Supporting Information

$Sn_{20}(Si^tBu_3)_{10}Cl_2$ – the largest metalloid group 14 cluster shows a raspberry-like arrangement of smaller units

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Content

1. Experimental section and crystal structure analysis

All reactions were carried out under rigorous exclusion of air and moisture using Schlenk techniques under standard nitrogen atmosphere. All solvents were dried and purified by standard procedures. Toluene was pre-dried with sodium and pentane was dried with CaH_2. All organic solvents were purified via distillation. EDX analysis was performed using solid samples at a HITACHI SU8030 scanning electron microscope with Bruker-EDX.

20 ml of a −78°C cold 0.2 M solution of Sn(I)Cl in toluene / PBu_3 (volume ratio 10:1; 4 mmol) was given to the −78°C precooled solid $NaSi^tBu_3$ (888 mg, 4 mmol). The dark red reaction mixture was slowly warmed up to room temperature while stirring, leading to a dark brown solution. The solution was filtered from the white precipitate and the solvent removed in vacuo to give a black oily residue. The residue was extracted by pentane and 15-Krone-5 (0.2 mL) was added. After few weeks at 6 °C black crystalline blocks of $[Sn_{20}(Si^tBu_3)_{10}Cl_2]$ were obtained from the black colored pentane extract.

The obtained single crystals (black blocks) are very sensitive and rapidly lose solvent molecules. Hence, the single crystal quality decreases rapidly when taken out of the mother liquor into mineral oil for selection and preparation of the single crystals for x-ray measurements. The elemental composition of the crystals was verified via EDX measurements (figure S2 and table S3). Single crystals of **1** only dissolve in C_6D_6 or THF-d_8 under decomposition to give a dark yellow solution, whereby the decomposition products tBu_3SiH, $(tBu_3Si)_2$ and further unknown compounds are observable within the proton NMR spectrum (see figure S3 and S4 in the supporting information).

Single crystals of **1** were taken directly from the mother liquor and selected in a drop of mineral oil under a light microscope. Due to rapid loss of solvent molecules, which can be observed under the microscope as rapidly loss of color and shape, one had to be quite fast

during the preparation process. After a few trials, a black block could be identified as suitable for X-ray structural analysis and was mounted on a Bruker APEXII diffractometer. The crystal was kept at 150.0 K during data collection. Using Olex2,[1] the structure was solved with the ShelXS[2] structure solution program using Direct Methods and refined with the ShelXL[3] refinement package using Least Squares minimisation. Using the implemented RLATT program, two crystal domains could be identified, which were integrated separately. The structure of the twin was refined using HKLF5 with a batch scaling factor of 0.4774.

Due to these twinning problems, a satisfying model for the co crystallized solvent molecules could not be found. Therefore the SQUEEZE program[4]was used to identify solvent accessible voids and solvent electrons therein.

Table S1 : Results of the SQUEEZE program

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	0.000	0.000	803	143	toluene
2	0.500	0.500	0.500	803	143	toluene

This fits to 3 toluene molecules per void, which are underoccupied in the large void and thus the toluene molecules cannot be refined properly.

Table S2 : Crystal data for **1**

Empirical formula	$C_{120}H_{270}Cl_2Si_{10}Sn_{20}$
Formula weight	4438.94
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	19.176(4)
b/Å	23.573(5)
c/Å	20.419(4)
α/°	90
β/°	92.820(4)
γ/°	90
Volume/Å^3	9219(3)
Z	2
ρ_{calc}g/cm^3	1.599
μ/mm^{-1}	2.781
F(000)	4328.0
Crystal size/mm^3	0.108 × 0.091 × 0.068
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.988 to 48.998
Index ranges	$-22 \leq h \leq 22$, $0 \leq k \leq 27$, $0 \leq l \leq 23$
Reflections collected	37661
Independent reflections	37661 [R_{int} = 0.0615, R_{sigma} = 0.1393]
Data/restraints/parameters	37661/30/731
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0708, wR_2 = 0.1513
Final R indexes [all data]	R_1 = 0.1368, wR_2 = 0.1901
Largest diff. peak/hole / e Å^{-3}	1.95/-1.31
CCDC	1911644

