942 0.685432 C 1.604569 -1.305114 0.280383 H -0.004148 -1.688499 1.472242 H 2.210180 -2.098964 0.702337 Ge -0.841000 0.262412 -0.030983 H -0.488382 0.760085 -1.412082 H -1.291900 1.313493 0.952836 F -2.293741 -0.695865 -0.282511 O 2.229963 -0.561195 -0.698971 H 3.075373 -0.968717 -0.912298 O 1.380379 1.893337 0.351649 H 1.420531 2.705691 -0.162129 H 1.947368 1.267717 -0.123153	C -0.531453 -1.108513 0.000000 C 0.313538 -2.155878 0.000000 H -1.583933 -1.351431 0.000000 H -0.054945 -3.175006 0.000000 Ge 0.000000 0.715137 0.000000 H -0.262012 1.504792 1.264037 H -0.262012 1.504792 -1.264037 F 1.776849 0.564209 0.000000 O 1.660831 -2.137601 0.000000 H 1.959937 -1.209408 0.000000 O -2.698909 1.057108 0.000000 H -3.088281 1.497154 0.762475 H -3.088281 1.497154 -0.762475
1SiF:HCN	1SiFOH _{rot} :HCN	1SiFOH:HCN
		
C -1.257265 1.139026 0.000183 C -2.457262 1.739471 -0.000271 H -0.368940 1.759253 0.000580 H -2.555653 2.818572 -0.000249 H -3.374098 1.163490 -0.000671 Si -1.109322 -0.717172 0.000145 H -0.488852 -1.265669 1.219637 H -0.488045 -1.265541 -1.219003 F -2.643129 -1.266358 -0.000415 C 2.856907 0.039196 0.000249 N 1.688270 0.017263 0.000970 H 3.926743 0.057931 -0.000401	C 1.083283 0.802948 0.847343 C 0.289651 1.789977 0.417433 H 1.530764 0.983164 1.818242 H 0.119404 2.695474 0.992055 Si 1.522225 -0.753886 -0.067499 H 0.857179 -0.897866 -1.370191 H 1.383429 -1.947462 0.783134 F 3.115960 -0.645347 -0.388640 O -0.406439 1.718235 -0.762795 H -0.733049 2.596846 -0.981857 C -2.360291 -0.833540 0.128987 N -1.250994 -1.152001 0.317083 H -3.365956 -0.517753 -0.054908	C -0.853278 0.902146 0.000874 C -2.052235 1.517679 0.000483 H -0.006667 1.574352 0.001669 H -2.137539 2.598000 0.000898 Si -0.576228 -0.925555 0.000179 H 0.030038 -1.483431 1.220716 H 0.029718 -1.482609 -1.220905 F -2.112987 -1.539460 0.000099 O -3.280685 0.953419 -0.000609 H -3.177385 -0.012004 -0.000831 C 3.186210 0.107927 -0.000617 N 2.037473 -0.105049 0.000128 H 4.238290 0.302932 -0.000613
1GeF:HCN	1GeFOH _{rot} :HCN	1GeFOH:HCN

