Supporting Information

Monomeric Siliconthiodichloride Trapped by a Lewis Base †

Sudipta Roy, Kartik Chandra Mondal,* Totan Mondal, Debasis Koley,* Birger Dittrich,* and Herbert W. Roesky*

Content:

1. Computational details
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1. Computational Details:

All geometry optimization were performed using the global-hybrid meta-GGA M06-2X[S1] functional with SVP[S2] basis set implemented in Gaussian09 suite of program.[S3] Geometries were fully optimized without symmetry constraints. Vibrational frequency calculations were computed in order to determine the nature of stationary point (minima or saddle point on the potential energy surface). Single point calculations were performed at higher basis set (TZVP)[S4] on M06-2X/SVP optimized geometries in order to perform NBO analysis. All the energy values reported in the manuscript are at M06-2X/TZVP//M06-2X/SVP level. The ^{13}C and ^{29}Si chemical shifts were calculated with GIAO[S5] method by a single point calculation using M06-2X/TZVP level of theory. The chemical shifts calculated by using the formula $\delta=\sigma_{ref}-\sigma$, where σ_{ref}= nuclear shielding constant of reference compound and σ = nuclear shielding constant of **3**. To compare ^{13}C and ^{29}Si, TMS taken as standard. The wavefunction file generated at M06-2X/TZVP//M06-2X/SVP level was used to perform QTAIM[S6] analysis in the AIMALL program suite. We have applied Bader's AIM (Atoms-in-molecule)[S7] concept to characterize the electron distribution in **3**. Any bonded pair of atoms has a bond path, *i.e.;* a connecting line with maximum electron density. The bond critical point (BCP) is a point on this line where the gradient $\nabla\rho(r)$ of the density is equal to zero. The magnitude of the electron density, $\rho(r)$ and its Laplacian, $\nabla^2\rho(r)$ at the BCP provide information about the strength and type of bond. The Laplacian indicates whether the density is locally concentrated ($\nabla^2\rho<0$) or depleted ($\nabla^2\rho>0$). Ellipticities at BCP represent the deviations of the bonding density from cylindrical symmetry. It is quantitatively expressed as $\varepsilon_{BCP} = \lambda_2/\lambda_1-1$, where λ_1 and λ_2 are eigenvalues of the

Hessian of ρ(r) at BCP. Optimized geometries and orbital diagrams are illustrated using Chemcraft and CYLview drawing.[S8]

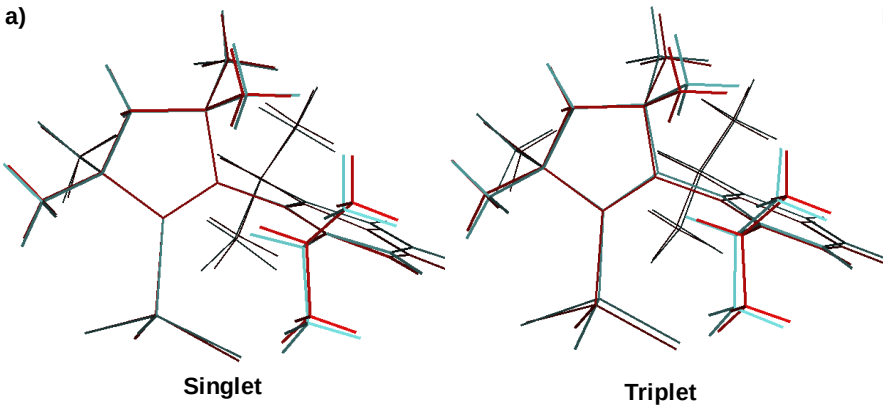
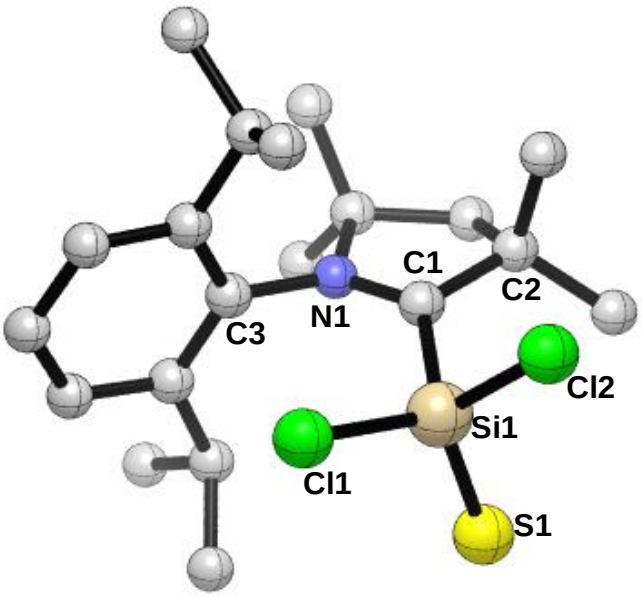


Figure. S1. a) Superposition of crystal structure of **3** with optimized geometries of different spin states at M06-2X/SVP level.

Table S1. Calculated geometrical parameters of compound **3** (in singlet and triplet electronic states)



	Crystal Structure	R/U-M06-2X/SVP	
		3	
		Singlet	Triplet
d (Si1-S1)	1.989	1.984	2.152
d (Si1-Cl1)	2.090	2.089	2.069

d (Si1-Cl2)	2.081	2.099	2.082
d (C1-Si1)	1.936	1.943	1.823
d (C1-N1)	1.298	1.303	1.377
d (C1-C2)	1.536	1.527	1.530
d (C3-N1)	1.472	1.454	1.431
A (C2-C1-N1)	109.6	109.9	108.9
A (C1-Si1-S1)	103.6	102.0	117.4
A (C1-Si1-Cl1)	113.1	110.1	114.9
A (C1-Si1-Cl2)	104.5	102.3	109.5
A (Cl1-Si1-S1)	115.9	119.0	107.3
A (Cl1-Si1-Cl2)	100.8	101.5	106.5
A (Cl2-Si1-S1)	118.8	120.6	99.7

Table S2. NBO Results of molecule **2a**[a] at M06-2X/TZVP//M06-2X/SVP level.

Bond	Occ.	Atomic contribution (Hyb.)	WBI
C1−Si1	1.945	Si1(sp^3) : 24%; C1(sp^2) : 76%	0.63
C1−N1	1.984	C1(sp^3) :36%; N1 (sp^2) : 64%	1.53
	1.957	C1(p) : 27%; N1(p) : 73%	
C1−C2	1.959	C1 (sp^2) : 48%; C2(sp^3) : 52%	0.98
Si1−S1	1.958	Si1(sp^2) : 37%; S1(sp^3) : 63%	1.43
Si1−Cl1	1.980	Si1(sp^3) : 25%; Cl2(sp^3) : 75%	0.81
Si1−Cl2	1.977	Si1(sp^3) : 25%; Cl1(sp^3) : 75%	0.78

[a] NBO occupancy (Occ.), orbital hybridization (Hyb.), Wiberg Bond Index (WBI).

Table S3. Lone pair occupancy of selected atoms in molecule **3** at M06-2X/TZVP//M06-2X/SVP level.

Atom	Lone pair	Occupancy
S1	1	1.971
	2	1.780
	3	1.722
Cl1	1	1.986

	2	1.946
	3	1.937
C12	1	1.987
	2	1.948
	3	1.938

Table S4. Topological parameters of selected bonds using AIMALL calculations at M06-2X/TZVP//M06-2X/SVP level of theory.

Bond	ρ (e/Å^3)	$\nabla^2\rho$ (e/Å^5)	ε_{BCP}	DI
Si1−S1	0.120	0.256	0.02	0.80
Si1−Cl1	0.089	0.231	0.03	0.46
Si1−Cl2	0.087	0.225	0.03	0.44
C1−Si1	0.097	0.242	0.12	0.38
C1−N1	0.347	-0.615	0.02	1.36
C1−C2	0.247	-0.598	0.02	0.94
C3−N1	0.254	-0.592	0.01	0.89

