Molecular structures of various alkyldichlorosilanes in the solid state

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Supporting Information

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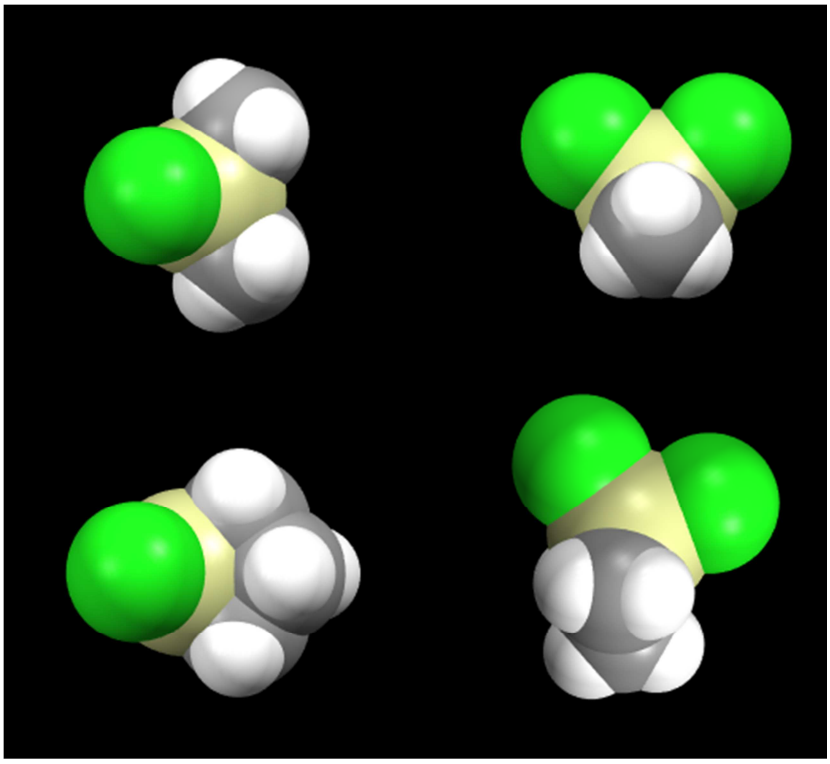

Figure S1: Space fill representations of dimethyldichlorosilane (top) and 1,1-dichlorosilacyclobutane (bottom).

Atomic coordinates and total energies (Hartree) of optimized molecular structures of $(CH_2)_3SiCl_2$, Me_2SiCl_2, $MeHSiCl_2$ and H_2SiCl_2 (B3LYP/6-311++G(d,p))

- $(CH_2)_3SiCl_2$: -1328.02983100 a.u.

Cl	1.72126	-1.28667	0.00004
Cl	0.69005	1.90783	-0.00004
Si	0.03854	-0.06780	0.00001
C	-1.33929	-0.42086	1.22309
H	-1.29220	-1.44001	1.61423
H	-1.52379	0.26515	2.04868
C	-2.32046	-0.30227	-0.00002
H	-3.09753	-1.06857	0.00004
H	-2.80866	0.67360	-0.00007
C	-1.33923	-0.42105	-1.22308
H	-1.52372	0.26476	-2.04883
H	-1.29204	-1.44029	-1.61401

- Me_2SiCl_2: -1289.95614044 a.u.

Cl	1.68300	-0.00000	-0.88953
Si	0.00000	-0.00000	0.34260
C	-0.00000	1.57050	1.34450
H	0.88745	1.61641	1.98184
H	-0.00000	2.44709	0.69307
Cl	-1.68300	0.00000	-0.88953
C	-0.00000	-1.57050	1.34450
H	-0.88745	-1.61641	1.98184
H	-0.00000	-2.44709	0.69307
H	0.88745	-1.61641	1.98184
H	-0.88745	1.61641	1.98184

- $MeHSiCl_2$: -1250.61141040 a.u.

Cl	-1.68795	-0.71315	-0.15038
Cl	1.68777	-0.71340	-0.15040
Si	0.00005	0.33091	0.45677
H	0.00013	0.33476	1.93060
C	0.00012	2.02628	-0.30551
H	0.00122	1.96208	-1.39614
H	0.88773	2.58196	0.00932
H	-0.88741	2.58205	0.00776

- H_2SiCl_2: -1211.26528010 a.u.

Cl	0.00000	1.69655	-0.40925
Si	0.00000	-0.00000	0.76886
Cl	-0.00000	-1.69655	-0.40925
H	1.23204	-0.00000	1.57525
H	-1.23204	0.00000	1.57525

Atomic coordinates of $(CH_2)_3SiCl_2$, Me_2SiCl_2, $MeHSiCl_2$ and H_2SiCl_2 from the potential energy surface scans of the Cl-Si-Cl angle variation (B3LYP/6-311++G(d,p))

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 101°

Cl	1.63555	-1.35453	0.00017
Cl	0.92244	1.78443	-0.00025
Si	-0.01450	-0.08019	0.00007
C	-1.41531	-0.30874	1.22355
H	-1.45339	-1.32578	1.62136
H	-1.53825	0.39531	2.04535
C	-2.38405	-0.11454	-0.00011
H	-3.21753	-0.81889	0.00015
H	-2.79534	0.89613	-0.00070
C	-1.41515	-0.30983	-1.22340
H	-1.53806	0.39348	-2.04584
H	-1.45316	-1.32722	-1.62031

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 102°

Cl	1.64336	-1.35066	0.00015
Cl	0.89526	1.80168	-0.00022
Si	-0.00674	-0.07862	0.00006
C	-1.40563	-0.32126	1.22347
H	-1.43425	-1.33898	1.62030
H	-1.53567	0.38087	2.04582
C	-2.37608	-0.13530	-0.00009
H	-3.20362	-0.84664	0.00013
H	-2.79597	0.87184	-0.00064
C	-1.40549	-0.32223	-1.22333
H	-1.53549	0.37923	-2.04626
H	-1.43403	-1.34026	-1.61935