																																																																																																																																																																																														
<table><tr><td>C</td><td>0.895532</td><td>1.374763</td><td>-0.000035</td></tr><tr><td>C</td><td>2.059772</td><td>2.035899</td><td>0.000019</td></tr><tr><td>H</td><td>-0.029845</td><td>1.937129</td><td>-0.000104</td></tr><tr><td>H</td><td>2.095955</td><td>3.118607</td><td>0.000054</td></tr><tr><td>H</td><td>3.003882</td><td>1.506639</td><td>0.000167</td></tr><tr><td>Ge</td><td>0.853802</td><td>-0.542561</td><td>0.000017</td></tr><tr><td>H</td><td>0.327922</td><td>-1.180075</td><td>-1.266831</td></tr><tr><td>H</td><td>0.328017</td><td>-1.179979</td><td>1.266961</td></tr><tr><td>F</td><td>2.563267</td><td>-0.956058</td><td>0.000000</td></tr><tr><td>C</td><td>-3.083135</td><td>0.044781</td><td>-0.000117</td></tr><tr><td>N</td><td>-1.916322</td><td>-0.017292</td><td>-0.000186</td></tr><tr><td>H</td><td>-4.151644</td><td>0.101253</td><td>0.000060</td></tr></table>	C	0.895532	1.374763	-0.000035	C	2.059772	2.035899	0.000019	H	-0.029845	1.937129	-0.000104	H	2.095955	3.118607	0.000054	H	3.003882	1.506639	0.000167	Ge	0.853802	-0.542561	0.000017	H	0.327922	-1.180075	-1.266831	H	0.328017	-1.179979	1.266961	F	2.563267	-0.956058	0.000000	C	-3.083135	0.044781	-0.000117	N	-1.916322	-0.017292	-0.000186	H	-4.151644	0.101253	0.000060	<table><tr><td>C</td><td>0.434301</td><td>0.819623</td><td>0.857481</td></tr><tr><td>C</td><td>-0.482837</td><td>1.686451</td><td>0.414345</td></tr><tr><td>H</td><td>0.818911</td><td>1.045674</td><td>1.845580</td></tr><tr><td>H</td><td>-0.803745</td><td>2.545863</td><td>0.995317</td></tr><tr><td>Ge</td><td>1.128254</td><td>-0.637742</td><td>-0.063308</td></tr><tr><td>H</td><td>0.533803</td><td>-0.853864</td><td>-1.389937</td></tr><tr><td>H</td><td>1.140977</td><td>-1.854529</td><td>0.765384</td></tr><tr><td>F</td><td>2.697682</td><td>-0.288844</td><td>-0.328014</td></tr><tr><td>O</td><td>-1.122592</td><td>1.534867</td><td>-0.789965</td></tr><tr><td>H</td><td>-1.568756</td><td>2.359532</td><td>-1.007874</td></tr><tr><td>C</td><td>-1.887041</td><td>-2.537922</td><td>0.589755</td></tr><tr><td>N</td><td>-0.860596</td><td>-2.008404</td><td>0.407113</td></tr><tr><td>H</td><td>-2.839599</td><td>-2.999683</td><td>0.745675</td></tr></table>	C	0.434301	0.819623	0.857481	C	-0.482837	1.686451	0.414345	H	0.818911	1.045674	1.845580	H	-0.803745	2.545863	0.995317	Ge	1.128254	-0.637742	-0.063308	H	0.533803	-0.853864	-1.389937	H	1.140977	-1.854529	0.765384	F	2.697682	-0.288844	-0.328014	O	-1.122592	1.534867	-0.789965	H	-1.568756	2.359532	-1.007874	C	-1.887041	-2.537922	0.589755	N	-0.860596	-2.008404	0.407113	H	-2.839599	-2.999683	0.745675	<table><tr><td>C</td><td>-0.677973</td><td>1.148464</td><td>-0.000265</td></tr><tr><td>C</td><td>-1.867325</td><td>1.779139</td><td>-0.000150</td></tr><tr><td>H</td><td>0.188719</td><td>1.792908</td><td>-0.000614</td></tr><tr><td>H</td><td>-1.928473</td><td>2.861364</td><td>-0.000375</td></tr><tr><td>Ge</td><td>-0.447025</td><td>-0.741658</td><td>-0.000074</td></tr><tr><td>H</td><td>0.078157</td><td>-1.376122</td><td>1.267515</td></tr><tr><td>H</td><td>0.077812</td><td>-1.376314</td><td>-1.267715</td></tr><tr><td>F</td><td>-2.156416</td><td>-1.276042</td><td>0.000196</td></tr><tr><td>O</td><td>-3.098960</td><td>1.232908</td><td>0.000366</td></tr><tr><td>H</td><td>-3.004532</td><td>0.261012</td><td>0.000666</td></tr><tr><td>C</td><td>3.294228</td><td>0.197967</td><td>-0.000079</td></tr><tr><td>N</td><td>2.152101</td><td>-0.045859</td><td>-0.000339</td></tr><tr><td>H</td><td>4.340457</td><td>0.422252</td><td>0.000245</td></tr></table>	C	-0.677973	1.148464	-0.000265	C	-1.867325	1.779139	-0.000150	H	0.188719	1.792908	-0.000614	H	-1.928473	2.861364	-0.000375	Ge	-0.447025	-0.741658	-0.000074	H	0.078157	-1.376122	1.267515	H	0.077812	-1.376314	-1.267715	F	-2.156416	-1.276042	0.000196	O	-3.098960	1.232908	0.000366	H	-3.004532	0.261012	0.000666	C	3.294228	0.197967	-0.000079	N	2.152101	-0.045859	-0.000339	H	4.340457	0.422252	0.000245																																				
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H	0.080284	-6.210167	0.891034																																																																																																																																																																																											
C	0.610610	0.291148	1.113261																																																																																																																																																																																											
C	0.618608	1.598646	0.826862																																																																																																																																																																																											
H	0.412811	0.042769	2.147853																																																																																																																																																																																											
H	0.455266	2.374679	1.567910																																																																																																																																																																																											
Si	0.954973	-1.040249	-0.135141																																																																																																																																																																																											
H	0.170814	-0.852343	-1.371923																																																																																																																																																																																											
H	0.726246	-2.368772	0.454620																																																																																																																																																																																											
F	2.513602	-0.968190	-0.572953																																																																																																																																																																																											
O	0.815052	2.041907	-0.454056																																																																																																																																																																																											
H	0.914225	2.999156	-0.451697																																																																																																																																																																																											
C	-2.373331	-0.530667	-0.005583																																																																																																																																																																																											
N	-2.254708	-1.517929	0.612537																																																																																																																																																																																											
C	-2.495337	0.698557	-0.775583																																																																																																																																																																																											
H	-1.504689	1.118492	-0.942442																																																																																																																																																																																											
H	-2.964120	0.490374	-1.734688																																																																																																																																																																																											
H	-3.103364	1.416975	-0.230141																																																																																																																																																																																											
C	0.537317	-0.985628	0.000890																																																																																																																																																																																											
C	1.669627	-0.254704	0.000499																																																																																																																																																																																											
H	0.696503	-2.054866	0.001685																																																																																																																																																																																											
H	2.648015	-0.720674	0.000914																																																																																																																																																																																											
Si	-1.184260	-0.312263	0.000195																																																																																																																																																																																											
H	-1.970448	-0.558620	1.220732																																																																																																																																																																																											
H	-1.969577	-0.558754	-1.220889																																																																																																																																																																																											
F	-0.948065	1.325638	0.000115																																																																																																																																																																																											
O	1.794757	1.091336	-0.000592																																																																																																																																																																																											
H	0.906900	1.484302	-0.000815																																																																																																																																																																																											
C	-2.169244	-4.087688	-0.000601																																																																																																																																																																																											
N	-1.779672	-2.986239	0.000144																																																																																																																																																																																											
C	-2.654774	-5.460238	-0.000596																																																																																																																																																																																											
H	-3.227488	-5.647737	0.904468																																																																																																																																																																																											
H	-3.291488	-5.625147	-0.866427																																																																																																																																																																																											
H	-1.813857	-6.148305	-0.039722																																																																																																																																																																																											
1GeF:ACN	1GeFOH _{rot} :ACN	1GeFOH:ACN																																																																																																																																																																																												
																																																																																																																																																																																														