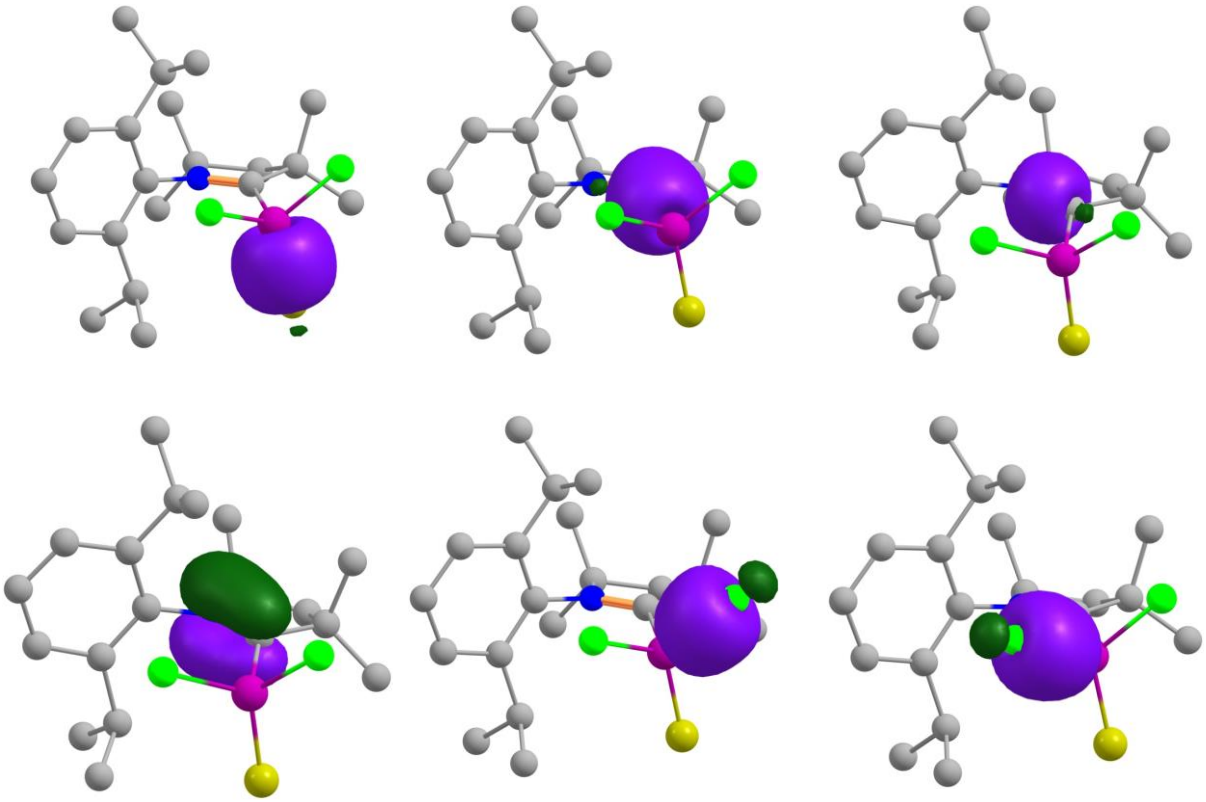


Figure S2. Selected NLMOs (Natural Localized Molecular Orbitals) of **3** (isosurface = 0.06 au) at M06-2X/TZVP//M06-2X/SVP level. Hydrogen atoms are omitted for clarity.

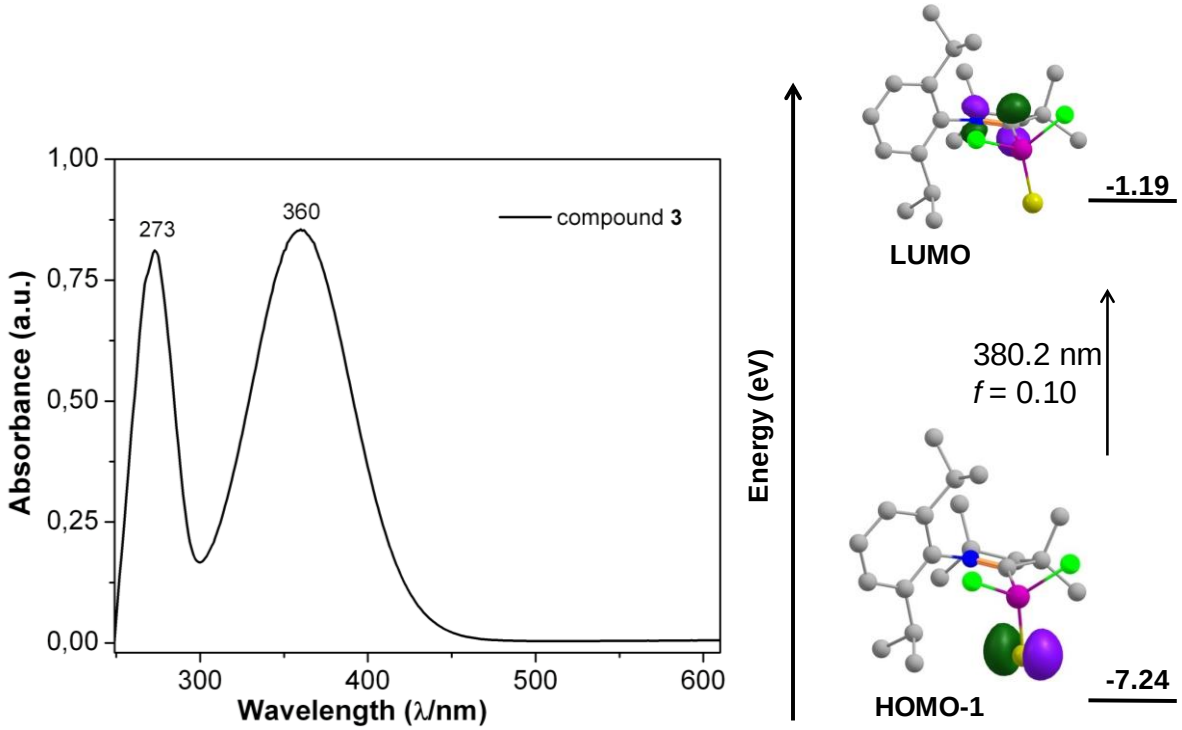


Figure S3. Uv-vis spectrum of compound **3** in THF (left). Calculated excitation energies, oscillator strength *f* and difference of the HOMO-1 and LUMO of **3** at B3LYP/TZVP//M06-2X/SVP level of theory (right).

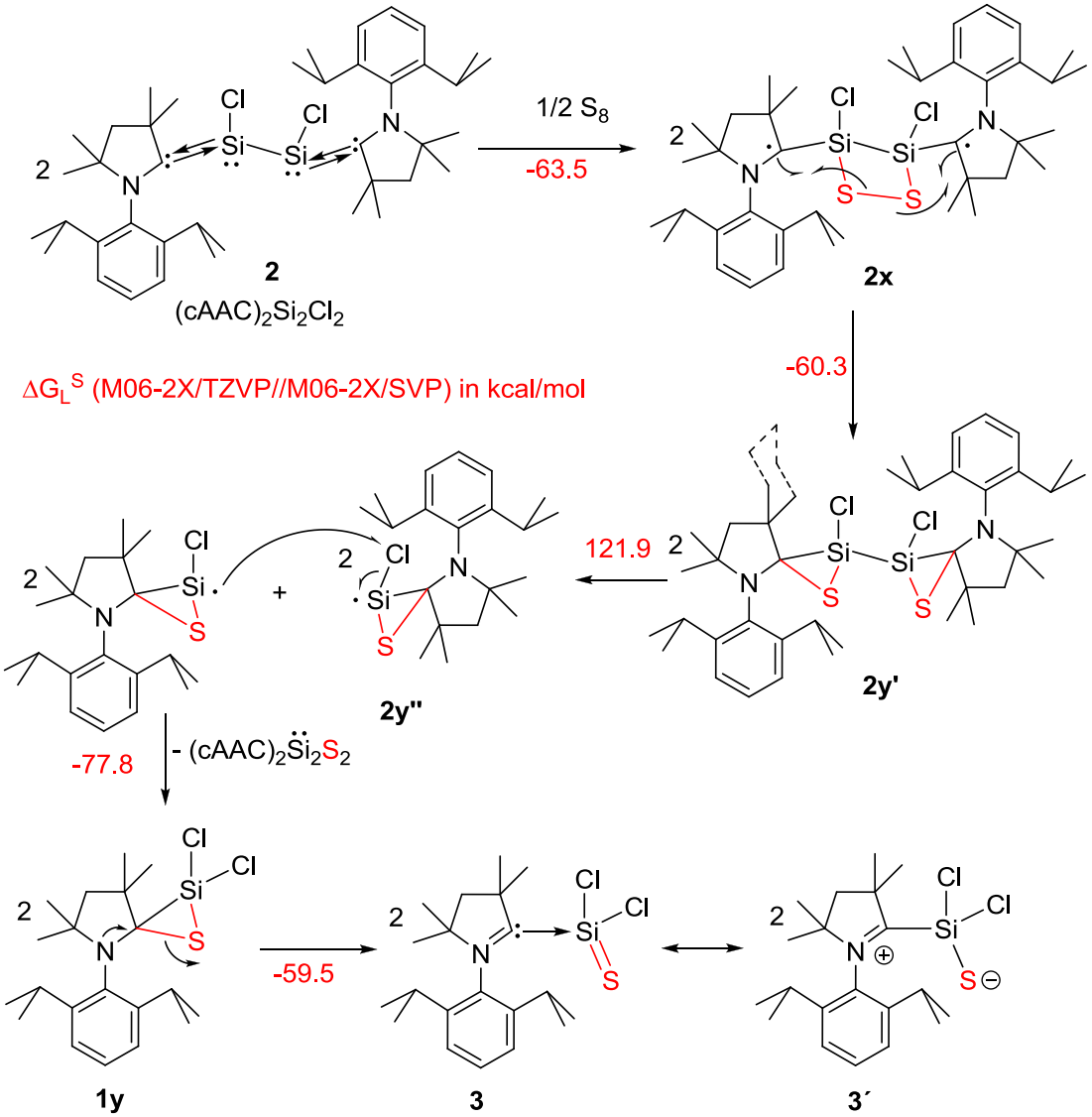
Table S5. Second order perturbation theory analysis of Fock matrix in NBO basis for compound **3**.

Donor NBO (i)	Acceptor NBO (j)	E(2)[a] (kcal/mol)	E(j)–E(i)[b] (a.u.)	F(i,j)[c] (a.u.)
LP(1) S1	RY* Si1	6.18	1.29	0.080
LP(2) S1	RY* Si1	8.00	0.79	0.074
LP(3) S1	RY* Si1	8.16	0.23	0.039

a E(2) means energy of hyperconjugative interaction (stabilization energy). *b* Energy difference between donor(i) and acceptor(j) NBO orbitals. *c* F(i.j) is the Fock matrix element between i and j NBO orbitals.

Table S6. NPA charge of selected atoms of **3 (3** in triplet state**)**.

Si1	C1	N1	C2	S1	C3	Cl1	Cl2
1.251 (1.309)	0.121 (-0.352)	-0.389 (-0.423)	-0.144 (-0.090)	-0.722 (-0.236)	0.101 (0.121)	-0.392 (-0.361)	-0.407 (-0.375)



Scheme S1. Alternative proposed mechanism for the formation of **3** from **2** reacting with sulfur.