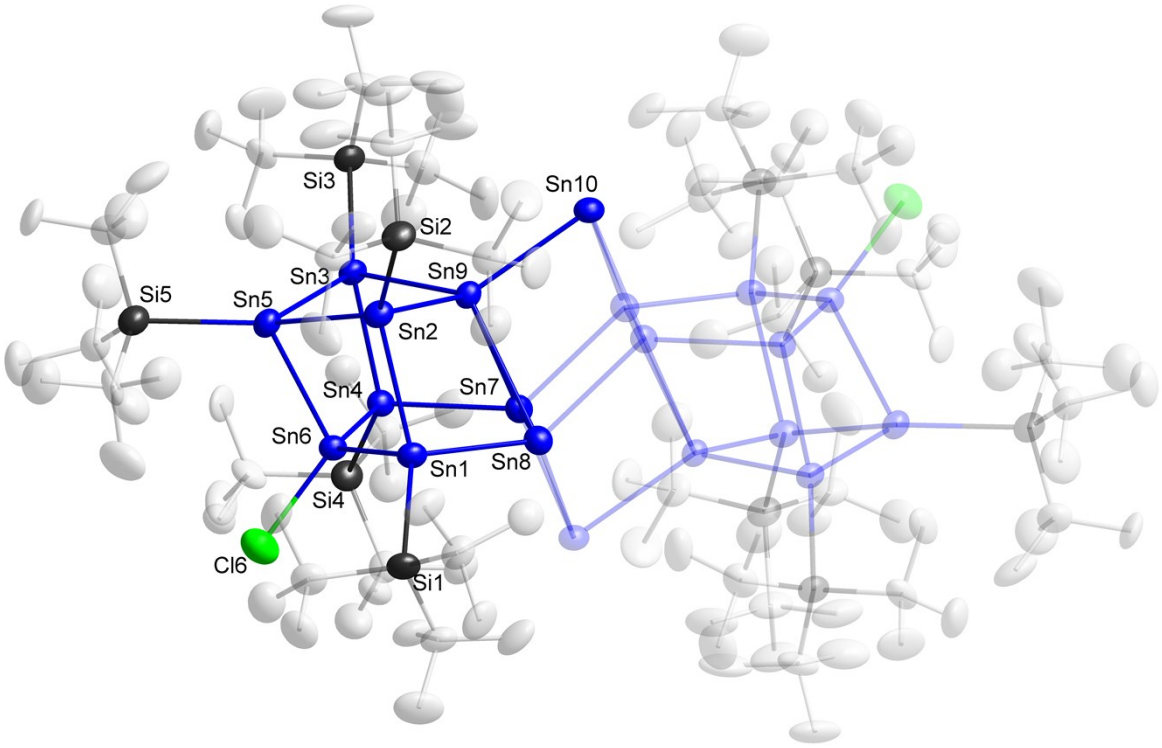
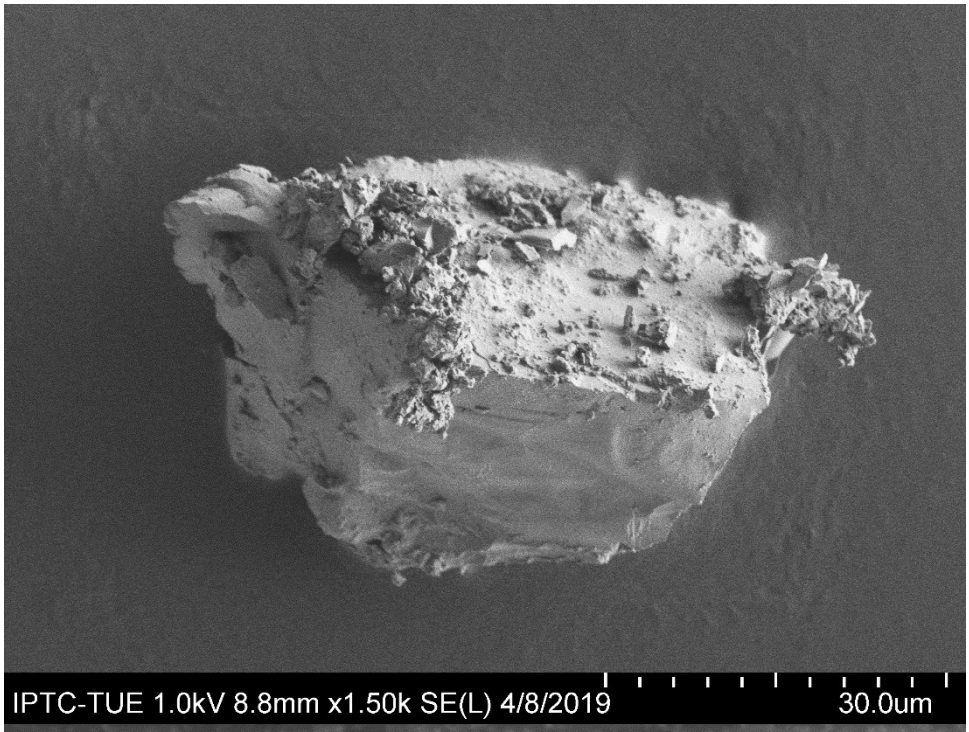
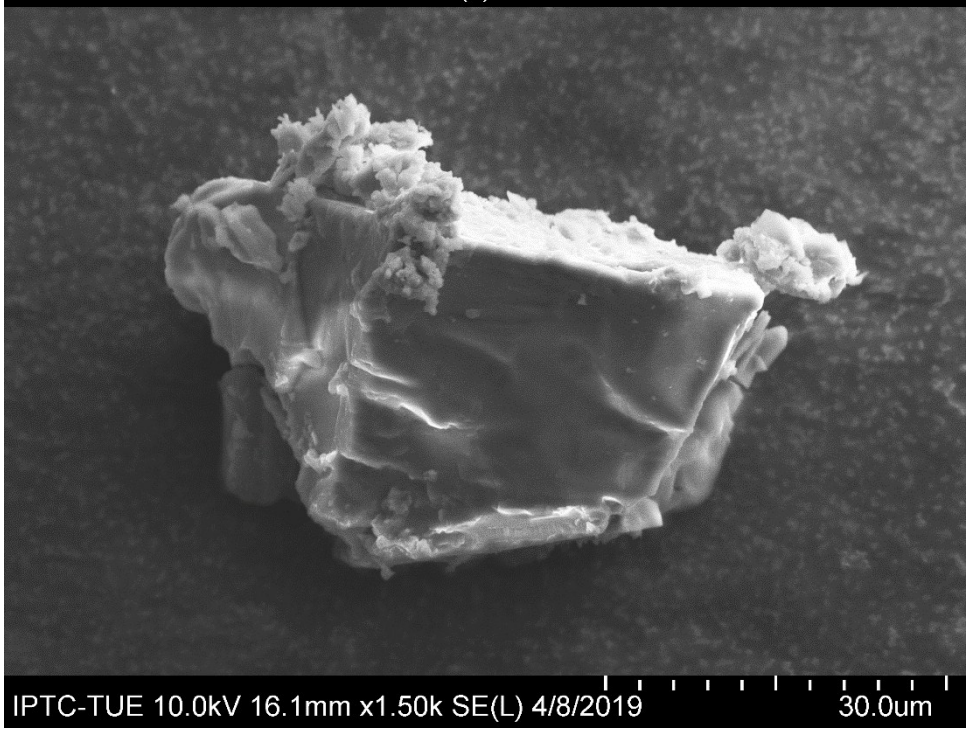