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 103°

Cl	1.65305	-1.34468	0.00014
Cl	0.86542	1.81952	-0.00020
Si	0.00110	-0.07708	0.00006
C	-1.39544	-0.33532	1.22338
H	-1.41361	-1.35373	1.61905
H	-1.53324	0.36454	2.04640
C	-2.36767	-0.15838	-0.00009
H	-3.18867	-0.87729	0.00012
H	-2.79686	0.84484	-0.00059
C	-1.39530	-0.33622	-1.22325
H	-1.53307	0.36304	-2.04680
H	-1.41341	-1.35491	-1.61817

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 104°

Cl	1.66477	-1.33631	0.00013
Cl	0.83260	1.83794	-0.00019
Si	0.00903	-0.07552	0.00005
C	-1.38464	-0.35112	1.22329
H	-1.39122	-1.37018	1.61762
H	-1.53097	0.34612	2.04707
C	-2.35873	-0.18413	-0.00008
H	-3.17246	-0.91127	0.00011
H	-2.79808	0.81469	-0.00055
C	-1.38450	-0.35195	-1.22317
H	-1.53080	0.34472	-2.04744
H	-1.39102	-1.37127	-1.61680

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 105°

Cl	1.67770	-1.32621	0.00007
Cl	0.79786	1.85652	-0.00008
Si	0.01708	-0.07387	0.00002
C	-1.37344	-0.36795	1.22317
H	-1.36741	-1.38718	1.61701
H	-1.52868	0.32691	2.04736
C	-2.34935	-0.21231	-0.00004
H	-3.15452	-0.94894	0.00007
H	-2.80049	0.78122	-0.00017
C	-1.37335	-0.36833	-1.22314
H	-1.52858	0.32621	-2.04760
H	-1.36719	-1.38770	-1.61661

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 106°

Cl	1.69264	-1.31351	0.00006
Cl	0.75988	1.87559	-0.00007
Si	0.02510	-0.07186	0.00001
C	-1.36133	-0.38647	1.22313
H	-1.34116	-1.40590	1.61595
H	-1.52674	0.30541	2.04785
C	-2.33922	-0.24353	-0.00003
H	-3.13487	-0.99045	0.00006
H	-2.80317	0.74409	-0.00015
C	-1.36124	-0.38681	-1.22311
H	-1.52665	0.30479	-2.04807
H	-1.34096	-1.40636	-1.61559

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 107°

Cl	1.70939	-1.29818	0.00005
Cl	0.71882	1.89494	-0.00006
Si	0.03316	-0.06957	0.00001
C	-1.34838	-0.40666	1.22311
H	-1.31256	-1.42605	1.61486
H	-1.52493	0.28182	2.04837
C	-2.32826	-0.27783	-0.00003
H	-3.11319	-1.03604	0.00005
H	-2.80630	0.70305	-0.00013
C	-1.34830	-0.40695	-1.22308
H	-1.52484	0.28128	-2.04856
H	-1.31237	-1.42644	-1.61455

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 108°

Cl	1.72832	-1.27958	0.00007
Cl	0.67388	1.91465	-0.00011
Si	0.04116	-0.06680	0.00003
C	-1.33423	-0.42906	1.22312
H	-1.28085	-1.44841	1.61293
H	-1.52330	0.25494	2.04932
C	-2.31614	-0.31556	-0.00004
H	-3.08942	-1.08570	0.00006
H	-2.80912	0.65792	-0.00035
C	-1.33414	-0.42953	-1.22304
H	-1.52317	0.25414	-2.04953
H	-1.28073	-1.44903	-1.61245

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 109°

Cl	1.74899	-1.25795	0.00004
Cl	0.62568	1.93426	-0.00005
Si	0.04937	-0.06394	0.00001
C	-1.31928	-0.45285	1.22309
H	-1.24678	-1.47110	1.61263
H	-1.52145	0.22722	2.04945
C	-2.30294	-0.35730	-0.00002
H	-3.06211	-1.14139	0.00004
H	-2.81360	0.60702	-0.00009
C	-1.31921	-0.45307	-1.22307
H	-1.52137	0.22681	-2.04960
H	-1.24663	-1.47139	-1.61239

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 110°

Cl	1.77220	-1.23201	0.00003
Cl	0.57255	1.95395	-0.00004
Si	0.05752	-0.06051	0.00001
C	-1.30270	-0.47924	1.22310
H	-1.20876	-1.49611	1.61160
H	-1.51957	0.19569	2.04994
C	-2.28804	-0.40341	-0.00002
H	-3.03155	-1.20240	0.00003
H	-2.81774	0.55061	-0.00008
C	-1.30263	-0.47943	-1.22309
H	-1.51949	0.19532	-2.05008
H	-1.20861	-1.49637	-1.61138

- $(CH_2)_3SiCl_2$: Cl-Si-Cl angle = 111°

Cl	1.79783	-1.20143	0.00004
Cl	0.51426	1.97342	-0.00007
Si	0.06558	-0.05641	0.00002
C	-1.28427	-0.50828	1.22315
H	-1.16637	-1.52331	1.60987
H	-1.51745	0.16013	2.05082
C	-2.27112	-0.45414	-0.00002
H	-2.99718	-1.26908	0.00004
H	-2.82141	0.48818	-0.00024
C	-1.28420	-0.50858	-1.22308
H	-1.51736	0.15962	-2.05094
H	-1.16630	-1.52370	-1.60954

- Me_2SiCl_2: Cl-Si-Cl angle = 101°

Cl	1.61415	-0.00000	-0.93650
Si	-0.00000	-0.00000	0.39410
C	-0.00000	1.57016	1.39311
H	0.88688	1.61564	2.03143
H	-0.00000	2.44540	0.74035
Cl	-1.61415	0.00000	-0.93650
C	-0.00000	-1.57016	1.39311
H	-0.88688	-1.61564	2.03143
H	-0.00000	-2.44540	0.74035
H	0.88688	-1.61564	2.03143
H	-0.88688	1.61564	2.03143

- Me_2SiCl_2: Cl-Si-Cl angle = 102°

Cl	1.62472	-0.00000	-0.92944
Si	-0.00000	0.00000	0.38623
C	0.00000	1.57010	1.38589
H	0.88696	1.61553	2.02407
H	0.00000	2.44564	0.73347
Cl	-1.62472	0.00000	-0.92944
C	-0.00000	-1.57010	1.38589
H	-0.88696	-1.61553	2.02407
H	-0.00000	-2.44564	0.73347
H	0.88696	-1.61553	2.02407
H	-0.88696	1.61553	2.02407