Table S7. Cartesian coordinates (in Å) of the optimized structures at M06-2X/SVP level of theory.

3(singlet)	Si	8.33646	12.89282	10.73153
	S	7.95873	13.27859	12.64070
	Cl	7.49834	11.19135	9.85575
	N	10.98772	11.67910	10.85077
	Cl	7.97693	14.34240	9.25612
	C	10.51831	10.33696	10.54461
	C	9.97726	9.51845	11.55564
	C	10.60140	9.91424	9.20032

	C	9.58745	8.22438	11.19188
	H	9.16471	7.56906	11.95524
	C	10.17702	8.61963	8.89681
	H	10.21994	8.27375	7.86297
	C	12.43234	11.91067	11.26503
	C	10.27550	12.76283	10.72129
	C	11.05715	10.81290	8.05909
	H	11.55105	11.68717	8.49215
	C	9.68922	7.77229	9.88426
	H	9.36705	6.76206	9.62776
	C	9.68696	9.96629	12.98214
	H	9.95241	11.02950	13.07829
	C	11.17392	13.99286	10.83570
	C	12.75150	11.10103	12.51508
	H	12.72673	10.02243	12.30542
	H	12.05540	11.32922	13.33173
	H	13.76672	11.36408	12.84494
	C	10.45736	9.14231	14.02209
	H	10.11658	8.09580	14.01224
	H	10.26516	9.54002	15.02940
	H	11.54166	9.13852	13.85585
	C	12.07255	10.12020	7.14518
	H	11.60007	9.32128	6.55498
	H	12.90112	9.67319	7.71337
	H	12.49248	10.84435	6.43176
	C	8.18402	9.85771	13.28086
	H	7.57877	10.37069	12.52499
	H	7.96736	10.32578	14.25179
	H	7.87455	8.80203	13.32960
	C	9.86774	11.33406	7.24261
	H	10.23109	11.89368	6.36767

	H	9.22213	12.00014	7.83005
	H	9.24420	10.50069	6.88497
	C	10.59828	15.18731	11.59762
	H	11.37129	15.97001	11.63992
	H	10.30168	14.90804	12.61509
	H	9.71513	15.59984	11.09153
	C	12.41024	13.41751	11.55127
	H	13.33961	13.90736	11.22775
	H	12.29813	13.58075	12.63324
	C	13.41483	11.50649	10.16467
	H	13.24796	10.46598	9.85202
	H	14.43097	11.57676	10.57659
	H	13.36807	12.15785	9.28412
	C	11.49961	14.44351	9.39414
	H	11.95736	13.64777	8.79192
	H	12.20930	15.28193	9.44654
	H	10.59146	14.78440	8.88096
3(triplet)	Si	8.43761	12.84610	10.63411
	S	7.38539	13.34341	12.44454
	Cl	7.51477	11.17992	9.82555
	N	11.03698	11.62143	10.82324
	Cl	7.87988	14.46463	9.44864
	C	10.55578	10.30865	10.51730
	C	9.97595	9.52085	11.53639
	C	10.59154	9.85544	9.17978
	C	9.50981	8.24548	11.20467
	H	9.06045	7.62302	11.98139
	C	10.10359	8.57693	8.89837
	H	10.12159	8.21380	7.86858
	C	12.44823	11.89336	11.22108
	C	10.25604	12.75134	10.71866

	C	11.06770	10.72640	8.02659
	H	11.49750	11.63826	8.45565
	C	9.57964	7.76942	9.90116
	H	9.20464	6.77308	9.66174
	C	9.74560	10.02755	12.95363
	H	10.12086	11.06062	13.00706
	C	11.14416	13.98533	10.88798
	C	12.86413	11.03235	12.41337
	H	12.82846	9.96271	12.15708
	H	12.22160	11.21345	13.28420
	H	13.89763	11.28132	12.69493
	C	10.47175	9.17596	14.00124
	H	10.05787	8.15629	14.02133
	H	10.33703	9.60726	15.00459
	H	11.54742	9.09466	13.80113
	C	12.14239	10.03095	7.18495
	H	11.72023	9.17881	6.63092
	H	12.96939	9.65126	7.80113
	H	12.55704	10.73031	6.44377
	C	8.24727	10.06466	13.29023
	H	7.65552	10.56932	12.51399
	H	8.08388	10.58189	14.24798
	H	7.84184	9.04568	13.38825
	C	9.89976	11.16082	7.13250
	H	10.27600	11.75005	6.28275
	H	9.17391	11.77489	7.68090
	H	9.36569	10.28620	6.72978
	C	10.53773	15.09891	11.74893
	H	11.29262	15.88226	11.91904
	H	10.20605	14.71206	12.72305
	H	9.67620	15.57092	11.25487

	C	12.37092	13.37985	11.60389
	H	13.30002	13.91606	11.35923
	H	12.21514	13.45909	12.69091
	C	13.44088	11.61966	10.08497
	H	13.34837	10.57975	9.74030
	H	14.46385	11.76209	10.46161
	H	13.30282	12.28986	9.22800
	C	11.51105	14.56389	9.50974
	H	11.93148	13.79597	8.84589
	H	12.25100	15.37284	9.61772
	H	10.61611	14.97270	9.02044
1	Si	7.62263	2.88030	2.96496
	Si	6.17405	4.50446	3.96943
	Cl	6.67079	2.51611	1.13724
	Cl	9.39674	3.84477	2.45036
	Cl	6.90204	4.54504	5.94126
	Cl	4.30348	3.59388	4.10135
	N	9.08893	1.07374	4.61972
	N	4.95310	6.62295	2.48917
	C	8.02207	1.27054	3.76792
	C	7.03934	0.09109	3.88262
	C	7.76274	-0.83469	4.88881
	H	8.29763	-1.62656	4.34079
	H	7.05702	-1.32583	5.57409
	C	8.78535	0.02783	5.64237
	C	5.64739	0.50607	4.37223
	H	5.68123	1.09546	5.29924
	H	5.14113	1.11399	3.60927
	C	6.85326	-0.64882	2.54499
	H	6.30643	-0.03461	1.81857

	H	7.81714	-0.93018	2.09936
	C	8.15000	0.66399	6.88649
	H	7.36921	1.38380	6.60238
	H	8.89619	1.19471	7.49053
	H	7.69831	-0.11697	7.51551
	C	10.02777	-0.76445	6.02928
	H	10.49577	-1.22678	5.14848
	H	9.74284	-1.56072	6.73187
	H	10.77598	-0.12266	6.51536
	C	10.42873	1.51603	4.35052
	C	11.02415	2.53294	5.12168
	C	12.33290	2.92416	4.82051
	H	12.80232	3.71182	5.41324
	C	13.03450	2.34819	3.76997
	H	14.04936	2.67681	3.54047
	C	12.43521	1.34828	3.01281
	H	12.98783	0.89298	2.18872
	C	11.14158	0.90454	3.29344
	C	10.29149	3.25145	6.23978
	H	9.23920	2.93582	6.20457
	C	10.87642	2.88820	7.60917
	H	10.91750	1.80097	7.76656
	H	10.27686	3.33277	8.41806
	H	11.90460	3.27201	7.70058
	C	10.31731	4.77045	6.04588
	H	9.96843	5.04045	5.04015
	H	11.33343	5.17388	6.17267
	H	9.66533	5.26067	6.78379
	C	10.55384	-0.20888	2.44397
	H	9.65809	-0.57624	2.95987

	C	10.12317	0.31304	1.06891
	H	10.98598	0.73705	0.53196
	H	9.36017	1.09890	1.15590
	H	9.70842	-0.50276	0.45674
	C	11.51213	-1.39465	2.29575
	H	11.00185	-2.23146	1.79612
	H	11.87811	-1.74585	3.27190
	H	12.38807	-1.13483	1.68287
	C	5.92498	6.23637	3.38986
	C	6.96060	7.36446	3.55430
	C	6.39196	8.46601	2.62964
	H	5.84268	9.20864	3.22977
	H	7.18896	9.00145	2.09357
	C	5.41607	7.77916	1.66303
	C	8.38077	6.95937	3.14811
	H	8.75240	6.16031	3.80463
	H	8.43979	6.59623	2.11409
	C	7.02994	7.88130	5.00347
	H	6.03407	8.12436	5.39790
	H	7.48867	7.13998	5.67042
	C	6.15354	7.27024	0.41736
	H	5.45558	6.85099	-0.31683
	H	6.87497	6.48542	0.68610
	H	6.69642	8.09737	-0.06337
	C	4.26609	8.69463	1.26447
	H	4.66886	9.56124	0.72076
	H	3.72296	9.05871	2.14804
	H	3.54773	8.17758	0.61305
	C	3.56731	6.24579	2.55893
	C	2.99632	5.39013	1.59526

	C	1.63562	5.08189	1.69656
	H	1.18352	4.42366	0.95267
	C	0.85633	5.57313	2.73454
	H	-0.19979	5.30760	2.80266
	C	1.43288	6.40405	3.68754
	H	0.82111	6.78843	4.50568
	C	2.77929	6.76655	3.61100
	C	3.79100	4.75493	0.46815
	H	4.85937	4.93235	0.66707
	C	3.57457	3.23870	0.40797
	H	2.53865	2.99630	0.12722
	H	3.79340	2.76724	1.37539
	H	4.23590	2.79243	-0.34872
	C	3.41937	5.37792	-0.88360
	H	4.07682	4.99935	-1.68085
	H	3.48593	6.47479	-0.87114
	H	2.38239	5.11776	-1.14785
	C	3.34207	7.69524	4.67244
	H	4.31069	8.05832	4.30824
	C	3.58539	6.94439	5.98623
	H	4.29579	6.11666	5.85389
	H	2.64180	6.52308	6.36654
	H	3.98831	7.62450	6.75278
	C	2.45692	8.92271	4.90771
	H	2.21927	9.43875	3.96574
	H	2.96914	9.63461	5.57194
	H	1.50663	8.65268	5.39178
	H	5.02947	-0.38830	4.54748
	H	6.27493	-1.57010	2.72099
	H	9.06036	7.81875	3.25675