Figure S1 : Presentation of the asymmetrical unit of **1** in the molecular structure (shown with 70% transparency)

2. EDX

The EDX measurements were performed at 9 different areas. Device: HITACHI SU8030 scanning electron microscope with Bruker-EDX.





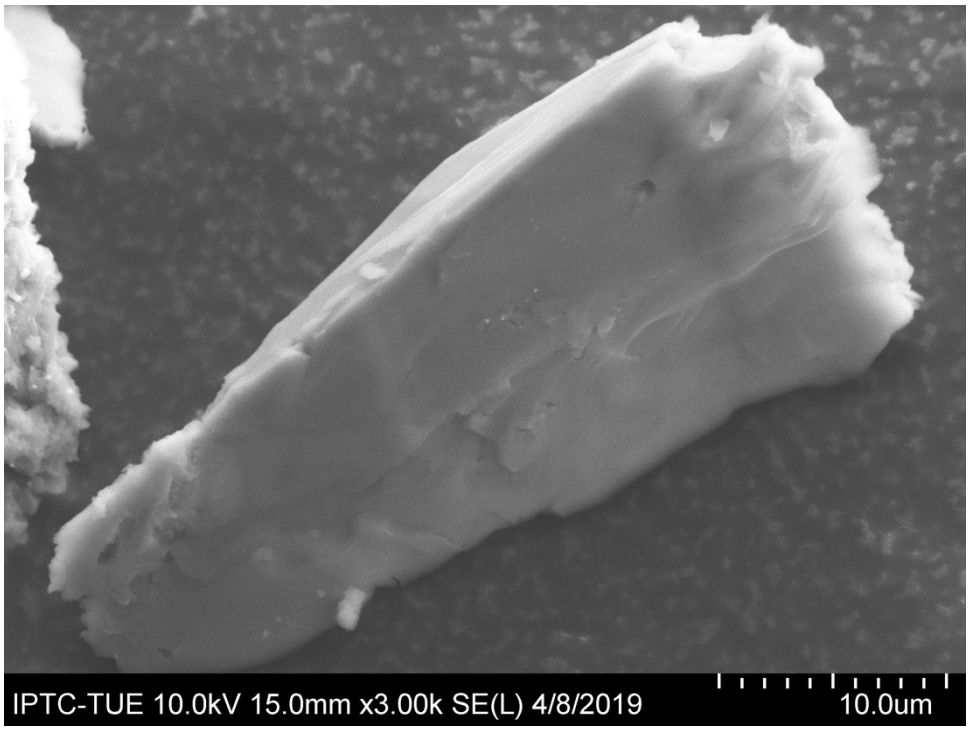


Figure S2**:** SEM-Images of a single crystal of **1** consisting of layers.

Table S3: Results of the EDX measurements of the crystallite at 9 different points:

Element	**Atom % calculated**	**Atoms calculated**	**Setpoint**
Sn	60.55	19.38	20
Si	32.33	10.34	10
Cl	7.12	2.28	2