<table><tr><td>C</td><td>1.168513</td><td>-0.514612</td><td>0.004023</td></tr><tr><td>C</td><td>1.872839</td><td>0.624016</td><td>0.006789</td></tr><tr><td>H</td><td>1.695773</td><td>-1.460428</td><td>0.006935</td></tr><tr><td>H</td><td>2.956131</td><td>0.619570</td><td>0.011805</td></tr><tr><td>H</td><td>1.379365</td><td>1.587309</td><td>0.003949</td></tr><tr><td>Ge</td><td>-0.749006</td><td>-0.484410</td><td>-0.004978</td></tr><tr><td>H</td><td>-1.411691</td><td>-0.985498</td><td>1.258999</td></tr><tr><td>H</td><td>-1.399782</td><td>-0.986438</td><td>-1.274765</td></tr><tr><td>F</td><td>-1.098098</td><td>1.239358</td><td>-0.007289</td></tr><tr><td>C</td><td>-0.309730</td><td>-4.440604</td><td>-0.001187</td></tr><tr><td>N</td><td>-0.328000</td><td>-3.272284</td><td>-0.001678</td></tr><tr><td>C</td><td>-0.287469</td><td>-5.896355</td><td>-0.000731</td></tr><tr><td>H</td><td>-0.808714</td><td>-6.271921</td><td>0.876457</td></tr><tr><td>H</td><td>-0.777966</td><td>-6.271984</td><td>-0.895450</td></tr></table>	C	1.168513	-0.514612	0.004023	C	1.872839	0.624016	0.006789	H	1.695773	-1.460428	0.006935	H	2.956131	0.619570	0.011805	H	1.379365	1.587309	0.003949	Ge	-0.749006	-0.484410	-0.004978	H	-1.411691	-0.985498	1.258999	H	-1.399782	-0.986438	-1.274765	F	-1.098098	1.239358	-0.007289	C	-0.309730	-4.440604	-0.001187	N	-0.328000	-3.272284	-0.001678	C	-0.287469	-5.896355	-0.000731	H	-0.808714	-6.271921	0.876457	H	-0.777966	-6.271984	-0.895450	<table><tr><td>C</td><td>0.261434</td><td>0.628827</td><td>1.151611</td></tr><tr><td>C</td><td>0.072872</td><td>1.902718</td><td>0.795730</td></tr><tr><td>H</td><td>0.103905</td><td>0.395970</td><td>2.195225</td></tr><tr><td>H</td><td>-0.214101</td><td>2.679873</td><td>1.496652</td></tr><tr><td>Ge</td><td>0.857945</td><td>-0.712267</td><td>-0.074601</td></tr><tr><td>H</td><td>0.124843</td><td>-0.690269</td><td>-1.399367</td></tr><tr><td>H</td><td>0.921350</td><td>-2.076859</td><td>0.566290</td></tr><tr><td>F</td><td>2.509766</td><td>-0.305703</td><td>-0.481444</td></tr><tr><td>O</td><td>0.203884</td><td>2.301821</td><td>-0.507434</td></tr><tr><td>H</td><td>0.184681</td><td>3.262911</td><td>-0.553620</td></tr><tr><td>C</td><td>-2.435959</td><td>-0.760518</td><td>-0.013888</td></tr><tr><td>N</td><td>-2.124985</td><td>-1.744081</td><td>0.540194</td></tr><tr><td>C</td><td>-2.786591</td><td>0.468160</td><td>-0.709960</td></tr><tr><td>H</td><td>-1.873997</td><td>0.988651</td><td>-0.996773</td></tr></table>	C	0.261434	0.628827	1.151611	C	0.072872	1.902718	0.795730	H	0.103905	0.395970	2.195225	H	-0.214101	2.679873	1.496652	Ge	0.857945	-0.712267	-0.074601	H	0.124843	-0.690269	-1.399367	H	0.921350	-2.076859	0.566290	F	2.509766	-0.305703	-0.481444	O	0.203884	2.301821	-0.507434	H	0.184681	3.262911	-0.553620	C	-2.435959	-0.760518	-0.013888	N	-2.124985	-1.744081	0.540194	C	-2.786591	0.468160	-0.709960	H	-1.873997	0.988651	-0.996773	<table><tr><td>C</td><td>-0.677973</td><td>1.148464</td><td>-0.000265</td></tr><tr><td>C</td><td>-1.867325</td><td>1.779139</td><td>-0.000150</td></tr><tr><td>H</td><td>0.188719</td><td>1.792908</td><td>-0.000614</td></tr><tr><td>H</td><td>-1.928473</td><td>2.861364</td><td>-0.000375</td></tr><tr><td>Ge</td><td>-0.447025</td><td>-0.741658</td><td>-0.000074</td></tr><tr><td>H</td><td>0.078157</td><td>-1.376122</td><td>1.267515</td></tr><tr><td>H</td><td>0.077812</td><td>-1.376314</td><td>-1.267715</td></tr><tr><td>F</td><td>-2.156416</td><td>-1.276042</td><td>0.000196</td></tr><tr><td>O</td><td>-3.098960</td><td>1.232908</td><td>0.000366</td></tr><tr><td>H</td><td>-3.004532</td><td>0.261012</td><td>0.000666</td></tr><tr><td>C</td><td>3.294228</td><td>0.197967</td><td>-0.000079</td></tr><tr><td>N</td><td>2.152101</td><td>-0.045859</td><td>-0.000339</td></tr><tr><td>C</td><td>4.717400</td><td>0.503059</td><td>0.000362</td></tr><tr><td>H</td><td>5.177202</td><td>0.109673</td><td>0.903689</td></tr></table>	C	-0.677973	1.148464	-0.000265	C	-1.867325	1.779139	-0.000150	H	0.188719	1.792908	-0.000614	H	-1.928473	2.861364	-0.000375	Ge	-0.447025	-0.741658	-0.000074	H	0.078157	-1.376122	1.267515	H	0.077812	-1.376314	-1.267715	F	-2.156416	-1.276042	0.000196	O	-3.098960	1.232908	0.000366	H	-3.004532	0.261012	0.000666	C	3.294228	0.197967	-0.000079	N	2.152101	-0.045859	-0.000339	C	4.717400	0.503059	0.000362	H	5.177202	0.109673	0.903689																				
C	1.168513	-0.514612	0.004023																																																																																																																																																																																											
C	1.872839	0.624016	0.006789																																																																																																																																																																																											
H	1.695773	-1.460428	0.006935																																																																																																																																																																																											
H	2.956131	0.619570	0.011805																																																																																																																																																																																											
H	1.379365	1.587309	0.003949																																																																																																																																																																																											
Ge	-0.749006	-0.484410	-0.004978																																																																																																																																																																																											
H	-1.411691	-0.985498	1.258999																																																																																																																																																																																											
H	-1.399782	-0.986438	-1.274765																																																																																																																																																																																											
F	-1.098098	1.239358	-0.007289																																																																																																																																																																																											
C	-0.309730	-4.440604	-0.001187																																																																																																																																																																																											
N	-0.328000	-3.272284	-0.001678																																																																																																																																																																																											