	H	7.64445	8.79548	5.03116
1x	Si	6.77857	2.17427	3.30476
	Si	6.46086	4.35924	4.47373
	Cl	4.66741	1.80188	3.46847
	Cl	6.93283	0.36629	2.01435
	Cl	7.82777	4.70872	6.09483
	Cl	4.77200	4.06313	5.84548
	N	9.15238	1.17641	4.81542
	N	4.77380	6.28896	2.99637
	C	7.85149	1.18994	4.65544
	C	7.16350	0.31866	5.70410
	C	8.35496	-0.35738	6.40329
	H	8.52798	-1.34261	5.94409
	H	8.17586	-0.51124	7.47553
	C	9.56510	0.53354	6.15081
	C	6.28236	1.16071	6.63988
	H	6.79179	2.04852	7.03939
	H	5.38794	1.51076	6.11013
	C	6.29693	-0.77802	5.05734
	H	5.41655	-0.37170	4.54871
	H	6.87351	-1.36552	4.32986
	C	9.67904	1.59362	7.25575
	H	8.86047	2.32349	7.21257
	H	10.63025	2.13170	7.22083
	H	9.63037	1.07132	8.22138
	C	10.85256	-0.26211	6.04655
	H	10.70393	-1.18159	5.47060
	H	11.16823	-0.54365	7.06122
	H	11.66124	0.32104	5.58549
	C	10.09831	1.62633	3.77708

	C	10.72731	2.89198	3.83776
	C	11.38530	3.35190	2.69327
	H	11.82194	4.35031	2.70959
	C	11.49055	2.57398	1.55130
	H	11.98274	2.96615	0.66024
	C	11.01022	1.27293	1.57144
	H	11.16188	0.62851	0.70474
	C	10.32877	0.75794	2.67664
	C	10.87866	3.71380	5.10551
	H	10.03656	3.48035	5.76250
	C	12.19934	3.31645	5.78721
	H	12.28713	2.23568	5.95843
	H	12.30383	3.83030	6.75557
	H	13.04722	3.61344	5.15148
	C	10.89031	5.23016	4.89940
	H	10.07037	5.54702	4.24567
	H	11.84265	5.56825	4.46262
	H	10.78069	5.72916	5.87370
	C	10.04787	-0.74077	2.65271
	H	9.28621	-0.97109	3.41475
	C	9.55735	-1.27139	1.29439
	H	10.40754	-1.43800	0.61625
	H	8.85189	-0.59064	0.81097
	H	9.06003	-2.24249	1.43211
	C	11.35561	-1.49321	2.97481
	H	11.15790	-2.56782	3.11071
	H	11.87243	-1.11438	3.86165
	H	12.05146	-1.38533	2.12959
	C	5.74385	6.08346	3.86087
	C	6.26180	7.43755	4.38444

	C	5.42582	8.45945	3.57750
	H	4.60890	8.85567	4.19963
	H	6.03377	9.31078	3.24303
	C	4.84808	7.68750	2.39255
	C	7.76337	7.71645	4.26917
	H	8.35943	6.96038	4.79559
	H	8.09391	7.76262	3.22329
	C	5.85124	7.51021	5.87186
	H	4.79489	7.23968	6.01250
	H	6.46144	6.84861	6.49718
	C	5.85328	7.68051	1.23582
	H	5.46152	7.17033	0.35104
	H	6.78839	7.18298	1.52789
	H	6.06892	8.72228	0.95801
	C	3.49978	8.21225	1.93026
	H	3.66376	9.15645	1.39217
	H	2.82933	8.41560	2.77199
	H	3.00270	7.51078	1.24545
	C	3.68621	5.35373	2.72615
	C	3.70567	4.47172	1.62602
	C	2.65797	3.55165	1.50632
	H	2.67314	2.84436	0.67773
	C	1.63065	3.49289	2.43391
	H	0.84655	2.74057	2.33689
	C	1.59013	4.41800	3.46898
	H	0.75114	4.40938	4.16742
	C	2.58323	5.38739	3.61796
	C	4.73915	4.50640	0.51239
	H	5.66040	4.96588	0.90827
	C	5.08718	3.11634	-0.03828

	H	4.28345	2.74544	-0.69297
	H	5.25329	2.37151	0.74887
	H	6.00453	3.17517	-0.63967
	C	4.19168	5.34613	-0.65496
	H	4.96499	5.48802	-1.42550
	H	3.82594	6.33281	-0.34359
	H	3.34265	4.82109	-1.11875
	C	2.31258	6.51059	4.61634
	H	3.15850	7.21133	4.58289
	C	2.12792	6.07298	6.07302
	H	3.05177	5.68469	6.51198
	H	1.36021	5.28833	6.15189
	H	1.78515	6.93281	6.66874
	C	1.04232	7.26545	4.17974
	H	1.01838	7.46412	3.10040
	H	0.95933	8.22192	4.71812
	H	0.14870	6.67110	4.42243
	H	5.96151	0.52887	7.48123
	H	5.96266	-1.44496	5.86744
	H	7.96296	8.69210	4.73748
	H	5.99220	8.54811	6.21072
	S	8.05534	5.07373	2.74403
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1y	Si	6.72877	4.59685	4.38990
	Cl	8.14532	4.16840	5.82550
	N	5.29042	6.64594	2.86329
	C	5.82653	6.22214	4.12826
	C	6.24721	7.51473	4.93023
	C	5.89405	8.63230	3.92871
	H	4.89191	9.03224	4.15155

	H	6.60785	9.46746	3.97996
	C	5.85147	7.97757	2.53766
	C	7.74724	7.54662	5.26335
	H	8.00075	6.80941	6.03566
	H	8.38109	7.35585	4.38708
	C	5.49196	7.68174	6.25260
	H	4.40138	7.66290	6.12195
	H	5.75807	6.88186	6.95816
	C	7.25796	7.83569	1.92878
	H	7.19369	7.53064	0.87621
	H	7.84694	7.07162	2.45473
	H	7.80440	8.78974	1.97476
	C	4.97461	8.77628	1.58275
	H	5.42916	9.76546	1.42496
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	H	4.87742	8.27925	0.60939
	C	4.15132	6.10604	2.18055
	C	4.32038	5.42563	0.95002
	C	3.19116	4.98939	0.24641
	H	3.32659	4.47476	-0.70685
	C	1.90924	5.19200	0.73506
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	H	0.73590	6.01580	2.33460
	C	2.83692	6.32365	2.67608
	C	5.67765	5.14356	0.32658
	H	6.44060	5.37693	1.08217
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	H	6.92906	5.81466	-1.32538
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	C	2.53512	7.07629	3.96291
	H	3.49552	7.30846	4.43517
	C	1.69982	6.23952	4.94136
	H	2.11664	5.23520	5.08424
	H	0.66767	6.12946	4.57479
	H	1.64811	6.73882	5.92113
	C	1.80528	8.40198	3.70793
	H	2.37231	9.08213	3.05986
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	H	0.83014	8.22317	3.22989
	H	8.00842	8.53993	5.65770
	H	5.76549	8.64710	6.70510
	S	4.78514	4.88755	5.04243
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	Si	5.59110	8.53905	5.57351
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	C	3.13080	8.26444	8.84456
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	C	3.66649	10.61103	8.00674

	C	2.52090	8.96390	6.50965
	C	4.30060	6.38864	10.06476
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	C	6.71091	7.33855	8.52329
	C	6.90958	6.00117	8.11815
	C	8.17880	5.44331	8.29208
	C	9.22492	6.18175	8.83075
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	C	7.77193	8.12018	9.02483
	C	5.84678	5.15323	7.43122
	C	5.57918	3.84306	8.18303
	C	6.25349	4.82852	5.98665
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	C	5.83945	12.96274	0.24469
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	C	7.05640	12.94285	3.01725
	C	6.28300	14.08638	3.31216
	C	6.92721	15.18470	3.88759
	C	8.28351	15.15183	4.18658
	C	9.01635	13.99963	3.93382
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	C	4.05634	14.32270	4.46615
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	C	10.56303	11.84267	2.45378
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	H	7.69707	11.38655	-0.79016
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	H	8.46034	12.25253	0.56241
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	H	8.76544	16.01899	4.64092
	H	10.07200	13.96135	4.20967
	H	4.43550	13.21551	2.67681
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	H	4.36036	13.54786	5.18019
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	H	3.28612	15.29251	2.00190

	H	8.66270	10.86530	2.67369
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	H	10.14103	11.71924	5.20978
	H	10.39874	12.31169	1.47336
	H	11.08357	10.88649	2.29609
	H	11.24245	12.49317	3.02509
2x	Si	6.71110	2.46184	3.82793
	Si	5.24917	4.27328	4.39421
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	N	5.18746	6.64426	2.82165
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	H	8.20181	-0.58703	7.47389
	C	9.51833	0.52606	6.11318
	C	6.18478	0.93197	6.78604
	H	6.69822	1.75223	7.30634
	H	5.29976	1.35802	6.29117
	C	6.24183	-0.88107	5.09805
	H	5.28511	-0.49648	4.72368
	H	6.77744	-1.35544	4.26324
	C	9.66143	1.56143	7.23634
	H	8.77520	2.20989	7.28197
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	H	9.76519	1.04640	8.20249
	C	10.82244	-0.24015	5.93198