3. NMR- and IR-Spectroscopy

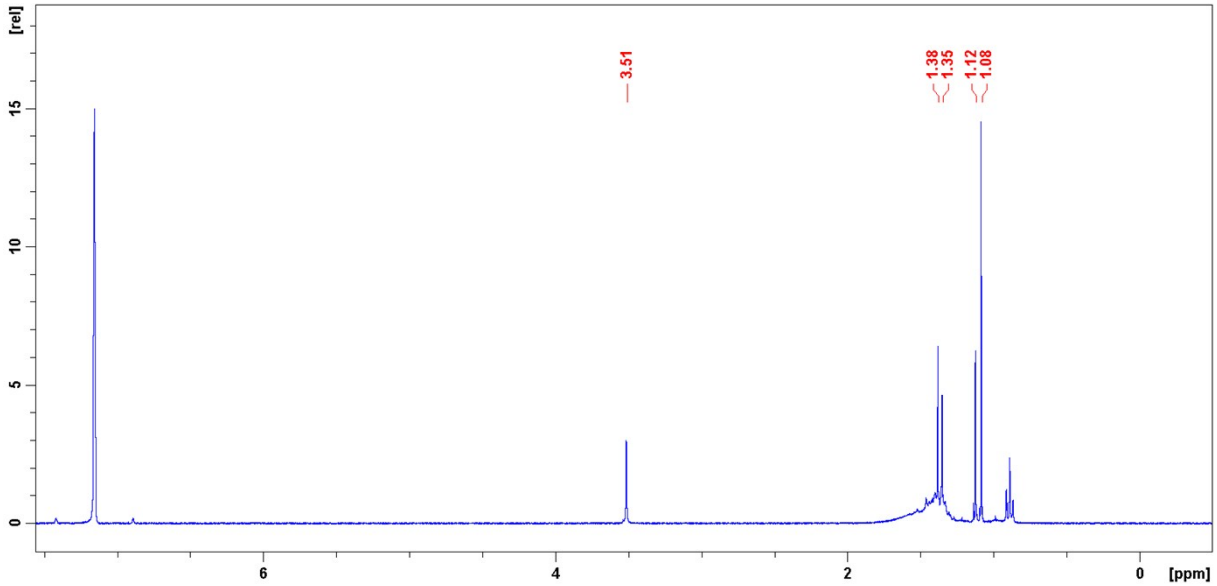


Figure S3: ^{1}H-NMR-spectrum of single crystal of **1** dissolved in C_6D_6 showing a decomposition of **1** to tBu$_3$SiH, (tBu$_3$Si)$_2$ and other unknown compounds in solution.

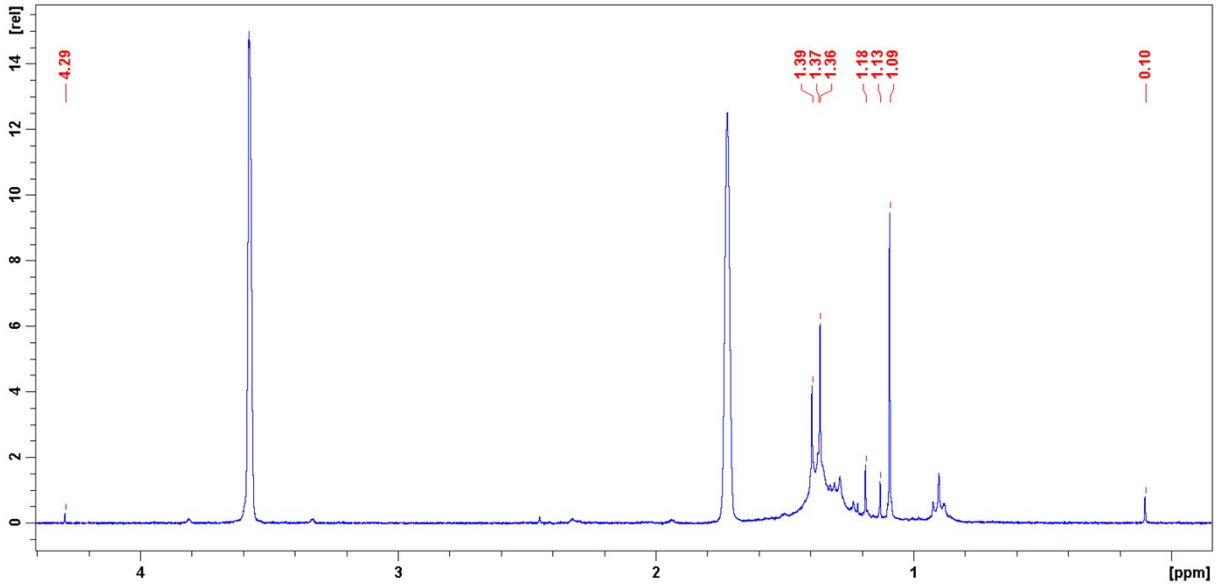


Figure S4: ^{1}H-NMR-spectrum of single crystal of **1** dissolved in THF-d_8 showing a decomposition of **1** to tBu$_3$SiH, (tBu$_3$Si)$_2$ and other unknown compounds in solution.

