

**Regioselective chelation in the reaction of *N*-trimethylsilyl-*N*-acetyl glycine  
*N'*,*N'*-dimethylamide with chloro(chloromethyl)dimethylsilane**

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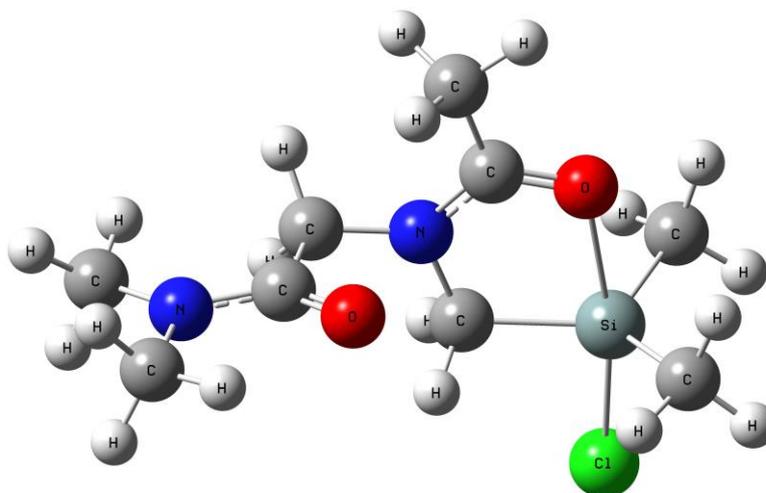
*The sums of electronic and zero-point energies are given.*

**Isolated molecule 2**

0 1

Cl	3.1355020	-2.1373360	-0.1977820
Si	2.3946060	-0.0914940	0.0984150
O	1.2985640	1.8414110	0.2718110
O	-2.0164070	0.0981030	1.3490560
N	-0.2704430	0.5565970	-0.6517200
N	-3.6934260	-0.6472050	0.0182990
C	0.6614940	-0.5572690	-0.5589990
H	0.7830730	-1.0206100	-1.5440330
H	0.2536530	-1.3224860	0.1123140
C	0.1336020	1.7272620	-0.1308300
C	-0.8177990	2.8818290	-0.0530970
H	-0.2680620	3.7480650	0.3085670
H	-1.6236700	2.6450680	0.6460390
H	-1.2547990	3.1148860	-1.0277280
C	3.5742080	0.8096900	-1.0408110
H	3.5120730	1.8905590	-0.9046520
H	3.3469010	0.5718560	-2.0846320
H	4.5973630	0.4760890	-0.8500720
C	2.6591050	0.0507440	1.9433400
H	2.5957350	1.0891680	2.2721530
H	3.6331450	-0.3633880	2.2145010
H	1.8962200	-0.5267550	2.4744110
C	-1.6340380	0.2674750	-1.0014220
H	-1.6223950	-0.5465970	-1.7298090

H	-2.0975590	1.1278510	-1.4947130
C	-2.4649560	-0.1111370	0.2374960
C	-4.2532160	-0.9351810	-1.2828360
H	-3.7478050	-0.3808550	-2.0714330
H	-5.3061490	-0.6374370	-1.2970710
H	-4.2004010	-2.0057620	-1.5178760
C	-4.4871080	-1.0673280	1.1548720
H	-3.9453820	-0.8174080	2.0646890
H	-4.6620510	-2.1485120	1.1216490
H	-5.4558270	-0.5564590	1.1529150
	-1363.069259		



**Isolated molecule 3**

0 1

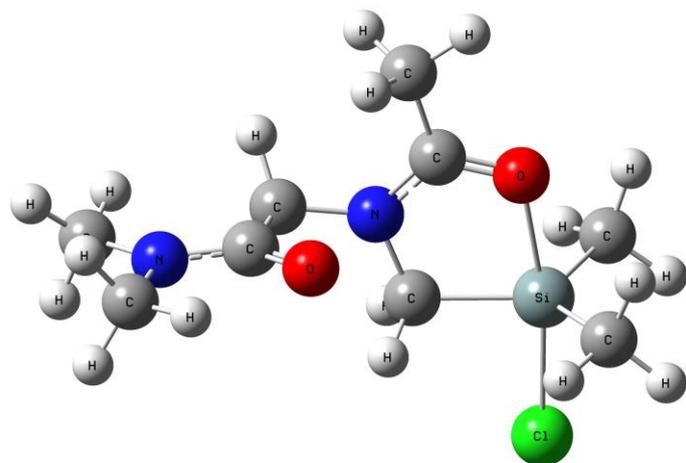
Cl	3.7879420	-0.9649900	-0.6560030
Si	1.8691210	-0.6738450	0.1651900
O	1.0814180	2.8228120	0.2873350
O	-1.2814350	-0.3259870	1.1814690
N	-0.1259210	1.2146690	-0.7345980
N	-3.0797750	-0.9274900	-0.0542890
C	1.1032720	0.5235450	-1.1052730
H	1.8633820	1.2887680	-1.2856590
H	0.9419580	-0.0005130	-2.0541380
C	-0.0092730	2.3660510	-0.0001810
C	-1.2887330	3.0508480	0.4220350
H	-1.0070540	3.9397610	0.9826880
H	-1.8913400	2.3998870	1.0607320
H	-1.8945350	3.3541240	-0.4374600
C	2.0586290	0.0681360	1.8562610
H	1.0650310	0.1721850	2.3014640
H	2.5126970	1.0588190	1.7920610
H	2.6699220	-0.5728500	2.4975140
C	1.0931630	-2.3742220	0.1889190
H	0.1222670	-2.3359220	0.6885530
H	1.7362460	-3.0666230	0.7399340
H	0.9653480	-2.7718340	-0.8220270
C	-1.3858350	0.5944810	-1.0224100
H	-1.2671660	-0.0243650	-1.9175610
H	-2.1335200	1.3539450	-1.2697400
C	-1.9088660	-0.2671270	0.1370960
C	-3.8516220	-0.9219610	-1.2757950
H	-3.4399060	-0.2343680	-2.0106520
H	-4.8827640	-0.6153170	-1.0677170
H	-3.8798750	-1.9234840	-1.7216870
C	-3.6072460	-1.7529980	1.0122760
H	-2.9597550	-1.6530130	1.8807130
H	-3.6430500	-2.8039570	0.7039020
H	-4.6215250	-1.4319610	1.2726840
	-1363.061448		