- Me_2SiCl_2: Cl-Si-Cl angle = 103°

Cl	1.63526	-0.00000	-0.92237
Si	-0.00000	-0.00000	0.37838
C	0.00000	1.57006	1.37863
H	0.88704	1.61547	2.01668
H	0.00000	2.44589	0.72653
Cl	-1.63526	0.00000	-0.92237
C	-0.00000	-1.57006	1.37863
H	-0.88704	-1.61547	2.01668
H	-0.00000	-2.44589	0.72653
H	0.88704	-1.61547	2.01668
H	-0.88704	1.61547	2.01668

- Me_2SiCl_2: Cl-Si-Cl angle = 104°

Cl	1.64577	-0.00000	-0.91528
Si	-0.00000	0.00000	0.37054
C	-0.00000	1.57005	1.37133
H	0.88713	1.61544	2.00924
H	-0.00000	2.44615	0.71953
Cl	-1.64577	0.00000	-0.91528
C	-0.00000	-1.57005	1.37133
H	-0.88713	-1.61544	2.00924
H	-0.00000	-2.44615	0.71953
H	0.88713	-1.61544	2.00924
H	-0.88713	1.61544	2.00924

- Me_2SiCl_2: Cl-Si-Cl angle = 105°

Cl	1.65623	-0.00000	-0.90817
Si	-0.00000	0.00000	0.36270
C	0.00000	1.57007	1.36400
H	0.88721	1.61545	2.00176
H	0.00000	2.44642	0.71246
Cl	-1.65623	0.00000	-0.90817
C	-0.00000	-1.57007	1.36400
H	-0.88721	-1.61545	2.00176
H	-0.00000	-2.44642	0.71246
H	0.88721	-1.61545	2.00176
H	-0.88721	1.61545	2.00176

- Me_2SiCl_2: Cl-Si-Cl angle = 106°

Cl	1.66664	-0.00000	-0.90104
Si	-0.00000	0.00000	0.35487
C	-0.00000	1.57012	1.35663
H	0.88730	1.61551	1.99423
H	-0.00000	2.44670	0.70533
Cl	-1.66664	0.00000	-0.90104
C	-0.00000	-1.57012	1.35663
H	-0.88730	-1.61551	1.99423
H	-0.00000	-2.44670	0.70533
H	0.88730	-1.61551	1.99423
H	-0.88730	1.61551	1.99423

- Me_2SiCl_2: Cl-Si-Cl angle = 107°

Cl	1.67700	-0.00000	-0.89388
Si	-0.00000	-0.00000	0.34704
C	0.00000	1.57020	1.34921
H	0.88740	1.61561	1.98665
H	0.00000	2.44698	0.69812
Cl	-1.67700	0.00000	-0.89388
C	-0.00000	-1.57020	1.34921
H	-0.88740	-1.61561	1.98665
H	-0.00000	-2.44698	0.69812
H	0.88740	-1.61561	1.98665
H	-0.88740	1.61561	1.98665

- Me_2SiCl_2: Cl-Si-Cl angle = 108°

Cl	1.68732	-0.00000	-0.88670
Si	-0.00000	0.00000	0.33921
C	-0.00000	1.57031	1.34175
H	0.88749	1.61576	1.97902
H	-0.00000	2.44728	0.69084
Cl	-1.68732	0.00000	-0.88670
C	-0.00000	-1.57031	1.34175
H	-0.88749	-1.61576	1.97902
H	-0.00000	-2.44728	0.69084
H	0.88749	-1.61576	1.97902
H	-0.88749	1.61576	1.97902

- Me_2SiCl_2: Cl-Si-Cl angle = 109°

Cl	1.69758	-0.00000	-0.87949
Si	-0.00000	0.00000	0.33139
C	0.00000	1.57046	1.33424
H	0.88759	1.61595	1.97134
H	0.00000	2.44758	0.68348
Cl	-1.69758	0.00000	-0.87949
C	-0.00000	-1.57046	1.33424
H	-0.88759	-1.61595	1.97134
H	-0.00000	-2.44758	0.68348
H	0.88759	-1.61595	1.97134
H	-0.88759	1.61595	1.97134

- Me_2SiCl_2: Cl-Si-Cl angle = 110°

Cl	1.70778	-0.00000	-0.87225
Si	-0.00000	0.00000	0.32356
C	0.00000	1.57063	1.32667
H	0.88769	1.61620	1.96359
H	0.00000	2.44790	0.67604
Cl	-1.70778	0.00000	-0.87225
C	-0.00000	-1.57063	1.32667
H	-0.88769	-1.61620	1.96359
H	-0.00000	-2.44790	0.67604
H	0.88769	-1.61620	1.96359
H	-0.88769	1.61620	1.96359

- Me_2SiCl_2: Cl-Si-Cl angle = 111°

Cl	1.71792	-0.00000	-0.86497
Si	-0.00000	0.00000	0.31572
C	0.00000	1.57084	1.31906
H	0.88780	1.61649	1.95579
H	0.00000	2.44822	0.66852
Cl	-1.71792	0.00000	-0.86497
C	-0.00000	-1.57084	1.31906
H	-0.88780	-1.61649	1.95579
H	-0.00000	-2.44822	0.66852
H	0.88780	-1.61649	1.95579
H	-0.88780	1.61649	1.95579

- $MeHSiCl_2$: Cl-Si-Cl angle = 101°

Cl	-1.60720	-0.76008	-0.14697
Cl	1.60699	-0.76039	-0.14700
Si	0.00006	0.40824	0.47730
H	0.00021	0.46579	1.94971
C	0.00015	2.07086	-0.34853
H	0.00158	1.96489	-1.43553
H	0.88701	2.63849	-0.05280
H	-0.88694	2.63829	-0.05488

- $MeHSiCl_2$: Cl-Si-Cl angle = 102°

Cl	-1.61768	-0.75411	-0.14744
Cl	1.61747	-0.75441	-0.14746
Si	0.00006	0.39836	0.47484
H	0.00020	0.44967	1.94753
C	0.00014	2.06519	-0.34318
H	0.00153	1.96444	-1.43073
H	0.88709	2.63137	-0.04504
H	-0.88699	2.63122	-0.04705