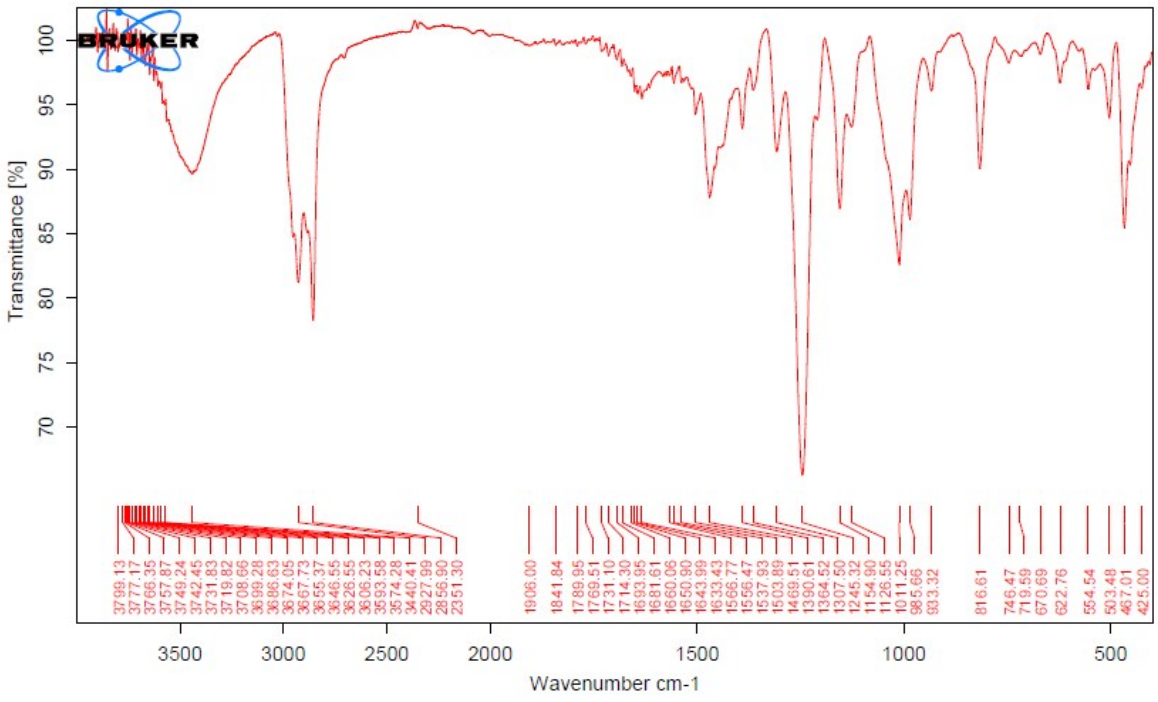


Figure S5**:** measured IR-spectrum of **1**

4. Quantum chemical calculations

Quantum-chemical calculations were carried out with the dispersion corrected RI-DFT-D3 version of the Turbomole program package by employing the BP86-functional. The basis sets were of TZVPP quality.[5]

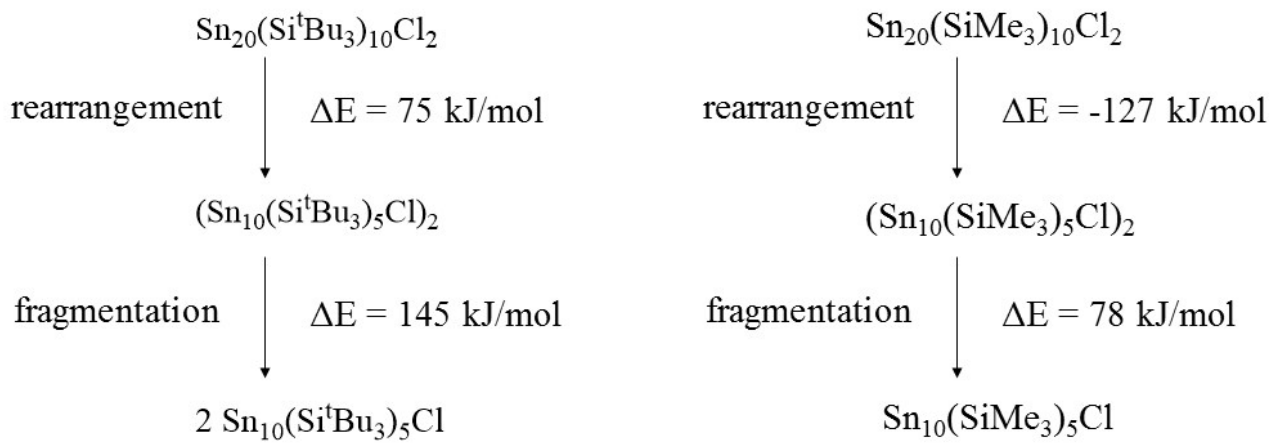


Figure S6: Energetic view on the calculated fragmentation mechanism for compound **1** and the model compound $Sn_{20}(SiMe_3)_{10}Cl_2$

All calculated structures were optimized and vibrational analyzed as an energetic minimal arrangement.

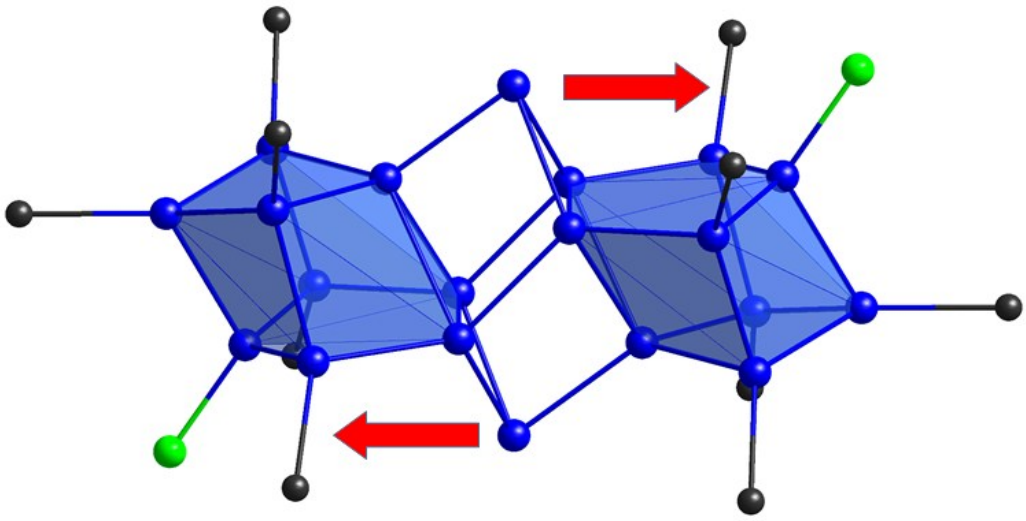


Figure S7: Postulated rearrangement process

Alternative reaction pathway:

$$Sn_{20}(Si^tBu_3)_{10}Cl_2 \xrightarrow{\Delta E = 791\ kJ/mol} Sn_8 + 2\ Sn_6(Si^tBu_3)_5Cl$$