**Molecule 2 in CHCl<sub>3</sub>**

0 1

Cl	3.1639330	-2.1263390	-0.2318950
Si	2.3509570	-0.0076620	0.1037780
O	1.3260290	1.7604450	0.2839490
O	-1.9930910	0.0129100	1.3535740
N	-0.2805900	0.5339220	-0.6398840
N	-3.7112570	-0.6233870	0.0161170
C	0.6631600	-0.5735890	-0.5862820
H	0.7944180	-0.9971910	-1.5864940
H	0.2641520	-1.3633980	0.0591620
C	0.1396090	1.6824920	-0.1144880
C	-0.7685250	2.8605960	-0.0067260
H	-0.1997180	3.7029220	0.3803020
H	-1.5886060	2.6303830	0.6776120
H	-1.1919100	3.1266790	-0.9782780
C	3.5914520	0.8264230	-1.0241160
H	3.5663220	1.9115360	-0.9044360
H	3.3702890	0.5856090	-2.0686050
H	4.5993400	0.4622510	-0.8120790
C	2.6610030	0.0016040	1.9491010
H	2.5902460	1.0139210	2.3522310
H	3.6461570	-0.4126410	2.1739860
H	1.9162460	-0.6221090	2.4532210
C	-1.6504190	0.2684080	-0.9969010
H	-1.6492070	-0.5257550	-1.7457510
H	-2.1010630	1.1478190	-1.4652660
C	-2.4720250	-0.1355990	0.2388360
C	-4.2993130	-0.8274810	-1.2916640
H	-3.7866030	-0.2529590	-2.0600900
H	-5.3401210	-0.4934280	-1.2713940
H	-4.2842170	-1.8866600	-1.5730870
C	-4.5118070	-1.0676570	1.1399600
H	-3.9539350	-0.8941360	2.0570660
H	-4.7359610	-2.1352940	1.0463700
H	-5.4554760	-0.5142850	1.1747200
	-1363.083955		



**Molecule 3 in CHCl<sub>3</sub>**

0 1

Cl	3.8072930	-0.8578340	-0.6517760
Si	1.8388300	-0.6854070	0.1448780
O	1.0937290	2.7984900	0.3304970
O	-1.1796640	-0.4885590	1.0904740
N	-0.1454090	1.2283510	-0.7095870
N	-3.0815690	-0.9275200	-0.0588230
C	1.0674660	0.5273880	-1.1073200
H	1.8332360	1.2812430	-1.3081780
H	0.8757320	0.0008910	-2.0481610
C	-0.0104980	2.3550810	0.0468710
C	-1.2740760	3.0420930	0.5059150
H	-0.9800320	3.8952860	1.1138650
H	-1.8972370	2.3738030	1.1055600
H	-1.8697920	3.4005790	-0.3386090
C	2.0192520	-0.0094410	1.8658150
H	1.0247040	0.0682320	2.3124350
H	2.4692100	0.9848720	1.8431710
H	2.6339780	-0.6743580	2.4789470
C	1.1754420	-2.4280400	0.0793790
H	0.1902510	-2.4663230	0.5492200
H	1.8457050	-3.1029630	0.6195060
H	1.0951560	-2.7828790	-0.9520020
C	-1.4180600	0.6300640	-1.0055810
H	-1.3304520	0.0800940	-1.9475670
H	-2.1686410	1.4056860	-1.1712350
C	-1.8880330	-0.3181570	0.1047810
C	-3.9561270	-0.7555520	-1.1998220
H	-3.4990540	-0.1429290	-1.9724790
H	-4.8955400	-0.2822210	-0.8940590
H	-4.1912650	-1.7312540	-1.6369030
C	-3.5815400	-1.8112190	0.9754620
H	-2.8694180	-1.8299950	1.7969250
H	-3.7107040	-2.8239230	0.5799640
H	-4.5500660	-1.4535280	1.3396180
	-1363.073195		