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	H	11.05866	-0.77305	6.86433
	H	11.65794	0.43389	5.69650
	C	9.97486	1.39844	3.74646
	C	10.80489	2.53653	3.70604
	C	11.68431	2.68836	2.62998
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	H	12.41624	1.90404	0.76126
	C	10.90076	0.64730	1.64200
	H	10.93763	-0.08220	0.83077
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	C	12.04902	3.63645	5.59579
	H	12.27244	2.64794	6.02067
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	H	12.90854	3.92401	4.97081
	C	10.55961	5.01158	4.12279
	H	9.67923	5.01372	3.46585
	H	11.43309	5.30785	3.52299
	H	10.42324	5.77322	4.90452
	C	9.16353	-0.81340	2.71015
	H	8.73091	-0.91594	3.71333
	C	8.01121	-0.68286	1.70807
	H	8.40379	-0.59004	0.68344
	H	7.39646	0.20581	1.90921
	H	7.36006	-1.56994	1.74324
	C	9.97393	-2.08451	2.43680
	H	9.33755	-2.97206	2.56977

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	H	10.35687	-2.10950	1.40589
	C	5.41144	6.06510	4.04955
	C	6.17527	7.03501	4.96090
	C	6.26444	8.30142	4.07728
	H	5.47053	9.00502	4.37328
	H	7.22631	8.82093	4.19746
	C	6.02628	7.86309	2.62284
	C	7.55510	6.47910	5.33629
	H	7.44940	5.55002	5.92228
	H	8.15362	6.25295	4.44637
	C	5.42495	7.37611	6.26084
	H	4.38109	7.65733	6.06129
	H	5.42203	6.53297	6.96125
	C	7.35312	7.50384	1.93954
	H	7.21163	7.30301	0.87097
	H	7.80092	6.60923	2.39628
	H	8.05987	8.34121	2.03593
	C	5.28970	8.92643	1.81804
	H	5.90787	9.83429	1.76508
	H	4.32966	9.18312	2.28816
	H	5.08837	8.58263	0.79369
	C	4.04800	6.33545	2.00384
	C	4.19198	5.66513	0.77140
	C	3.04402	5.39165	0.02228
	H	3.14610	4.87458	-0.93357
	C	1.77929	5.72963	0.48560
	H	0.89453	5.48536	-0.10441
	C	1.64787	6.37810	1.70765
	H	0.65404	6.64662	2.07101

	C	2.76759	6.70982	2.47497
	C	5.53287	5.19446	0.23763
	H	6.27547	5.32900	1.03668
	C	5.52455	3.70555	-0.12514
	H	4.83636	3.50069	-0.95939
	H	5.22820	3.08285	0.72907
	H	6.53206	3.39229	-0.43628
	C	5.94960	6.02239	-0.98482
	H	6.96969	5.75849	-1.30281
	H	5.91601	7.10374	-0.78829
	H	5.27077	5.82304	-1.82872
	C	2.55586	7.46436	3.77763
	H	3.53739	7.81482	4.12156
	C	1.97292	6.55283	4.86285
	H	2.64025	5.70965	5.09184
	H	1.00435	6.14132	4.53875
	H	1.80753	7.11649	5.79406
	C	1.67423	8.70331	3.58648
	H	2.04292	9.34276	2.77087
	H	1.65469	9.29948	4.51098
	H	0.63482	8.42924	3.35219
	H	5.83137	0.20679	7.53548
	H	6.02623	-1.65746	5.84967
	H	8.10866	7.20129	5.95721
	H	5.92397	8.22883	6.74900
	S	3.77760	3.31816	3.12900
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2y	Si	8.46588	12.85801	10.56036
	S	7.98904	13.31973	12.45898
	N	11.05515	11.68470	10.87409

	Cl	8.21022	14.33245	9.03598
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	C	10.01858	9.53939	11.58433
	C	10.55963	9.94989	9.21227
	C	9.65758	8.23257	11.23557
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	C	10.17163	8.63940	8.92469
	H	10.19097	8.29526	7.88919
	C	12.50940	11.84683	11.26953
	C	10.40693	12.80323	10.70634
	C	10.90888	10.86724	8.04902
	H	11.29621	11.81068	8.45109
	C	9.74982	7.77538	9.92823
	H	9.46257	6.75156	9.68427
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	C	11.34935	13.98780	10.84222
	C	12.82951	11.02218	12.50839
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	H	13.86913	11.22851	12.80124
	C	10.45794	9.17700	14.06707
	H	10.09778	8.13698	14.06507
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	H	11.54500	9.15197	13.92136
	C	11.98115	10.27552	7.12865
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	H	12.26737	11.01154	6.36324
	C	8.21260	9.92419	13.26416

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	H	7.97720	10.38959	14.23212
	H	7.87990	8.87490	13.29293
	C	9.64740	11.20723	7.24312
	H	9.89601	11.89614	6.42235
	H	8.88039	11.68887	7.86504
	H	9.21106	10.29647	6.80528
	C	10.76334	15.16484	11.62211
	H	11.53104	15.94901	11.70892
	H	10.43592	14.85647	12.62264
	H	9.89016	15.58107	11.10014
	C	12.56021	13.35549	11.55766
	H	13.51261	13.79817	11.23271
	H	12.46064	13.52045	12.64070
	C	13.42765	11.40038	10.13179
	H	13.25388	10.34252	9.88772
	H	14.46958	11.50562	10.46439
	H	13.30029	11.99822	9.22152
	C	11.71224	14.47058	9.42127
	H	12.19246	13.68919	8.81692
	H	12.41949	15.30793	9.51228
	H	10.81713	14.81929	8.89161
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	C	4.53041	7.92439	1.27451
	C	3.75073	5.97984	2.56788

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	H	6.30931	9.00592	1.70477
	C	3.95844	4.83240	3.54822
	H	4.96788	4.92740	3.97526
	C	3.33844	7.88752	0.54887
	H	3.18380	8.60197	-0.26091
	C	2.57026	5.99567	1.81633
	H	1.81531	5.22831	1.99892
	C	2.35781	6.94140	0.82304
	H	1.43456	6.92682	0.24173
	C	2.92407	4.84331	4.68053
	H	1.91471	4.66772	4.27796
	H	2.90167	5.79429	5.22706
	H	3.13736	4.03749	5.39880
	C	5.05215	10.31129	0.58894
	H	5.87653	11.02753	0.45921
	H	4.41205	10.66584	1.41072
	H	4.45790	10.33291	-0.33662
	C	6.13836	7.77185	4.31476
	C	3.89756	3.47536	2.83223
	H	2.87929	3.27250	2.46579
	H	4.16821	2.67161	3.53288
	H	4.58093	3.43144	1.97430
	C	6.42859	8.39762	-0.32103
	H	5.77748	8.12769	-1.16640
	H	7.00774	7.50428	-0.04523
	H	7.13499	9.17252	-0.65695
	C	9.24227	5.71420	3.73768
	H	9.72953	5.33186	2.82933
	H	8.75171	4.87321	4.24756

	H	10.02575	6.12006	4.39650
	C	8.96383	7.92637	2.61459
	H	9.35534	7.51440	1.67322
	H	9.80272	8.31838	3.20995
	H	8.29646	8.76326	2.36735
	Si	7.44750	4.98333	-1.42324
	N	8.73776	2.93621	-2.93470
	C	7.59744	3.39174	-2.40535
	C	6.41624	2.75852	-3.15042
	C	9.97966	3.00443	-2.21324
	C	10.20317	2.01349	-1.23343
	C	10.88981	4.05688	-2.41509
	C	9.17892	0.93289	-0.92155
	H	8.48893	0.86526	-1.77472
	C	10.64326	5.19140	-3.39473
	H	9.62954	5.06692	-3.80152
	C	11.37760	2.08022	-0.48345
	H	11.56403	1.33132	0.28797
	C	12.05915	4.07235	-1.64590
	H	12.77812	4.88177	-1.78802
	C	12.30537	3.09604	-0.69049
	H	13.21712	3.13281	-0.09213
	C	11.65772	5.15333	-4.54437
	H	12.66372	5.40689	-4.17568
	H	11.72425	4.15793	-5.00708
	H	11.39270	5.88392	-5.32358
	C	9.81617	-0.44655	-0.73771
	H	9.03400	-1.21401	-0.64392
	H	10.46298	-0.71142	-1.58753
	H	10.42527	-0.49194	0.17712

	C	8.57474	2.26812	-4.26429
	C	10.68442	6.56028	-2.70562
	H	11.69389	6.78376	-2.32721
	H	10.41429	7.34931	-3.42322
	H	9.98569	6.60618	-1.85887
	C	8.34469	1.32284	0.30484
	H	8.99116	1.47406	1.18315
	H	7.79754	2.26088	0.13025
	H	7.61562	0.53228	0.54118
	C	5.49567	3.78942	-3.81600
	H	5.04608	4.45045	-3.05982
	H	6.03732	4.41826	-4.53553
	H	4.68025	3.27054	-4.34359
	C	5.59090	1.92173	-2.15716
	H	5.10635	2.55719	-1.40454
	H	4.81858	1.36322	-2.70997
	H	6.22888	1.19471	-1.63280
	C	7.11022	1.81562	-4.16865
	H	6.61605	1.82969	-5.15067
	H	7.07402	0.78099	-3.79327
	C	9.55913	1.11762	-4.43568
	H	9.45666	0.37146	-3.63575
	H	9.36894	0.62018	-5.39757
	H	10.59638	1.48380	-4.43637
	C	8.74771	3.27408	-5.40709
	H	8.10295	4.15216	-5.25701
	H	9.78629	3.61439	-5.49299
	C	7.57213	7.36381	4.69298
	H	8.13249	8.20162	5.13369
	H	7.53337	6.55661	5.44051