Figure S8: Energetics of the direct dissociation of **1** into the subunits $Sn_6(SitBu_3)_5Cl$ and Sn_8 which might be seen as another alternative dissociation pathway. However, this pathway is strongly endothermic by 791 kJ/mol and thus much less probable

4.1 $Sn_{20}(Si^tBu_3)_{10}Cl_2$

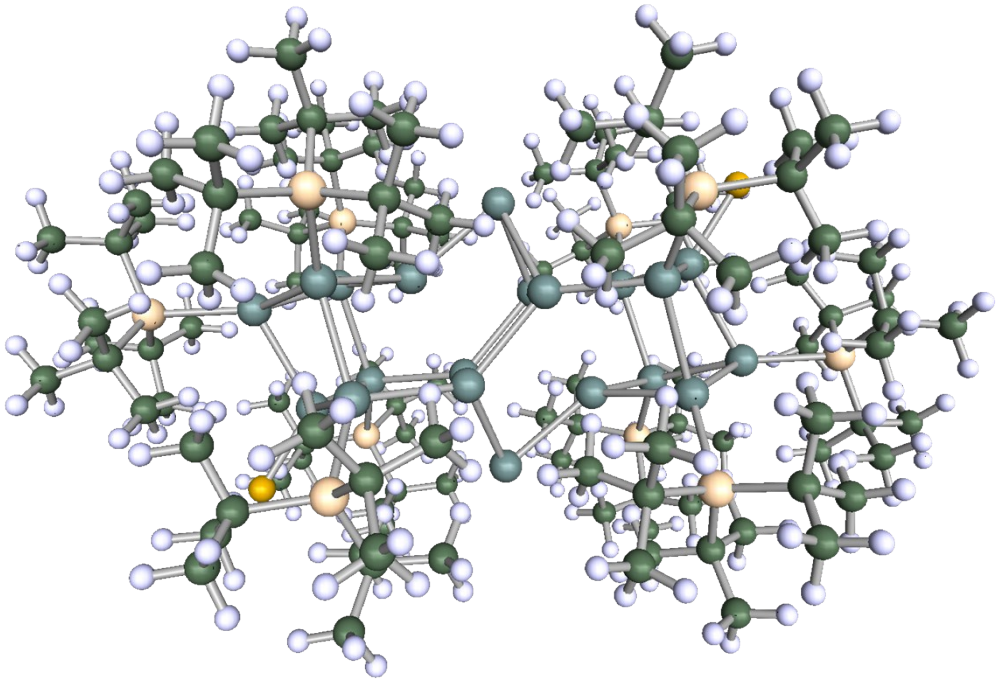


Figure S9: Optimized structure of $Sn_{20}(Si^tBu_3)_{10}Cl_2$

Point group used: C_1

Total energy: -8623.33395889009 Hartree

HOMO-LUMO-gap: 1.194 eV

XYZ positions of all atoms in $Sn_{20}(Si^tBu_3)_{10}Cl_2$

```
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Sn 4.128830 -1.804033 -2.382827
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Si 6.270181 2.558740 -0.526340
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4.2 $(Sn_{10}(Si^tBu_3)_5Cl)_2$

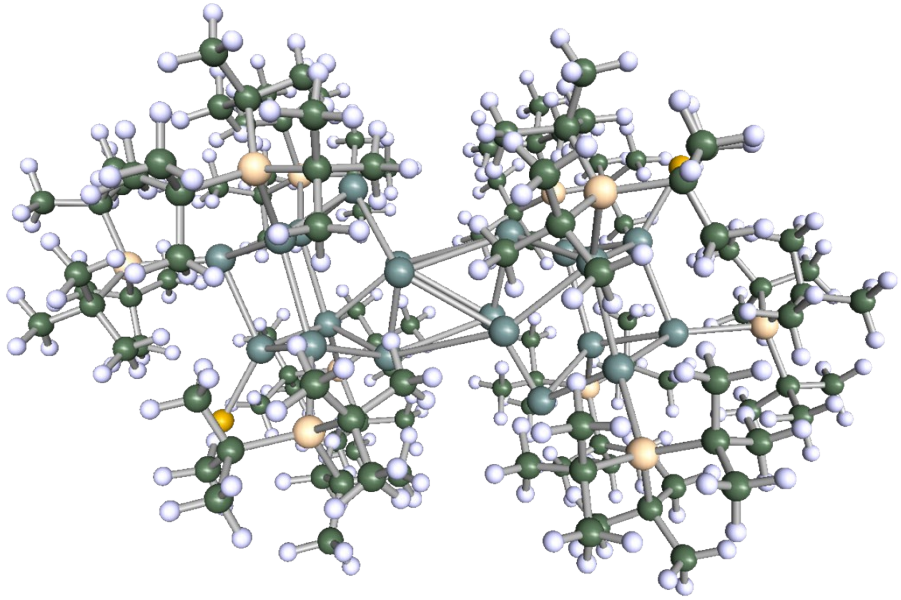

Figure S10: Optimized structure of $(Sn_{10}(Si^tBu_3)_5Cl)_2$

Point group used: C_1

Total energy: -8623.30519171019 Hartree

HOMO-LUMO-gap: 0.842 eV

XYZ positions of all atoms in $(Sn_{10}(Si^tBu_3)_5Cl)_2$

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Sn 4.254024 -1.910871 -2.931514
Sn 3.623870 1.508778 -5.047392
Sn 2.072816 -0.376977 -0.796124
Si 6.158897 2.844196 -1.015281
Sn 3.974680 -1.257454 -5.930862
Sn 1.349698 -2.676622 -2.744244
Si 5.722544 -3.980553 -1.753285
Sn 0.695475 1.515156 -5.188231
Cl 4.717000 3.430018 -6.171829
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Sn 0.369896 0.090843 2.696794
Sn 1.535361 2.247240 -2.253516
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C 5.262922 4.602991 -0.892653
C 6.538739 2.081211 0.768879
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H 4.256289 1.496430 6.022475
H 3.468319 1.612644 7.604635
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4.3 $Sn_{10}(Si^tBu_3)_5Cl$

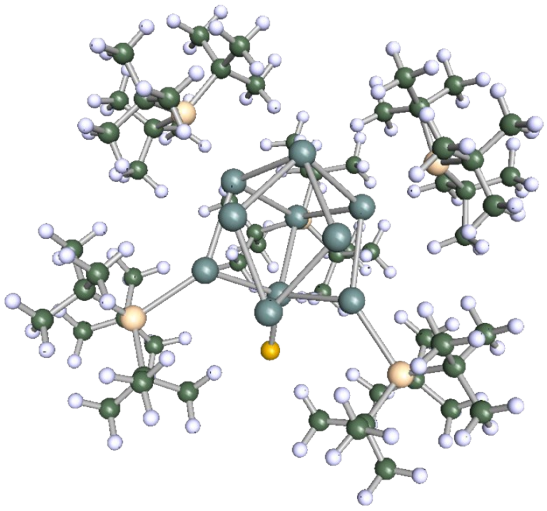

Figure S11: Optimized structure of $Sn_{10}(Si^tBu_3)_5Cl$

Point group used: C_1

Total energy: -4311.16961962133 Hartree

HOMO-LUMO-gap: 1.441 eV

XYZ positions of all atoms in $Sn_{10}(Si^tBu_3)_5Cl$

Sn 0.542109 0.084346 2.009459
Sn -1.339029 -2.255739 1.553477
Sn -1.953109 0.389016 0.184259
Sn -0.429378 -1.580530 4.474154
Sn -1.149028 2.665573 2.106579
Sn -4.253383 -1.123535 1.671056
Sn -0.618778 1.475717 4.819168
Sn -3.358185 -1.562602 4.425087
Si 0.976045 -3.722076 5.502240
Sn -4.048353 1.882832 2.313680
Si -5.955472 -2.886542 0.403204
Sn -3.664551 1.209736 5.300405
Si 1.273231 3.144275 6.050104
H 2.295146 2.086686 3.279829
Cl -4.420434 -3.491727 5.563962
C 2.896365 -3.276685 5.343106