C	-0.287469	-5.896355	-0.000731																																																																																																																																																																																											
H	-0.808714	-6.271921	0.876457																																																																																																																																																																																											
H	-0.777966	-6.271984	-0.895450																																																																																																																																																																																											
C	0.261434	0.628827	1.151611																																																																																																																																																																																											
C	0.072872	1.902718	0.795730																																																																																																																																																																																											
H	0.103905	0.395970	2.195225																																																																																																																																																																																											
H	-0.214101	2.679873	1.496652																																																																																																																																																																																											
Ge	0.857945	-0.712267	-0.074601																																																																																																																																																																																											
H	0.124843	-0.690269	-1.399367																																																																																																																																																																																											
H	0.921350	-2.076859	0.566290																																																																																																																																																																																											
F	2.509766	-0.305703	-0.481444																																																																																																																																																																																											
O	0.203884	2.301821	-0.507434																																																																																																																																																																																											
H	0.184681	3.262911	-0.553620																																																																																																																																																																																											
C	-2.435959	-0.760518	-0.013888																																																																																																																																																																																											
N	-2.124985	-1.744081	0.540194																																																																																																																																																																																											
C	-2.786591	0.468160	-0.709960																																																																																																																																																																																											
H	-1.873997	0.988651	-0.996773																																																																																																																																																																																											
C	-0.677973	1.148464	-0.000265																																																																																																																																																																																											
C	-1.867325	1.779139	-0.000150																																																																																																																																																																																											
H	0.188719	1.792908	-0.000614																																																																																																																																																																																											
H	-1.928473	2.861364	-0.000375																																																																																																																																																																																											
Ge	-0.447025	-0.741658	-0.000074																																																																																																																																																																																											
H	0.078157	-1.376122	1.267515																																																																																																																																																																																											
H	0.077812	-1.376314	-1.267715																																																																																																																																																																																											
F	-2.156416	-1.276042	0.000196																																																																																																																																																																																											
O	-3.098960	1.232908	0.000366																																																																																																																																																																																											
H	-3.004532	0.261012	0.000666																																																																																																																																																																																											
C	3.294228	0.197967	-0.000079																																																																																																																																																																																											
N	2.152101	-0.045859	-0.000339																																																																																																																																																																																											
C	4.717400	0.503059	0.000362																																																																																																																																																																																											
H	5.177202	0.109673	0.903689																																																																																																																																																																																											