	C	5.97826	9.28245	4.10804
	H	6.79397	9.71741	3.51852
	H	5.98128	9.77293	5.09163
	H	5.02086	9.51150	3.61652
	C	5.12634	7.33549	5.36964
	H	4.10199	7.57773	5.05105
	H	5.33048	7.87680	6.30485
	H	5.19383	6.25999	5.57596
	H	8.46663	2.79469	-6.35607
	S	8.88982	5.04671	0.23851
	S	5.65909	4.88706	-0.14955
2y'	Si	6.62530	2.95240	3.84042
	Si	6.38240	5.17231	4.73558
	Cl	7.99059	3.15449	2.23264
	Cl	8.46047	5.52261	5.19488
	N	8.56531	1.06446	5.02434
	N	5.10867	6.95432	2.82189
	C	7.60125	1.93090	5.20891
	C	7.09819	1.84560	6.65393
	C	7.62884	0.47490	7.10062
	H	6.84398	-0.27710	6.93019
	H	7.88777	0.45918	8.16844
	C	8.83114	0.15419	6.21784
	C	7.75028	3.00397	7.44395
	H	8.81596	3.14392	7.21323
	H	7.23166	3.95209	7.24976
	C	5.58337	1.91118	6.86156
	H	5.16203	2.87096	6.53410
	H	5.07196	1.10605	6.32113
	C	10.16975	0.49880	6.86260

	H	10.22968	1.55000	7.17047
	H	10.99432	0.27835	6.17216
	H	10.29603	-0.13046	7.75463
	C	8.84394	-1.31261	5.81295
	H	7.89497	-1.60510	5.34791
	H	8.97595	-1.91214	6.72559
	H	9.67272	-1.54164	5.12880
	C	9.44247	0.90761	3.86985
	C	10.64085	1.65497	3.81430
	C	11.55334	1.34676	2.80065
	H	12.48681	1.90941	2.74554
	C	11.28857	0.36747	1.85374
	H	12.01884	0.14564	1.07406
	C	10.07251	-0.30005	1.88542
	H	9.84103	-1.03430	1.11191
	C	9.12254	-0.04820	2.88049
	C	10.97645	2.85185	4.69813
	H	10.16542	2.99627	5.42757
	C	12.30595	2.69908	5.44875
	H	12.35605	1.79604	6.06838
	H	12.46584	3.57026	6.10088
	H	13.14684	2.66449	4.73986
	C	11.05368	4.12172	3.83643
	H	10.12895	4.27898	3.26980
	H	11.89383	4.05052	3.12856
	H	11.21990	5.00030	4.47648
	C	7.78290	-0.76368	2.76266
	H	7.14516	-0.46668	3.60839
	C	7.05855	-0.31701	1.48377
	H	7.60516	-0.66502	0.59260

	H	6.95290	0.77237	1.43627
	H	6.04736	-0.74903	1.46283
	C	7.92752	-2.29158	2.73264
	H	6.93288	-2.75972	2.77204
	H	8.52730	-2.68757	3.56164
	H	8.40298	-2.61852	1.79550
	C	5.96087	6.83540	3.80711
	C	6.34880	8.22243	4.32683
	C	5.15840	9.07283	3.84628
	H	4.42151	9.12482	4.66099
	H	5.45929	10.09981	3.59294
	C	4.53233	8.35088	2.64452
	C	7.66184	8.60217	3.60605
	H	8.47593	7.93588	3.92128
	H	7.58051	8.55212	2.51287
	C	6.56556	8.40076	5.82957
	H	5.66744	8.13521	6.39718
	H	7.39224	7.77877	6.19482
	C	4.89480	8.98180	1.29658
	H	4.66167	8.30115	0.46506
	H	5.94566	9.28708	1.23286
	H	4.28320	9.88610	1.17419
	C	3.01154	8.33096	2.74884
	H	2.65874	9.37196	2.72097
	H	2.66867	7.88123	3.68796
	H	2.56374	7.79829	1.90089
	C	4.84288	5.83650	1.92389
	C	5.77083	5.63396	0.87397
	C	5.60582	4.51055	0.06392
	H	6.32447	4.32284	-0.73518

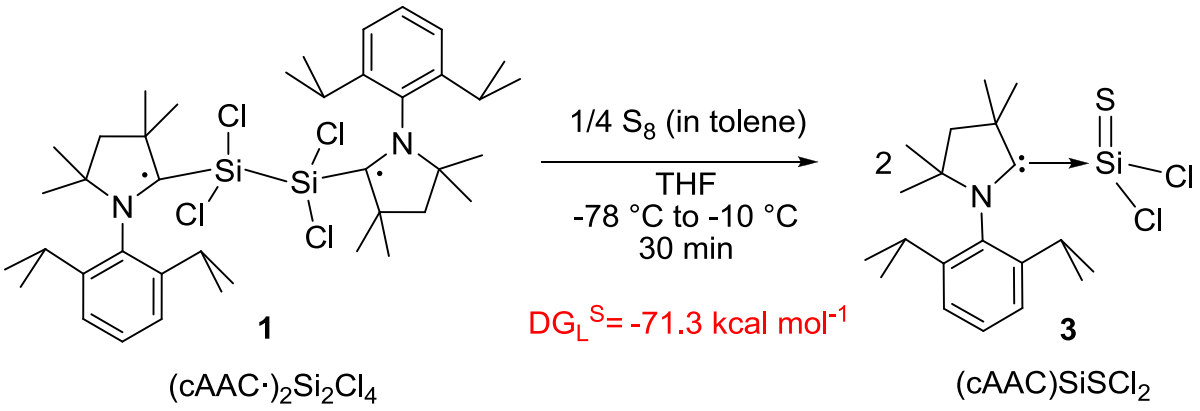
	C	4.56245	3.61817	0.27733
	H	4.46612	2.72907	-0.34698
	C	3.65529	3.84695	1.30174
	H	2.85354	3.12873	1.47741
	C	3.76632	4.95177	2.15402
	C	6.91335	6.59771	0.57889
	H	6.69536	7.51997	1.11463
	C	8.28040	6.13068	1.08294
	H	8.59994	5.20993	0.57523
	H	8.27103	5.92370	2.16389
	H	9.02943	6.91410	0.88727
	C	6.98356	6.95720	-0.90829
	H	7.71168	7.76674	-1.06597
	H	6.00804	7.28692	-1.29529
	H	7.31271	6.10054	-1.51446
	C	2.71068	5.12913	3.23762
	H	3.03171	5.95354	3.88814
	C	2.55056	3.90476	4.14241
	H	3.48246	3.64958	4.65423
	H	2.22819	3.02052	3.57237
	H	1.78585	4.12147	4.90386
	C	1.34463	5.44334	2.60633
	H	1.38648	6.22236	1.83493
	H	0.62962	5.75738	3.38152
	H	0.93922	4.53721	2.13054
	H	7.65051	2.78428	8.51717
	H	5.39155	1.81309	7.94200
	H	7.92488	9.63363	3.88320
	H	6.81858	9.45760	6.00829
	S	5.02289	5.49564	6.19524

	S	5.13393	1.64133	3.52683
2y''	Si	7.11258	4.42726	3.74827
	Cl	8.26391	3.82090	5.46058
	N	5.19391	6.79786	2.88616
	C	5.71086	6.27312	4.04236
	C	6.26925	7.41528	4.92515
	C	5.99859	8.65691	4.04089
	H	5.08479	9.16725	4.38340
	H	6.82155	9.38389	4.08881
	C	5.77569	8.14245	2.60745
	C	7.75658	7.29479	5.27340
	H	7.94847	6.40639	5.88761
	H	8.39077	7.23608	4.37718
	C	5.47773	7.47890	6.23835
	H	4.39362	7.52641	6.05680
	H	5.68070	6.58744	6.84809
	C	7.10316	8.00387	1.85145
	H	6.93467	7.69717	0.81071
	H	7.75247	7.25645	2.32839
	H	7.62635	8.97093	1.84088
	C	4.82189	9.02298	1.81330
	H	5.27713	10.01610	1.68889
	H	3.86195	9.14394	2.33053
	H	4.62909	8.60238	0.81573
	C	4.10057	6.23586	2.14133
	C	4.33948	5.45990	0.99192
	C	3.24254	4.95674	0.28374
	H	3.41961	4.35427	-0.60964
	C	1.94183	5.19946	0.70254
	H	1.09885	4.79353	0.14129