C 0.390087 -3.868231 7.387178
C 0.503230 -5.333473 4.456086
Si -5.514680 3.956381 1.132802
C -7.589622 -2.921631 1.519630
C -5.076205 -4.657554 0.330759
C -6.291031 -2.154793 -1.403232
Si -5.308714 1.523412 7.548060
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C 1.332170 2.641602 7.964656
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C 1.189888 -5.326653 3.075792
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C -3.969368 -4.690117 -0.741820
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C -6.098880 -5.767090 -0.005554
C -6.940070 -3.198718 -2.338835
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C 1.347405 1.107853 8.111951
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4.4 Model compound $Sn_{20}(SiMe_3)_{10}Cl_2$

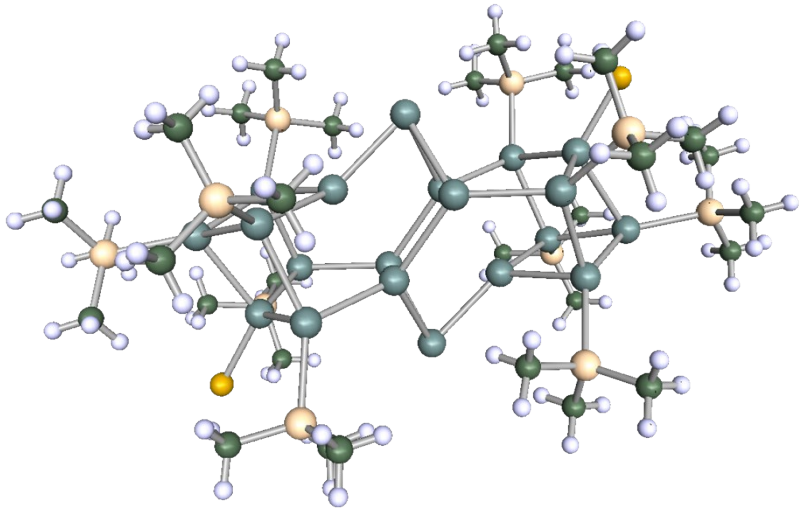

Figure S12: Optimized structure of $Sn_{20}(SiMe_3)_{10}Cl_2$

Point group used: C_i

Total energy: -5083.58207024395 Hartree

HOMO-LUMO-gap: 0.918 eV

XYZ positions of all atoms

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Si 6.296325 2.693394 -1.778800
Sn 3.599021 -1.031583 -5.165551
Sn 1.178316 -1.723425 -1.965582
Si 5.008954 -3.482116 -0.800453
Sn 0.008678 1.238846 -4.435683
Cl 3.749926 3.561655 -5.261541
Sn -0.476152 0.899461 -1.608885
Sn 0.041469 3.484680 -0.082655
Sn 0.742931 -1.562757 -4.891859
Si 5.293043 -0.890648 -7.169270
Si -0.732633 3.452806 -5.644513
Si -0.697323 -2.773128 -6.733312
Sn -4.192096 -1.139416 1.511699
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Sn -2.856655 -1.591502 4.071444
Sn -1.982978 -1.355157 -0.317716
Sn -3.599021 1.031583 5.165551
Sn -1.178316 1.723425 1.965582
Sn -0.008678 -1.238846 4.435683
Cl -3.749926 -3.561655 5.261541
Sn 0.476152 -0.899461 1.608885
Sn -0.041469 -3.484680 0.082655
Sn -0.742931 1.562757 4.891859
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C 5.704421 4.486581 -1.868053
C 7.547986 2.462782 -0.375384
C 0.173663 3.559944 -7.302036
C -2.609293 3.544072 -5.885309
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C 5.303799 -2.457703 -8.234355
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H 6.563102 5.158821 -2.019346
H 5.187436 4.792164 -0.948603
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H 7.985870 2.785150 -3.615505
H 7.336918 1.133701 -3.459211
H 6.368243 2.404929 -4.256691
H 3.741134 0.442111 -8.626077
H 5.444204 0.774568 -9.023889
H 4.700399 1.509518 -7.577944
H 7.353879 -1.408172 -5.827034
H 7.745774 -0.447250 -7.275026
H 7.029133 0.340461 -5.848974
H 6.002776 -2.336315 -9.076328
H 4.307352 -2.664218 -8.647561