H	0.740835	-6.249083	0.017120	H	-3.369917	0.238822	-1.598791	H	5.190359	0.050801	-0.867943
				H	-3.370906	1.109062	-0.053416	H	4.862308	1.580093	-0.034383
1SiCl:NH ₃				1SiCl ^{OH} _{rot} :NH ₃				1SiCl ^{OH} :NH ₃			
											
C	1.095167	-0.731259	0.000000	C	-0.491842	-0.573575	-0.807380	C	-1.107255	-0.473659	-0.217195
C	1.849557	0.377623	0.000000	C	-1.004335	-1.613478	-0.142663	C	-0.971865	-1.801331	-0.004522
H	1.611438	-1.685059	0.000000	H	-0.199308	-0.797008	-1.826867	H	-1.981757	-0.241566	-0.815047
H	2.931781	0.322809	0.000000	H	-1.142985	-2.591506	-0.590638	H	-1.700965	-2.501397	-0.397573
H	1.402372	1.362959	0.000000	Si	-0.043061	1.112678	-0.138758	Si	-0.059849	0.936976	0.381482
Si	-0.774910	-0.711290	0.000000	H	0.211882	1.257371	1.304331	H	-0.205759	1.410444	1.771199
H	-1.418302	-1.189563	1.235305	H	-0.518691	2.287314	-0.891337	H	0.402384	1.929318	-0.605239
H	-1.418302	-1.189563	-1.235305	Cl	1.999197	1.146693	-0.828108	Cl	1.866472	-0.050791	0.678200
Cl	-1.271818	1.339364	0.000000	O	-1.403215	-1.520891	1.174691	O	-0.014988	-2.451506	0.676044
N	-0.442103	-3.329875	0.000000	H	-1.627560	-2.399945	1.495160	H	0.700262	-1.819852	0.887073
H	-1.374962	-3.726998	0.000000	N	-2.202859	1.187580	0.622380	N	-1.990426	2.154469	0.181112
H	0.032963	-3.700903	0.815281	H	-2.393526	2.007374	1.187663	H	-1.842856	3.102149	0.511978
H	0.032963	-3.700903	-0.815281	H	-2.355066	0.359931	1.191295	H	-2.722909	1.742815	0.749943
				H	-2.873673	1.171043	-0.137500	H	-2.341842	2.217595	-0.768501
1GeCl:NH ₃				1GeCl ^{OH} _{rot} :NH ₃				1GeCl ^{OH} :NH ₃			
											
C	1.121389	-0.706885	0.000000	C	-0.470510	-0.745006	-0.784396	C	-1.090792	-0.720888	-0.278839
C	1.871981	0.400688	0.000000	C	-1.081598	-1.749197	-0.153450	C	-0.963499	-2.026726	0.023447
H	1.620254	-1.668954	0.000000	H	-0.228328	-0.926821	-1.823323	H	-1.929840	-0.488648	-0.921258
H	2.953810	0.345494	0.000000	H	-1.342809	-2.680344	-0.644593	H	-1.679730	-2.755086	-0.339780
H	1.421524	1.384709	0.000000	Ge	0.164381	0.871955	0.023544	Ge	0.015633	0.716785	0.312731
Ge	-0.801114	-0.672801	0.000000	H	0.204729	0.913491	1.530148	H	-0.151130	1.209395	1.734029
H	-1.463693	-1.155850	1.270964	H	-0.188613	2.148395	-0.701784	H	0.384091	1.759185	-0.716434
H	-1.463693	-1.155850	-1.270964	Cl	2.318424	0.713119	-0.476771	Cl	2.011637	-0.292366	0.565079
Cl	-1.274890	1.467963	0.000000	O	-1.447636	-1.666228	1.170309	O	-0.016693	-2.620627	0.772053
N	-0.443996	-3.416230	0.000000	H	-1.740010	-2.533436	1.467962	H	0.712778	-1.988038	0.920292
H	-1.371552	-3.825371	0.000000	N	-2.349577	1.127008	0.648295	N	-2.184206	1.990444	0.182661
H	0.034571	-3.784990	0.814078	H	-2.629411	1.882750	1.262335	H	-2.114941	2.917009	0.588835
H	0.034571	-3.784990	-0.814078	H	-2.524949	0.251528	1.129980	H	-2.859297	1.472555	0.734530
				H	-2.954551	1.155024	-0.163705	H	-2.582219	2.103163	-0.743074
2T											
2SiF:NH ₃				2SiF ^{OH} _{rot} :NH ₃				2SiF ^{OH} :NH ₃			
											
C	2.170619	-0.133927	-1.206331	C	-2.153710	-1.404922	0.574309	C	2.139203	1.399535	-0.515103
C	2.869897	-0.121297	-0.000193	C	-2.885093	-0.304401	0.134583	C	2.886295	0.328034	-0.024876
C	2.170679	-0.139635	1.205906	C	-2.220922	0.814930	-0.360133	C	2.249798	-0.844831	0.360925
C	0.776402	-0.165945	1.022281	C	-0.828105	0.827991	-0.411301	C	0.859640	-0.952235	0.272411
C	0.053749	-0.174030	-0.000244	C	-0.061654	-0.259723	0.020018	C	0.074261	0.134173	-0.155150
C	0.776340	-0.160249	-1.202756	C	-0.762123	-1.374351	0.507072	C	0.753062	1.292166	-0.570398
H	2.709907	-0.125984	-2.145132	H	-2.661664	-2.280531	0.955744	H	2.630376	2.303809	-0.849220
H	3.952028	-0.101170	-0.000173	H	-3.966563	-0.311840	0.171310	H	3.964524	0.397717	0.038530
H	2.710018	-0.136116	2.144707	H	-2.783822	1.674943	-0.707580	H	2.810615	-1.699207	0.716614