- $MeHSiCl_2$: Cl-Si-Cl angle = 103°

Cl	-1.62811	-0.74814	-0.14790
Cl	1.62791	-0.74843	-0.14792
Si	0.00006	0.38849	0.47233
H	0.00019	0.43339	1.94528
C	0.00014	2.05951	-0.33779
H	0.00149	1.96402	-1.42586
H	0.88717	2.62424	-0.03723
H	-0.88704	2.62412	-0.03918

- $MeHSiCl_2$: Cl-Si-Cl angle = 104°

Cl	-1.63851	-0.74216	-0.14835
Cl	1.63831	-0.74245	-0.14837
Si	0.00006	0.37862	0.46978
H	0.00017	0.41692	1.94295
C	0.00013	2.05383	-0.33236
H	0.00144	1.96364	-1.42092
H	0.88726	2.61706	-0.02936
H	-0.88710	2.61698	-0.03124

- $MeHSiCl_2$: Cl-Si-Cl angle = 105°

Cl	-1.64886	-0.73617	-0.14879
Cl	1.64866	-0.73645	-0.14881
Si	0.00006	0.36875	0.46717
H	0.00016	0.40028	1.94055
C	0.00013	2.04814	-0.32688
H	0.00140	1.96330	-1.41592
H	0.88735	2.60986	-0.02144
H	-0.88715	2.60981	-0.02325

- $MeHSiCl_2$: Cl-Si-Cl angle = 106°

Cl	-1.65916	-0.73018	-0.14921
Cl	1.65897	-0.73044	-0.14923
Si	0.00006	0.35887	0.46452
H	0.00015	0.38345	1.93806
C	0.00013	2.04245	-0.32136
H	0.00135	1.96298	-1.41085
H	0.88744	2.60262	-0.01345
H	-0.88721	2.60260	-0.01520

- $MeHSiCl_2$: Cl-Si-Cl angle = 107°

Cl	-1.66941	-0.72416	-0.14963
Cl	1.66922	-0.72442	-0.14965
Si	0.00006	0.34898	0.46181
H	0.00014	0.36643	1.93549
C	0.00012	2.03675	-0.31579
H	0.00131	1.96270	-1.40571
H	0.88753	2.59533	-0.00541
H	-0.88728	2.59536	-0.00710

- $MeHSiCl_2$: Cl-Si-Cl angle = 108°

Cl	-1.67961	-0.71814	-0.15004
Cl	1.67942	-0.71839	-0.15006
Si	0.00005	0.33908	0.45904
H	0.00013	0.34922	1.93283
C	0.00012	2.03103	-0.31017
H	0.00126	1.96246	-1.40049
H	0.88763	2.58802	0.00270
H	-0.88735	2.58807	0.00108

- $MeHSiCl_2$: Cl-Si-Cl angle = 109°

Cl	-1.68975	-0.71211	-0.15043
Cl	1.68957	-0.71235	-0.15045
Si	0.00005	0.32917	0.45622
H	0.00013	0.33181	1.93006
C	0.00012	2.02531	-0.30451
H	0.00122	1.96225	-1.39520
H	0.88773	2.58065	0.01087
H	-0.88742	2.58074	0.00931

- $MeHSiCl_2$: Cl-Si-Cl angle = 110°

Cl	-1.69983	-0.70606	-0.15082
Cl	1.69965	-0.70629	-0.15083
Si	0.00005	0.31926	0.45333
H	0.00012	0.31421	1.92720
C	0.00011	2.01957	-0.29879
H	0.00117	1.96208	-1.38983
H	0.88784	2.57325	0.01910
H	-0.88749	2.57337	0.01761

- $MeHSiCl_2$: Cl-Si-Cl angle = 111°

Cl	-1.70985	-0.69999	-0.15118
Cl	1.70968	-0.70022	-0.15120
Si	0.00005	0.30933	0.45038
H	0.00011	0.29639	1.92423
C	0.00010	2.01382	-0.29302
H	0.00112	1.96194	-1.38439
H	0.88794	2.56580	0.02741
H	-0.88758	2.56594	0.02598

- H_2SiCl_2: Cl-Si-Cl angle = 101°

Cl	0.00000	1.59957	-0.45410
Si	0.00000	-0.00000	0.86446
Cl	-0.00000	-1.59957	-0.45410
H	1.23314	-0.00000	1.66846
H	-1.23314	0.00000	1.66846

- H_2SiCl_2: Cl-Si-Cl angle = 102°

Cl	0.00000	1.60996	-0.44937
Si	-0.00000	0.00000	0.85433
Cl	-0.00000	-1.60996	-0.44937
H	1.23287	-0.00000	1.65888
H	-1.23287	0.00000	1.65888

- H_2SiCl_2: Cl-Si-Cl angle = 103°

Cl	-0.00000	1.62030	-0.44463
Si	-0.00000	0.00000	0.84420
Cl	-0.00000	-1.62030	-0.44463
H	1.23264	-0.00000	1.64921
H	-1.23264	0.00000	1.64921

- H_2SiCl_2: Cl-Si-Cl angle = 104°

Cl	-0.00000	1.63060	-0.43988
Si	0.00000	0.00000	0.83407
Cl	-0.00000	-1.63060	-0.43988
H	1.23246	-0.00000	1.63947
H	-1.23246	0.00000	1.63947

- H_2SiCl_2: Cl-Si-Cl angle = 105°

Cl	-0.00000	1.64086	-0.43513
Si	0.00000	0.00000	0.82394
Cl	-0.00000	-1.64086	-0.43513
H	1.23231	-0.00000	1.62966
H	-1.23231	0.00000	1.62966

- H_2SiCl_2: Cl-Si-Cl angle = 106°

Cl	-0.00000	1.65106	-0.43037
Si	-0.00000	-0.00000	0.81379
Cl	-0.00000	-1.65106	-0.43037
H	1.23220	-0.00000	1.61976
H	-1.23220	0.00000	1.61976

- H_2SiCl_2: Cl-Si-Cl angle = 107°

Cl	0.00000	1.66122	-0.42560
Si	-0.00000	-0.00000	0.80363
Cl	-0.00000	-1.66122	-0.42560
H	1.23213	-0.00000	1.60980
H	-1.23213	0.00000	1.60980