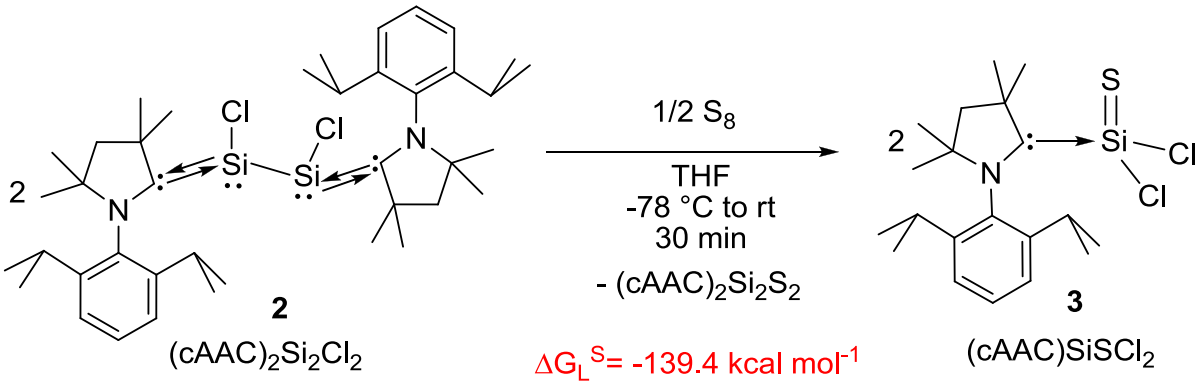
	C	1.71977	5.96110	1.84432
	H	0.69632	6.14803	2.17543
	C	2.78073	6.49612	2.57793
	C	5.73438	5.13144	0.49420
	H	6.45317	5.53769	1.21926
	C	5.95650	3.61727	0.42914
	H	5.33244	3.15688	-0.35204
	H	5.70784	3.14051	1.38810
	H	7.00873	3.39447	0.19820
	C	6.00333	5.77822	-0.86864
	H	7.04698	5.61416	-1.17582
	H	5.81328	6.86155	-0.85018
	H	5.35200	5.34414	-1.64270
	C	2.45923	7.32736	3.81045
	H	3.39424	7.79002	4.15456
	C	1.92151	6.45414	4.95010
	H	2.63296	5.66436	5.22513
	H	0.97766	5.97246	4.65109
	H	1.71881	7.06906	5.84032
	C	1.46458	8.45365	3.50389
	H	1.77140	9.05711	2.63762
	H	1.36806	9.12030	4.37352
	H	0.46362	8.05102	3.28856
	H	8.06313	8.18071	5.84999
	H	5.77613	8.37205	6.80884
	S	5.11175	4.73072	4.66745

2. Synthesis

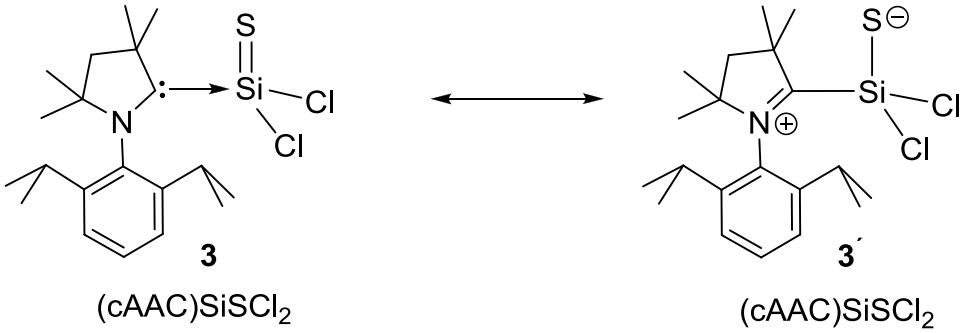
All reactions and handling of reagents were performed under an atmosphere of dry nitrogen or argon using standard Schlenk techniques or a glove box where the O_2 and H_2O levels were usually kept below 1 ppm. Ligand Me_2-cAAC, $(cAAC\cdot)_2Si_2Cl_4$ (**1**) and $(cAAC)_2Si_2Cl_2$ (**2**) were prepared according to literature methods.[S9a-c] Solvents were purified with the M-Braun solvent drying system. Solution NMR spectra were recorded on Bruker Avance 200, Bruker Avance 300, and Bruker Avance 500 MHz NMR spectrometers. Deuterated NMR solvent C_6D_6 was dried by stirring for 2 days over Na/K alloy followed by distillation in vacuum and degassed. EI-MS spectra were obtained with a Finnigan MAT 8230 or a Varian MAT CH5 instrument (70 eV) by EI-MS methods. Elemental analyses were performed by the Analytisches Labor des Instituts für Anorganische Chemie der Universität Göttingen. Melting points were measured in sealed glass tubes on a Büchi B-540 melting point apparatus.



Scheme S2. Synthesis of compound **3** from **1**.



Scheme S3. Synthesis of compound **3** from and **2**.



Scheme S4. Resonance structures of compound **3**.

3. Crystal structure

The molecular structure of **3** was elucidated by single-crystal X-ray diffraction. Crystallographic data are summarized in the supplementary information; CCDC number 1410475 contains full information on space group and other crystallographic details. The structure of **3** was measured at Microdiffractometer at PetraIII. Radiation source: monochromated X-rays beamline PX11A@PetraIII. Data integration was performed with the XDS program.[S10]

Intensity data for all three compounds were corrected for absorption and scaled with SADABS.[S11] Synchrotron data from XDS integration were converted with XDS2SAD (G. Sheldrick) prior to use with SADABS (Absorption correction: empirical (using intensity measurements)

SADABS version 2015/1, multi-scan. (G. M. Sheldrick, 2015)). The crystal was measured at a temperature of 80 K. Structure was solved by direct method and that of **3** refined by full-matrix least-squares methods on F^2 with the program SHELXL12[S12] using anisotropic displacement parameters for all non-hydrogen atoms. Anomalous dispersion for the chosen wavelength was adjusted with the DISP command for the synchroton data. Unmerged intensity data and the SHELXL refinement instructions are included in the CIF file.

Minor disorder at in the five-membered ring system of the cAAC ligand of **3**, affecting C3, C7 and C8 becomes visible in the Fourier residual map. We have therefore attempted to refine this disorder, but occupancy refinement gave a value of less than 5% for the minor component and did not lead to a stable refinement of anisotropic displacement parameters even when restraints were used. Neither did the *R*1(*F*) factor improve upon introducing split positions. We therefore did not further consider the disorder model.

Table S8. Crystal data and structure refinement of (cAAC)$SiSCl_2$ (**3**)

Compound	$(cAAC)_2SiSCl_2$ (cAAC = :C(CH_2) (CMe_2)$_2$N-2,6-*i*$Pr_2C_6H_3$) (**3**) at T = 100 K
Empirical formula	$C_{20}H_{31}NSiSCl_2$
CCDC no.	1410475
Molecular weight	416.51
Crystal size [mm]	0.18 × 0.17 × 0.09
Wavelength [Å]	0.4765
Crystal system	orthorhombic
Space group	*Pbca*
a [Å]	16.115 (5)
b [Å]	16.040 (7)
c [Å]	17.0193 (17)
α [°]	90.0
β [°]	90.0
γ [°]	90.0
V [nm^3]	4399 (2)
Z	8
Temperature [K]	80
ρ [Mg m^{-3}]	1.258
μ [mm^{-1}]	0.15
F (000)	1776
θ-area [°]	1.4 to 17.3
Total number reflect.	60455
Unique reflections	4415
reflections with $I > 2\sigma(I)$	3482
R_{int}	0.113
Number of restraints	0
Parameters	234
*R*1 [$I>2\sigma(I)$]	0.0444
*wR*2 [$I>2\sigma(I)$]	0.1047
*R*1 [all data]	0.0624
*wR*2 [all data]	0.1137
GooF	1.03
Extinction coefficient	
Largest diff. peak / hole	
max. / min. [10^3·e·nm^{-3}]	0.68 and - 0.40

Table S9. Bond lengths [Å] and bond angle [°] of (cAAC)$SiSCl_2$ (**3**)

Cl1—Si1	2.0904 (11)	C9—C14	1.417 (3)

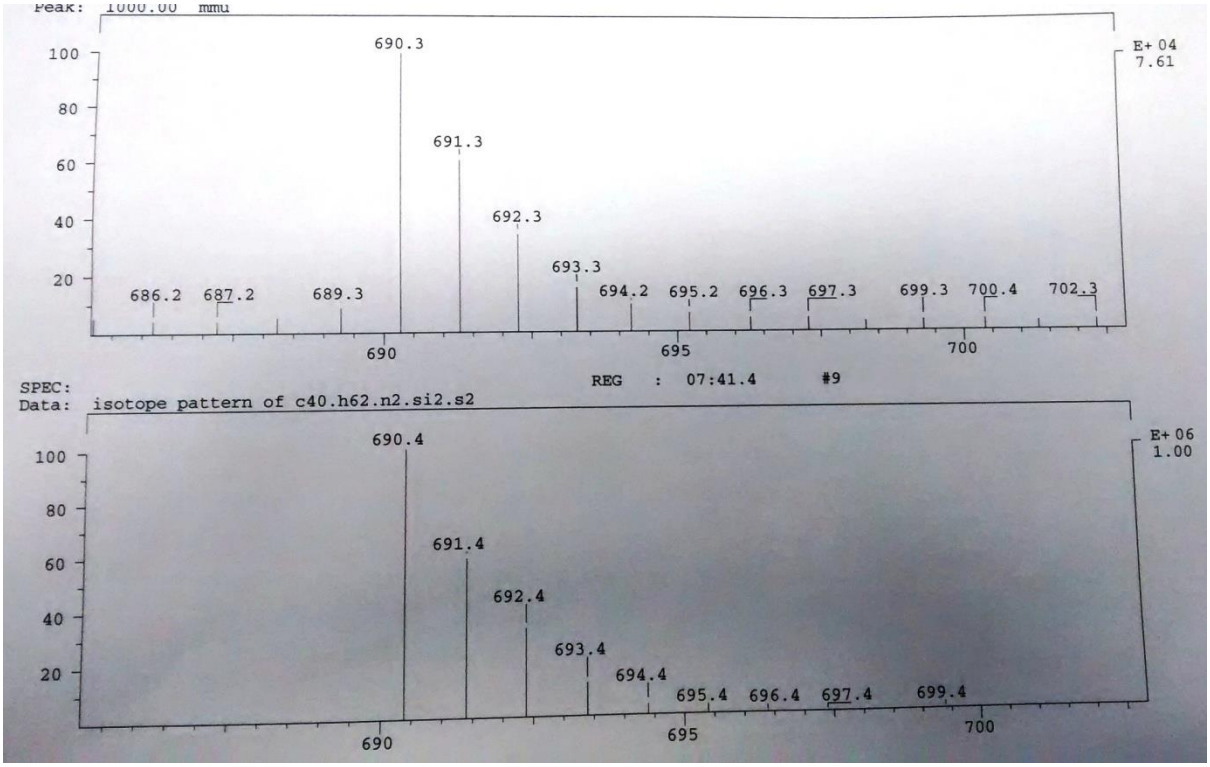
Cl2—Si1	2.0806 (11)	C10—C11	1.399 (3)
S1—Si1	1.9895 (10)	C10—C15	1.528 (3)
Si1—C1	1.936 (3)	C11—C12	1.384 (4)
N1—C1	1.298 (3)	C11—H11	0.9500
N1—C9	1.471 (3)	C12—C13	1.379 (4)
N1—C4	1.553 (3)	C12—H12	0.9500
C1—C2	1.537 (3)	C13—C14	1.395 (4)
C2—C6	1.521 (4)	C13—H13	0.9500
C2—C5	1.542 (4)	C14—C18	1.520 (3)
C2—C3	1.543 (4)	C15—C16	1.534 (4)
C3—C4	1.527 (4)	C15—C17	1.536 (4)
C3—H3A	0.9900	C15—H15	1.0000
C3—H3B	0.9900	C16—H16A	0.9800
C4—C7	1.518 (4)	C16—H16B	0.9800
C4—C8	1.527 (4)	C16—H16C	0.9800
C5—H5A	0.9800	C17—H17A	0.9800
C5—H5B	0.9800	C17—H17B	0.9800
C5—H5C	0.9800	C17—H17C	0.9800
C6—H6A	0.9800	C18—C20	1.535 (4)
C6—H6B	0.9800	C18—C19	1.538 (4)
C6—H6C	0.9800	C18—H18	1.0000
C7—H7A	0.9800	C19—H19A	0.9800
C7—H7B	0.9800	C19—H19B	0.9800
C7—H7C	0.9800	C19—H19C	0.9800