H	0.246595	-0.183828	2.148908	Si	1.822818	-0.367677	-0.042190	Si	-1.803936	-0.002819	-0.167502
Si	-1.819091	-0.201536	-0.000282	H	2.442371	-0.876661	1.199145	H	-2.535786	0.759985	-1.195724
H	-2.418662	0.283723	-1.256660	H	2.565916	0.612622	-0.853377	H	-2.481852	-0.284621	1.115095
H	-2.418840	0.280005	1.257436	F	1.981238	-1.714858	-0.985744	F	-1.928999	-1.548609	-0.805756
F	-2.213560	-1.791069	-0.002601	N	1.679427	1.527332	1.306208	N	-1.773803	2.057715	0.856309
N	-1.293667	2.341226	0.003449	H	2.585912	1.902361	1.562292	H	-2.691137	2.259282	1.240986
H	-2.052739	3.013957	0.005220	H	1.182744	2.228649	0.765492	H	-1.119449	2.009348	1.630755
H	-0.717147	2.531824	0.815558	H	1.159122	1.361978	2.160345	H	-1.501529	2.852324	0.288800
H	-0.718747	2.534303	-0.809207	H	-0.200180	-2.244594	0.826726	H	0.185884	2.128017	-0.965672
H	0.246467	-0.173670	-2.149426	O	-0.151580	1.935084	-0.891429	O	0.321227	-2.150657	0.645532
				H	-0.796918	2.543857	-1.270403	H	-0.542261	-2.246374	0.211177
2GeF: NH ₃				2GeF ^{OH} _{rot} :NH ₃				2GeF ^{OH} :NH ₃			
											
C	2.529405	-0.194449	-1.206310	C	-2.411556	-1.433917	0.679483	C	2.428984	1.448802	-0.517979
C	3.227928	-0.206278	0.000046	C	-3.193207	-0.417907	0.135169	C	3.199491	0.400391	-0.014459
C	2.529476	-0.192758	1.206426	C	-2.584541	0.687945	-0.452382	C	2.592981	-0.783398	0.386149
C	1.135329	-0.164402	1.203391	C	-1.193979	0.771503	-0.495335	C	1.205515	-0.928318	0.300905
C	0.419715	-0.149468	0.000088	C	-0.385630	-0.232514	0.040819	C	0.406242	0.136416	-0.147164
C	1.135257	-0.166092	-1.203237	C	-1.022766	-1.333629	0.625921	C	1.046069	1.306729	-0.578023
H	3.068589	-0.210431	-2.144739	H	-2.878299	-2.297315	1.133924	H	2.898830	2.361746	-0.858050
H	4.309969	-0.228964	0.000029	H	-4.273064	-0.480650	0.163596	H	4.275763	0.496714	0.048482
H	3.068717	-0.207420	2.144845	H	-3.188484	1.482196	-0.877760	H	3.175184	-1.617748	0.754168
H	0.603608	-0.158512	2.148619	Ge	1.544914	-0.218084	-0.026840	Ge	-1.512438	-0.049641	-0.157375
Ge	-1.502963	-0.101139	0.000085	H	2.199670	-0.634503	1.272310	H	-2.270743	0.631906	-1.271564
H	-2.108706	0.388207	-1.296328	H	2.224373	0.824519	-0.878781	H	-2.213783	-0.265567	1.166249
H	-2.108716	0.389061	1.296159	F	1.815885	-1.685895	-0.988581	F	-1.574899	-1.769025	-0.714934
F	-1.961358	-1.806235	0.000618	N	1.157089	1.892759	1.356669	N	-1.518115	2.240095	0.809416
N	-0.808365	2.511487	-0.000998	H	1.959728	2.437098	1.650756	H	-2.339671	2.378151	1.388279
H	-1.472001	3.278262	-0.002617	H	0.608652	2.461017	0.719530	H	-0.707101	2.284094	1.417841
H	-0.211736	2.633175	0.809929	H	0.589096	1.717936	2.177450	H	-1.459149	3.035821	0.184015
H	-0.210284	2.630983	-0.811183	H	-0.417429	-2.136331	1.030888	H	0.452807	2.122617	-0.975508
H	0.603479	-0.161538	-2.148443	O	-0.563861	1.861454	-1.062469	O	0.687387	-2.126166	0.689144
				H	-1.227738	2.395695	-1.514825	H	-0.172497	-2.248340	0.242835
2SiCl: NH ₃				2SiCl ^{OH} _{rot} :NH ₃				2SiCl ^{OH} :NH ₃			
											