- H_2SiCl_2: Cl-Si-Cl angle = 108°

Cl	-0.00000	1.67132	-0.42082
Si	0.00000	-0.00000	0.79346
Cl	-0.00000	-1.67132	-0.42082
H	1.23210	-0.00000	1.59975
H	-1.23210	0.00000	1.59975

- H_2SiCl_2: Cl-Si-Cl angle = 109°

Cl	0.00000	1.68135	-0.41603
Si	0.00000	0.00000	0.78327
Cl	-0.00000	-1.68135	-0.41603
H	1.23210	-0.00000	1.58963
H	-1.23210	0.00000	1.58963

- H_2SiCl_2: Cl-Si-Cl angle = 110°

Cl	-0.00000	1.69134	-0.41123
Si	0.00000	-0.00000	0.77306
Cl	-0.00000	-1.69134	-0.41123
H	1.23213	-0.00000	1.57943
H	-1.23213	0.00000	1.57943

- H_2SiCl_2: Cl-Si-Cl angle = 111°

Cl	0.00000	1.70125	-0.40641
Si	0.00000	0.00000	0.76282
Cl	-0.00000	-1.70125	-0.40641
H	1.23220	-0.00000	1.56916
H	-1.23220	0.00000	1.56916

Total energies (Hartree) of $(CH_2)_3SiCl_2$, Me_2SiCl_2, $MeHSiCl_2$ and H_2SiCl_2 from the potential energy surface scans of the Cl-Si-Cl angle variation (B3LYP/6-311++G(d,p))

Cl-Si-Cl (deg)	$MeHSiCl_2$	Me_2SiCl_2	$(CH_2)_3SiCl_2$	H_2SiCl_2
101	-1250.60940935	-1289.95470635	-1328.02833576	-1211.26245372
102	-1250.60990663	-1289.95512261	-1328.02876092	-1211.26304642
103	-1250.61032831	-1289.95546410	-1328.02911065	-1211.26356357
104	-1250.61067704	-1289.95573334	-1328.02938801	-1211.26400780
105	-1250.61095530	-1289.95593274	-1328.02959614	-1211.26438160
106	-1250.61116546	-1289.95606461	-1328.02973765	-1211.26468738
107	-1250.61130978	-1289.95613113	-1328.02981470	-1211.26492737
108	-1250.61139041	-1289.95613437	-1328.02982878	-1211.26510373
109	-1250.61140938	-1289.95607630	-1328.02978139	-1211.26521851
110	-1250.61136864	-1289.95595877	-1328.02967362	-1211.26527363
111	-1250.61126998	-1289.95578355	-1328.02950702	-1211.26527092

Si–Cl, Si–C and Si–H Natural Bond Orbital (NBO) compositions and Natural Charges (NCs) from NBO analyses of $(CH_2)_3SiCl_2$, Me_2SiCl_2, $MeHSiCl_2$ and H_2SiCl_2

The data of NBO compositions are reported in the following order:

Line 1: Number of NBO; (electronic occupancy); bonding character; atom 1; atom 2

*Line 2: (% atomic orbital contribution from atom 1); orbital coefficient*atom; atomic orbital hybrid composition (s, p, d hybrid contributions)*

*Line 3: (% atomic orbital contribution from atom 2); orbital coefficient*atom; atomic orbital hybrid composition (s, p, d hybrid contributions)*

- $(CH_2)_3SiCl_2$: NBO composition

25. (1.97500) BD (1)Cl 1-Si 3
    (73.55%) 0.8576*Cl 1 s(20.34%)p 3.90(79.30%)d 0.02(0.36%)
    (26.45%) 0.5143*Si 3 s(20.39%)p 3.81(77.58%)d 0.10(2.03%)
26. (1.97495) BD (1)Cl 2-Si 3
    (73.68%) 0.8584*Cl 2 s(20.18%)p 3.94(79.46%)d 0.02(0.36%)
    (26.32%) 0.5131*Si 3 s(20.09%)p 3.88(77.90%)d 0.10(2.00%)
27. (1.96543) BD (1)Si 3- C 4
    (30.48%) 0.5521*Si 3 s(29.83%)p 2.32(69.26%)d 0.03(0.90%)
    (69.52%) 0.8338* C 4 s(23.26%)p 3.29(76.60%)d 0.01(0.14%)
28. (1.96543) BD (1)Si 3- C 10
    (30.48%) 0.5521*Si 3 s(29.84%)p 2.32(69.26%)d 0.03(0.90%)
    (69.52%) 0.8338* C 10 s(23.26%)p 3.29(76.60%)d 0.01(0.14%)

Atom	Natural Charge
Cl 1	-0.34164
Cl 2	-0.34808
Si 3	1.43938
C 4	-0.85710
H 5	0.23445
H 6	0.23830
C 7	-0.39812
H 8	0.21094
H 9	0.20622
C 10	-0.85710
H 11	0.23831
H 12	0.23445

- Me_2SiCl_2: NBO composition

24. (1.97733) BD (1)Cl 1-Si 2
(73.87%) 0.8595*Cl 1 s(20.00%)p 3.98(79.64%)d 0.02(0.36%)
(26.13%) 0.5112*Si 2 s(19.55%)p 4.01(78.36%)d 0.11(2.09%)
26. (1.97733) BD (1)Si 2-Cl 6
(73.87%) 0.8595*Cl 6 s(20.00%)p 3.98(79.64%)d 0.02(0.36%)
(26.13%) 0.5112*Si 2 s(19.55%)p 4.01(78.36%)d 0.11(2.09%)
25. (1.97774) BD (1)Si 2- C 3
(30.63%) 0.5535*Si 2 s(30.46%)p 2.26(68.79%)d 0.02(0.76%)
(69.37%) 0.8329* C 3 s(27.98%)p 2.57(71.87%)d 0.01(0.15%)
27. (1.97774) BD (1)Si 2- C 7
(30.63%) 0.5535*Si 2 s(30.46%)p 2.26(68.79%)d 0.02(0.76%)
(69.37%) 0.8329* C 7 s(27.98%)p 2.57(71.87%)d 0.01(0.15%)

Atom	Natural Charge
Cl 1	-0.36276
Si 2	1.46576
C 3	-1.10177
H 4	0.24071
H 5	0.25023
Cl 6	-0.36276
C 7	-1.10177
H 8	0.24071
H 9	0.25023
H 10	0.24071
H 11	0.24071