C8—H8A	0.9800	C20—H20A	0.9800
C8—H8B	0.9800	C20—H20B	0.9800
C8—H8C	0.9800	C20—H20C	0.9800
C9—C10	1.404 (3)		
C1—Si1—S1	103.58 (8)	C10—C9—C14	122.3 (2)
C1—Si1—Cl2	104.55 (8)	C10—C9—N1	120.5 (2)
S1—Si1—Cl2	118.79 (5)	C14—C9—N1	117.1 (2)
C1—Si1—Cl1	113.07 (8)	C11—C10—C9	117.4 (2)
S1—Si1—Cl1	115.89 (4)	C11—C10—C15	117.0 (2)
Cl2—Si1—Cl1	100.79 (5)	C9—C10—C15	125.5 (2)
C1—N1—C9	124.1 (2)	C12—C11—C10	121.3 (2)
C1—N1—C4	114.8 (2)	C12—C11—H11	119.3
C9—N1—C4	120.85 (18)	C10—C11—H11	119.3
N1—C1—C2	109.6 (2)	C13—C12—C11	120.2 (2)
N1—C1—Si1	127.60 (18)	C13—C12—H12	119.9
C2—C1—Si1	122.05 (18)	C11—C12—H12	119.9
C6—C2—C1	116.4 (2)	C12—C13—C14	121.6 (2)
C6—C2—C5	108.1 (2)	C12—C13—H13	119.2
C1—C2—C5	107.2 (2)	C14—C13—H13	119.2
C6—C2—C3	110.2 (2)	C13—C14—C9	117.1 (2)
C1—C2—C3	102.3 (2)	C13—C14—C18	118.3 (2)
C5—C2—C3	112.7 (2)	C9—C14—C18	124.5 (2)
C4—C3—C2	107.3 (2)	C10—C15—C16	110.7 (2)
C4—C3—H3A	110.2	C10—C15—C17	111.6 (2)

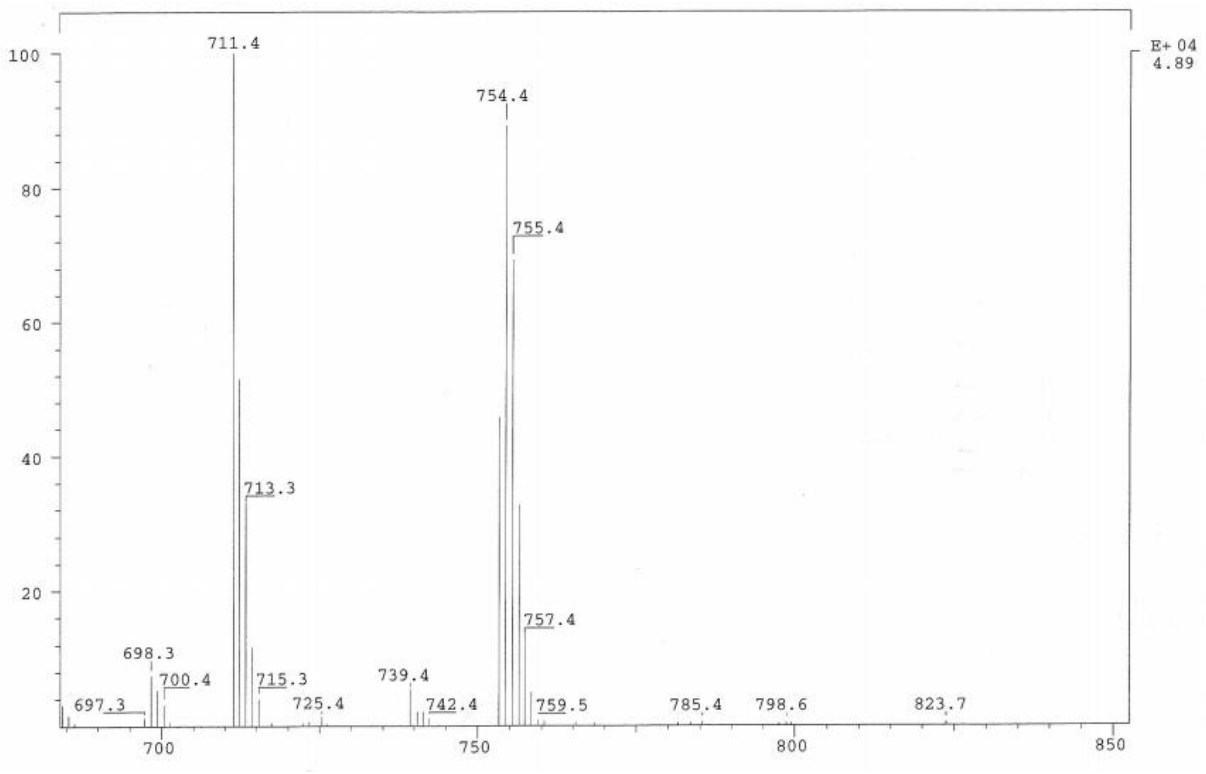
C2—C3—H3A	110.2	C16—C15—C17	108.3 (2)
C4—C3—H3B	110.2	C10—C15—H15	108.7
C2—C3—H3B	110.2	C16—C15—H15	108.7
H3A—C3—H3B	108.5	C17—C15—H15	108.7
C7—C4—C3	114.9 (2)	C15—C16—H16A	109.5
C7—C4—C8	107.9 (2)	C15—C16—H16B	109.5
C3—C4—C8	110.7 (2)	H16A—C16—H16B	109.5
C7—C4—N1	112.1 (2)	C15—C16—H16C	109.5
C3—C4—N1	100.36 (19)	H16A—C16—H16C	109.5
C8—C4—N1	110.73 (19)	H16B—C16—H16C	109.5
C2—C5—H5A	109.5	C15—C17—H17A	109.5
C2—C5—H5B	109.5	C15—C17—H17B	109.5
H5A—C5—H5B	109.5	H17A—C17—H17B	109.5
C2—C5—H5C	109.5	C15—C17—H17C	109.5
H5A—C5—H5C	109.5	H17A—C17—H17C	109.5
H5B—C5—H5C	109.5	H17B—C17—H17C	109.5
C2—C6—H6A	109.5	C14—C18—C20	111.4 (2)
C2—C6—H6B	109.5	C14—C18—C19	111.4 (2)
H6A—C6—H6B	109.5	C20—C18—C19	110.0 (2)
C2—C6—H6C	109.5	C14—C18—H18	108.0
H6A—C6—H6C	109.5	C20—C18—H18	108.0
H6B—C6—H6C	109.5	C19—C18—H18	108.0
C4—C7—H7A	109.5	C18—C19—H19A	109.5
C4—C7—H7B	109.5	C18—C19—H19B	109.5

H7A—C7—H7B	109.5	H19A—C19—H19B	109.5
C4—C7—H7C	109.5	C18—C19—H19C	109.5
H7A—C7—H7C	109.5	H19A—C19—H19C	109.5
H7B—C7—H7C	109.5	H19B—C19—H19C	109.5
C4—C8—H8A	109.5	C18—C20—H20A	109.5
C4—C8—H8B	109.5	C18—C20—H20B	109.5
H8A—C8—H8B	109.5	H20A—C20—H20B	109.5
C4—C8—H8C	109.5	C18—C20—H20C	109.5
H8A—C8—H8C	109.5	H20A—C20—H20C	109.5
H8B—C8—H8C	109.5	H20B—C20—H20C	109.5

4. EI mass spectra of byproducts:



For $(cAAC)_2Si_2S_2$ (top, experimental; bottom, simulated isotope pattern)



For $(cAAC)_2Si_2S_4$

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