C	-2.341600	-0.518262	1.206635	C	-1.977507	-1.694358	0.783166	C	2.577333	0.723009	-0.911252
C	-3.018967	-0.690996	0.000143	C	-2.925024	-0.959005	0.074342	C	3.068979	-0.394144	-0.234948
C	-2.341290	-0.519996	-1.206420	C	-2.543692	0.201992	-0.592619	C	2.201065	-1.224851	0.464117
C	-0.990925	-0.172605	-1.203978	C	-1.215794	0.622774	-0.545908	C	0.835031	-0.937840	0.505974
C	-0.295630	0.010812	-0.000016	C	-0.239108	-0.096643	0.150222	C	0.323139	0.213930	-0.115132
C	-0.991238	-0.170867	1.204030	C	-0.652685	-1.265106	0.807519	C	1.218789	1.016456	-0.841926
H	-2.862880	-0.657150	2.145307	H	-2.265128	-2.600072	1.299927	H	3.243668	1.354973	-1.483248
H	-4.066864	-0.961595	0.000199	H	-3.956230	-1.284389	0.034296	H	4.124579	-0.630637	-0.268627
H	-2.862328	-0.660235	-2.145025	H	-3.275072	0.778270	-1.149404	H	2.556705	-2.112570	0.970541
H	-0.474026	-0.049439	-2.149785	Si	1.579573	0.390098	0.237270	Si	-1.485406	0.688885	0.025609
Si	1.513697	0.478734	-0.000102	H	2.191877	0.274645	1.573621	H	-2.003132	1.614590	-0.995488
H	1.974236	1.099314	1.252356	H	2.111756	1.384583	-0.706134	H	-2.131070	0.645775	1.349320
H	1.974396	1.098579	-1.252861	Cl	2.436070	-1.379193	-0.632626	Cl	-2.376034	-1.153510	-0.714620

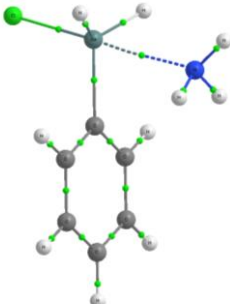
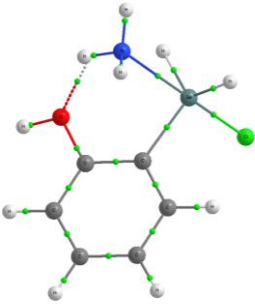
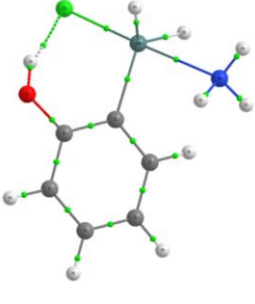
Cl	2.531168	-1.370479	0.000465	N	0.742409	2.317450	1.184274	N	-0.673150	2.622585	0.947351
N	0.312896	2.824335	-0.000863	H	1.463798	2.988460	1.424691	H	-1.410856	3.242500	1.267284
H	0.846272	3.686981	-0.001589	H	0.132307	2.737323	0.488988	H	-0.119711	2.360449	1.757153
H	-0.294471	2.842980	-0.812681	H	0.193436	2.138729	2.017896	H	-0.063077	3.156223	0.337569
H	-0.293725	2.843890	0.811490	H	0.087975	-1.860318	1.329225	H	0.841916	1.882826	-1.376996
H	-0.474579	-0.046321	2.149789	O	-0.817309	1.781823	-1.186885	O	0.044222	-1.808756	1.201293
				H	-1.547467	2.093017	-1.735401	H	-0.838505	-1.816252	0.789722
2GeCl: NH ₃				2GeCl ^{OH} _{rot} :NH ₃				2GeCl ^{OH} ₂ :NH ₃			
											
C	-2.637042	-0.554527	1.206615	C	2.303836	-1.630786	-0.898869	C	2.802653	0.707423	-0.946966
C	-3.317302	-0.712328	-0.000079	C	3.215469	-0.948793	-0.096088	C	3.341668	-0.366976	-0.238395
C	-2.637504	-0.552370	-1.206747	C	2.790425	0.125066	0.681519	C	2.512440	-1.216842	0.484411
C	-1.280520	-0.231855	-1.204512	C	1.451725	0.512178	0.655135	C	1.135103	-0.990151	0.518693
C	-0.587142	-0.066841	-0.000023	C	0.518070	-0.157228	-0.137497	C	0.581959	0.116245	-0.141348
C	-1.280058	-0.234007	1.204437	C	0.968555	-1.233936	-0.909812	C	1.431462	0.939259	-0.892664
H	-3.160757	-0.683846	2.145007	H	2.627643	-2.468159	-1.501955	H	3.442345	1.354433	-1.531881
H	-4.370281	-0.962297	-0.000099	H	4.254864	-1.248347	-0.069737	H	4.407067	-0.555896	-0.264243
H	-3.161575	-0.680019	-2.145172	H	3.496224	0.659184	1.308390	H	2.908119	-2.071400	1.017004
H	-0.760228	-0.115249	-2.148871	Ge	-1.356208	0.298363	-0.180529	Ge	-1.295022	0.507622	-0.008607
Ge	1.282060	0.379639	0.000036	H	-1.941003	0.288923	-1.574321	H	-1.842484	1.429672	-1.070502
H	1.755511	1.010407	1.289096	H	-1.859818	1.333301	0.791127	H	-1.904808	0.563217	1.372585
H	1.755360	1.011108	-1.288735	Cl	-2.235227	-1.560759	0.639666	Cl	-2.144776	-1.470159	-0.644261
Cl	2.297058	-1.564998	-0.000490	N	-0.322215	2.480959	-1.127175	N	-0.397690	2.712448	0.917693
N	-0.016300	2.827143	0.000862	H	-0.928049	3.252282	-1.382502	H	-1.072970	3.281401	1.417278
H	0.426043	3.739534	0.001607	H	0.251022	2.780032	-0.345123	H	0.301277	2.414118	1.590180
H	-0.624339	2.789345	-0.809759	H	0.297043	2.307381	-1.910393	H	0.078625	3.320773	0.261186
H	-0.624734	2.788206	0.811133	H	0.255016	-1.783182	-1.513373	H	1.011688	1.773981	-1.443904
H	-0.759407	-0.119108	2.148806	O	1.001033	1.581156	1.402153	O	0.378261	-1.868418	1.240934
				H	1.703318	1.848894	2.007175	H	-0.500953	-1.935064	0.826433