- $MeHSiCl_2$: NBO composition

23. (1.98018) BD (1)Cl 1-Si 3
(73.36%) 0.8565*Cl 1 s(19.39%)p 4.14(80.24%)d 0.02(0.37%)
(26.64%) 0.5161*Si 3 s(19.75%)p 3.96(78.13%)d 0.11(2.12%)
24. (1.98019) BD (1)Cl 2-Si 3
(73.36%) 0.8565*Cl 2 s(19.39%)p 4.14(80.24%)d 0.02(0.37%)
(26.64%) 0.5161*Si 3 s(19.75%)p 3.96(78.13%)d 0.11(2.12%)
25. (1.97755) BD (1)Si 3- H 4
(42.33%) 0.6506*Si 3 s(30.07%)p 2.30(69.18%)d 0.02(0.75%)
(57.67%) 0.7594* H 4 s(99.62%)p 0.00(0.38%)
26. (1.98027) BD (1)Si 3- C 5
(31.35%) 0.5599*Si 3 s(30.50%)p 2.25(68.74%)d 0.03(0.77%)
(68.65%) 0.8286* C 5 s(27.49%)p 2.63(72.38%)d 0.00(0.13%)

Atom	Natural Charge
Cl 1	-0.35566
Cl 2	-0.35561
Si 3	1.24009
H 4	-0.17099
C 5	-1.09420
H 6	0.24822
H 7	0.24408
H 8	0.24407

- H_2SiCl_2: NBO composition

22. (1.98216) BD (1)Cl 1-Si 2
    (72.97%) 0.8542*Cl 1 s(19.06%)p 4.23(80.57%)d 0.02(0.37%)
    (27.03%) 0.5199*Si 2 s(20.07%)p 3.88(77.78%)d 0.11(2.15%)
23. (1.98216) BD (1)Si 2-Cl 3
    (27.03%) 0.5199*Si 2 s(20.07%)p 3.88(77.78%)d 0.11(2.15%)
    (72.97%) 0.8542*Cl 3 s(19.06%)p 4.23(80.57%)d 0.02(0.37%)
24. (1.97912) BD (1)Si 2- H 4
    (43.01%) 0.6558*Si 2 s(30.22%)p 2.28(68.98%)d 0.03(0.80%)
    (56.99%) 0.7549* H 4 s(99.67%)p 0.00(0.33%)
25. (1.97912) BD (1)Si 2- H 5
    (43.01%) 0.6558*Si 2 s(30.22%)p 2.28(68.98%)d 0.03(0.80%)
    (56.99%) 0.7549* H 5 s(99.67%)p 0.00(0.33%)

Atom	Natural Charge
Cl 1	-0.34839
Si 2	1.01288
Cl 3	-0.34839
H 4	-0.15805
H 5	-0.15805

Intermolecular Cl···Cl and Cl···H contacts in the crystal structures of $(CH_2)_3SiCl_2$, $(CH_2)_4SiCl_2$, $(CH_2)_5SiCl_2$, Me_2SiCl_2, $MeHSiCl_2$ and $MeSiCl_3$

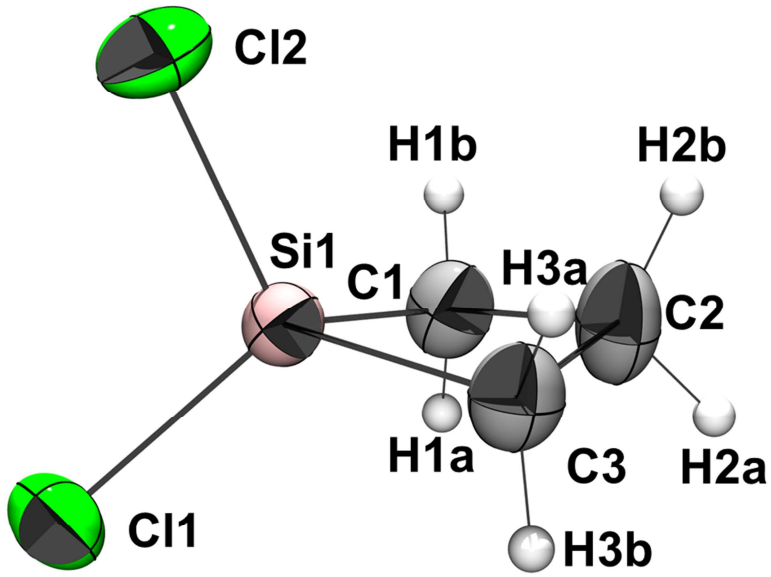

Figure S2: Molecular structure with atom labels of $(CH_2)_3SiCl_2$.

Intermolecular contacts (Cl···Cl < 3.8 Å, Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Si1–Cl1···Cl1*	3.552(1)	138.2(1)	3–x, –y, 1–z
Cl1···H1b*–C1*	3.13	162	x+0.5, 0.5–y, z+0.5
Cl1···H2a*–C2*	3.15	129	x+0.5, 0.5–y, z–0.5
Cl1···H2b*–C2*	3.39	129	x+1, y, z
Cl1···H3b*–C3*	3.27	116	x+0.5, 0.5–y, z–0.5
Cl1···H3a*–C3*	3.07	139	x+1, y, z
Cl1···H3a*–C3*	3.28	146	2–x, –y, 1–z
Cl2···H1b*–C1*	3.39	110	1.5–x, y–0.5, 0.5–z
Cl2···H1a*–C1*	3.35	128	x–0.5, 0.5–y, z–0.5
Cl2···H2b*–C2*	3.13	114	1.5–x, y–0.5, 0.5–z

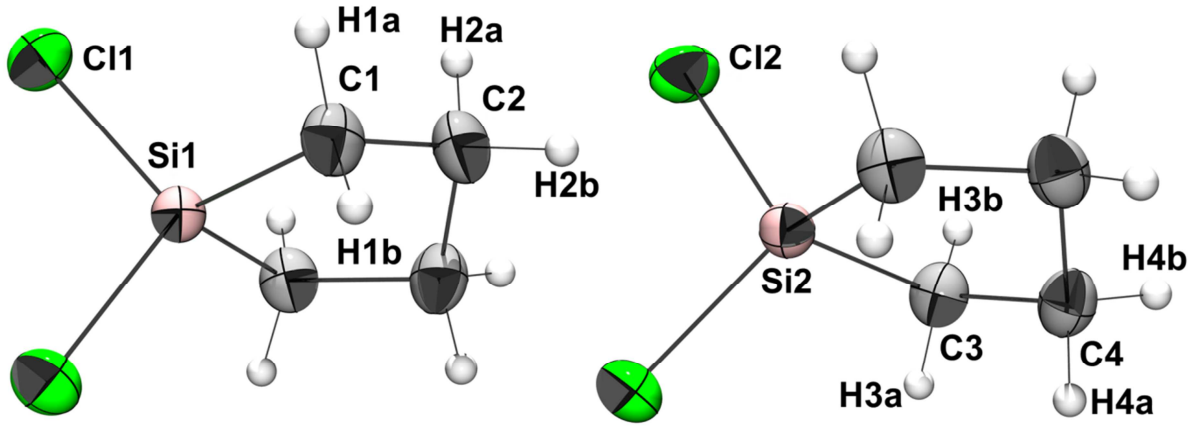

Figure S3: Molecular structure with atom labels of $(CH_2)_4SiCl_2$.

Intermolecular contacts (Cl···Cl < 3.8 Å, Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Si1–Cl1···Cl1*	3.693(1)	138.3(1)	2–x, 1–y, –z
Si1–Cl1···Cl2*	3.663(1)	153.6(1)	x, 1–y, z–0.5
Si2–Cl2···Cl1*	3.663(1)	97.9(1)	x, 1–y, z+0.5
Cl1···H3a*–C3*	3.34	127	1–x, 1–y, –z
Cl1···H4a*–C4*	3.31	137	1–x, 1–y, –z
Cl1···H1b*–C1*	3.12	135	x, 2–y, z–0.5
Cl1···H2a*–C2*	3.34	130	2–x, 2–y, –z
Cl1···H2b*–C2*	3.26	119	x, 2–y, z–0.5
Cl2···H3a*–C3*	3.20	147	1–x, 1–y, –z
Cl2···H4b*–C4*	3.40	126	x, y+1, z
Cl2···H1a–C1	3.38	102	(x, y, z)
Cl2···H2a*–C2*	3.13	149	x, 2–y, z+0.5

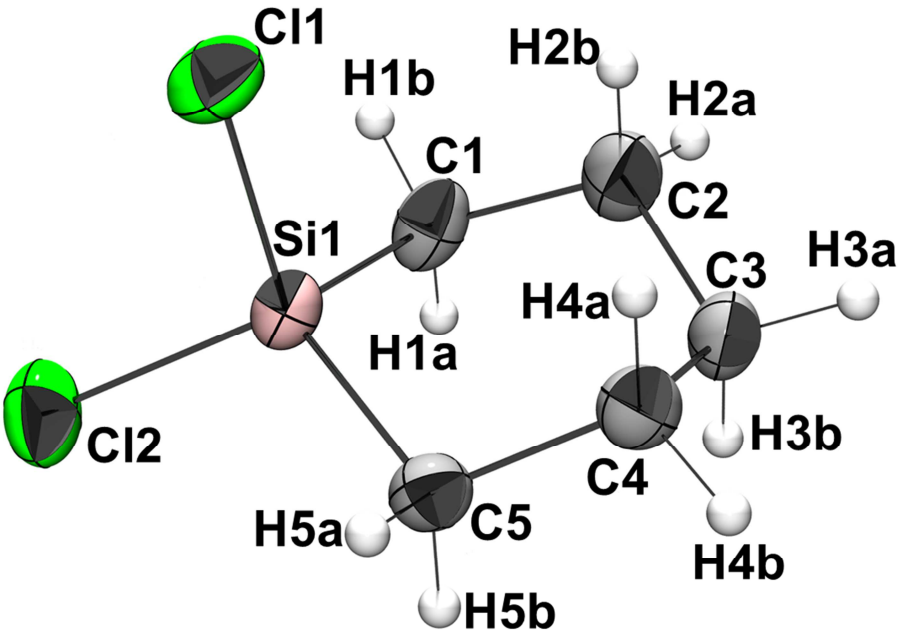

Figure S4: Molecular structure with atom labels of $(CH_2)_5SiCl_2$.

Intermolecular contacts (Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Cl1···H3a*–C3*	3.24	143	x+0.5, 1–y, 1–z
Cl1···H1a*–C1*	3.29	145	x+0.5, 0.5–y, z–0.5
Cl1···H3b*–C3*	3.26	145	x+0.5, 0.5–y, z–0.5
Cl1···H1b*–C1*	2.95	145	2–x, –y, 1–z
Cl1···H4b*–C4*	3.07	134	1.5–x, y–0.5, 0.5–z
Cl2···H5b*–C5*	3.34	147	1–x, –y, 1–z
Cl2···H3a*–C3*	3.36	130	x, y–1, z
Cl2···H4b*–C4*	3.22	126	x, y–1, z
Cl2···H5a*–C5*	3.04	139	1.5–x, y–0.5, 0.5–z

Note: This structure exhibits a short intramolecular contact (Cl1···H4a 3.17 Å, 109 deg).

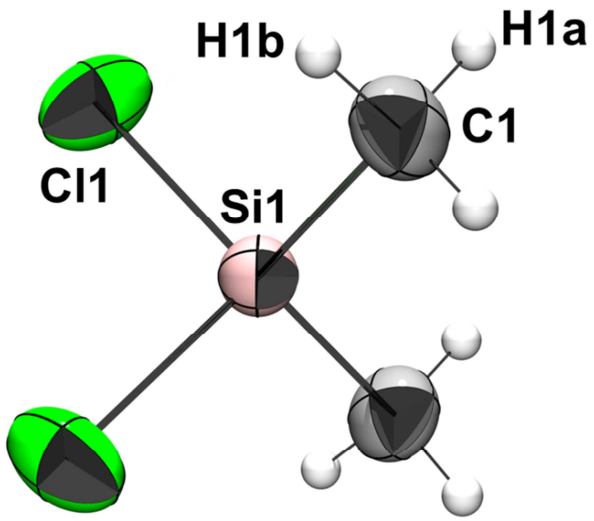

Figure S5: Molecular structure with atom labels of Me_2SiCl_2.