Table S2. Molecular electrostatic potential maxima corresponding to the σ -hole on the tetrel atom, in kcal/mol, on the 0.001 a.u. electron density isosurface at the MP2/aug-cc-pVTZ computational level.

	F	Cl
1SiX:NH ₃	0.0156	0.0150
1SiX ^{OH} :NH ₃	0.0173	0.0161
1SiX ^{OH} _{rot} :NH ₃	0.0088	0.0087
1GeX: NH ₃	0.0183	0.0165
1GeX ^{OH} :NH ₃	0.0203	0.0176
1GeX ^{OH} _{rot} :NH ₃	0.0115	-
2SiX:NH ₃	0.0108	0.0093
2SiX ^{OH} :NH ₃	0.0148	-

2SiX ^{OH} _{rot} :NH ₃	0.0093	0.0114
2GeX: NH ₃	0.0136	0.0105
2GeX ^{OH} :NH ₃	0.0169	0.0130
2GeX ^{OH} _{rot} :NH ₃	0.0123	0.0094

Table S3. Electron density, Laplacian, and total energy density, H at the bond critical point, in a.u. and intermolecular distance, in Å, at the MP2/aug-cc-pVTZ computational level.

Complex	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Distance
1SiF:NH ₃	0.0270	0.0489	-0.0050	2.518
1SiF ^{OH} :NH ₃	0.0405	0.0817	-0.0135	2.276
1SiF ^{OH} _{rot} :NH ₃	0.0372	0.0626	-0.0119	2.335
1GeF: NH ₃	0.0241	0.0641	-0.0009	2.661
1GeF ^{OH} :NH ₃	0.0366	0.0916	-0.0051	2.450
1GeF ^{OH} _{rot} :NH ₃	0.0289	0.0742	-0.0022	2.570
1SiCl:NH ₃	0.0224	0.0452	-0.0024	2.640
1SiCl ^{OH} :NH ₃	0.0401	0.0718	-0.0135	2.291
1SiCl ^{OH} _{rot} :NH ₃	0.0406	0.0707	-0.0140	2.291
1GeCl: NH ₃	0.0199	0.0539	0.0000	2.767
1GeCl ^{OH} :NH ₃	0.0305	0.0769	-0.0028	2.545
1GeCl ^{OH} _{rot} :NH ₃	0.0274	0.0696	-0.0018	2.603
1SiF:H ₂ O	0.0117	0.0364	0.0006	2.885
1SiF ^{OH} :H ₂ O	0.0142	0.0417	0.0002	2.765
1SiF ^{OH} _{rot} :H ₂ O	0.0125	0.0364	0.0005	2.883
1GeF:H ₂ O	0.0137	0.0474	0.0012	2.829
1GeF ^{OH} :H ₂ O	0.0166	0.0572	0.0011	2.720
1GeF ^{OH} _{rot} :H ₂ O	0.0158	0.0509	0.0009	2.782
1SiF:HCN	0.0101	0.0336	0.0010	2.991
1SiF ^{OH} :HCN	0.0123	0.0386	0.0007	2.873
1SiF ^{OH} _{rot} :HCN	-	-	-	-
1GeF:HCN	0.0129	0.0449	0.0013	2.898
1GeF ^{OH} :HCN	0.0158	0.0536	0.0011	2.789
1GeF ^{OH} _{rot} :ACN	0.0132	0.0458	0.0013	2.891

2T				
Complex	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}	Distance
2SiF:NH ₃	0.0241	0.0468	-0.0033	2.596
2SiF ^{OH} :NH ₃	0.0396	0.0665	-0.0135	2.301
2SiF ^{OH} _{rot} :NH ₃	0.0377	0.0641	-0.0122	2.330
2GeF: NH ₃	0.0224	0.0602	-0.0005	2.703
2GeF ^{OH} :NH ₃	0.0301	0.0762	-0.0026	2.485
2GeF ^{OH} _{rot} :NH ₃	0.0345	0.0843	-0.0043	2.553
2SiCl:NH ₃	0.0229	0.0452	-0.0026	2.635
2SiCl ^{OH} :NH ₃	0.0408	0.0691	-0.0141	2.291
2SiCl ^{OH} _{rot} :NH ₃	0.0399	0.0666	-0.0136	2.305
2GeCl: NH ₃	0.0200	0.0539	0.0000	2.771
2GeCl ^{OH} :NH ₃	0.0303	0.0749	-0.0028	2.554
2GeCl ^{OH} _{rot} :NH ₃	0.0280	0.0708	-0.0020	2.594