Intermolecular contacts (Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Cl1···H1b*–C1*	3.40	147	x, –y, –z
Cl1···H1b*–C1*	3.40	147	x, –y, z+0.5
Cl1···H1a*–C1*	3.33	135	0.5–x, 0.5–y, z+0.5
Cl1···H1a*–C1*	3.33	135	0.5–x, 0.5–y, –z
Cl1···H1a*–C1*	3.18	148	0.5–x, y–0.5, z
Cl1···H1a*–C1*	3.18	148	0.5–x, y–0.5, 0.5–z

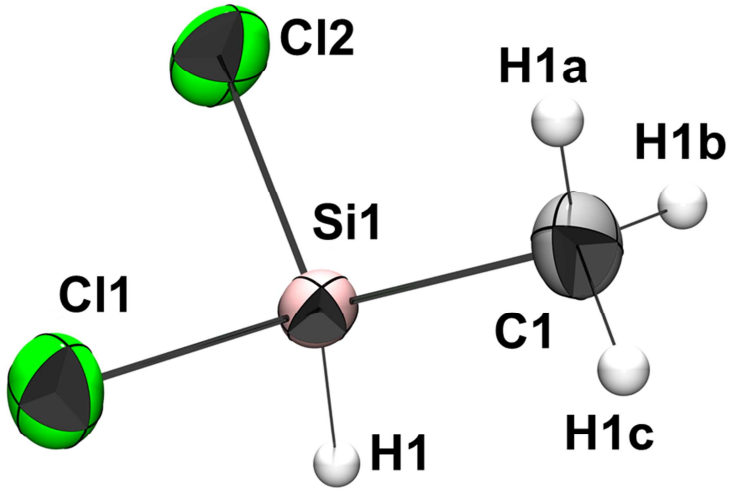

Figure S6: Molecular structure with atom labels of $MeHSiCl_2$.

Intermolecular contacts (Cl···Cl < 3.8 Å, Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Si1–Cl1···Cl1*	3.607(1)	158.3(1)	2–x, 2–y, –z
Cl1···H1c*–C1*	3.20	138	2–x, 1–y, –z
Cl1···H1b*–C1*	3.20	125	x+1, y+1, z
Cl1···H1a*–C1*	3.22	151	1–x, 1–y, –z
Cl1···H1c*–C1*	3.30	132	x, y+1, z
Cl1···H1*–Si1*	3.38	132	2–x, 2–y, 1–z
Cl2···H1b*–C1*	3.35	140	x, y+1, z
Cl2···H1b*–C4*	3.22	135	1–x, 1–y, 1–z

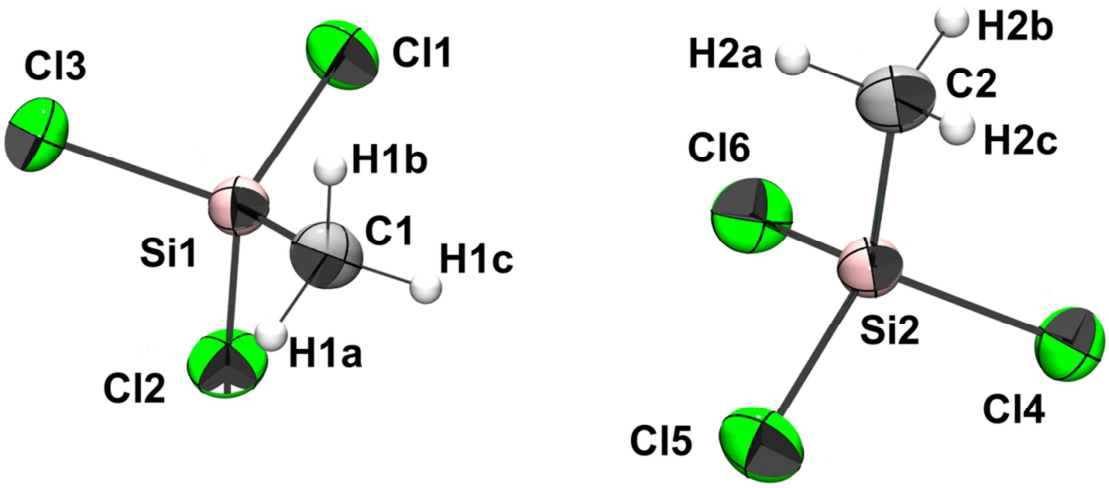

Figure S7: Molecular structure with atom labels of $MeSiCl_3$.

Intermolecular contacts (Cl···Cl < 3.8 Å, Cl···H < 3.4 Å):

Contact	Separation (Å)	Angle (deg)	* symmetry operation
Si1–Cl2···Cl4*	3.793(2)	101.5(1)	x–1, 1–y, z+0.5
Si2–Cl4···Cl2*	3.793(2)	153.9(1)	x+1, 1–y, z–0.5
Si2–Cl4···Cl6*	3.766(2)	100.2(1)	x, 1–y, z–0.5
Si2–Cl6···Cl4*	3.766(2)	134.0(1)	x, 1–y, z+0.5
Cl1···H1c*–C1*	3.19	135	x, 1–y, z+0.5
Cl1···H2a*–C2*	3.15	140	x, –y, z+0.5
Cl1···H1b*–C1*	3.30	126	x, –y, z+0.5
Cl2···H1a*–C1*	3.30	130	x, 1–y, z+0.5
Cl2···H1b*–C1*	3.20	140	x, y+1, z
Cl3···H2b*–C2*	3.14	144	x–1, y, z
Cl3···H2c*–C2*	3.20	129	x–1, –y, z+0.5
Cl3···H1a*–C1*	3.16	131	x, –y, z+0.5
Cl4···H2c*–C2*	3.34	127	x, y+1, z
Cl4···H1a*–C1*	3.14	146	x+1, y, z
Cl5···H1b*–C1*	3.08	137	x, –y, z–0.5
Cl5···H2a*–C2*	3.20	140	x, –y, z–0.5
Cl6···H1c–C1	3.18	150	(x, y, z)
Cl6···H2a*–C2*	3.32	127	x, y+1, z
Cl6···H2c*–C2*	3.08	148	x, –y, z+0.5