H 5.620030 -3.334081 -7.652635
H 7.186665 -4.020642 -1.928959
H 7.412494 -2.772944 -0.682332
H 7.220588 -4.478414 -0.209176
H 3.034889 -4.985263 -1.116669
H 4.438003 -5.896270 -0.509279
H 4.345851 -5.443693 -2.229629
H 4.817620 -3.696160 1.683367
H 5.002225 -1.983788 1.221850
H 3.432689 -2.794236 1.019447
C -0.079247 -4.545188 -7.002276
C -2.507812 -2.805903 -6.171697
C -0.554803 -1.797091 -8.353547
H -3.134490 -3.287154 -6.938140
H -2.890132 -1.789169 -6.007303
H -2.622717 -3.367552 -5.234845
H -0.677920 -5.040060 -7.782339
H 0.971594 -4.554370 -7.321531
H -0.160495 -5.139975 -6.082509
H -0.901368 -0.763147 -8.221696
H 0.484039 -1.764546 -8.708819
H -1.169573 -2.267914 -9.136206
Si -6.296325 -2.693394 1.778800
Si -5.008954 3.482116 0.800453
Si -5.293043 0.890648 7.169270
Si 0.732633 -3.452806 5.644513
Si 0.697323 2.773128 6.733312
C -7.071016 -2.199209 3.436646
C -5.704421 -4.486581 1.868053
C -7.547986 -2.462782 0.375384
C -0.173663 -3.559944 7.302036
C 2.609293 -3.544072 5.885309
C 0.137425 -4.839058 4.502649
C -4.739542 -0.601249 8.195888
C -5.303799 2.457703 8.234355
C -7.019171 0.573521 6.457563
C -4.521897 2.932701 -0.947562
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H 3.134387 -3.461480 4.924294
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H -0.959592 -4.829002 4.437461
H 0.450233 -5.816762 4.900563
H 0.544105 -4.734909 3.486980
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H 0.072409 -4.508036 7.805026
H 0.100128 -2.735846 7.974288
H -5.016167 -4.613182 2.715259
H -6.563102 -5.158821 2.019346
H -5.187436 -4.792164 0.948603
H -8.425734 -3.104742 0.547132
H -7.113238 -2.733689 -0.596193
H -7.893649 -1.421897 0.317315
H -7.985870 -2.785150 3.615505
H -7.336918 -1.133701 3.459211
H -6.368243 -2.404929 4.256691
H -3.741134 -0.442111 8.626077
H -5.444204 -0.774568 9.023889
H -4.700399 -1.509518 7.577944
H -7.353879 1.408172 5.827034
H -7.745774 0.447250 7.275026
H -7.029133 -0.340461 5.848974
H -6.002776 2.336315 9.076328
H -4.307352 2.664218 8.647561
H -5.620030 3.334081 7.652635
H -7.186665 4.020642 1.928959
H -7.412494 2.772944 0.682332
H -7.220588 4.478414 0.209176
H -3.034889 4.985263 1.116669
H -4.438003 5.896270 0.509279
H -4.345851 5.443693 2.229629
H -4.817620 3.696160 -1.683367
H -5.002225 1.983788 -1.221850
H -3.432689 2.794236 -1.019447
C 0.079247 4.545188 7.002276
C 2.507812 2.805903 6.171697
C 0.554803 1.797091 8.353547
H 3.134490 3.287154 6.938140
H 2.890132 1.789169 6.007303
H 2.622717 3.367552 5.234845
H 0.677920 5.040060 7.782339
H -0.971594 4.554370 7.321531
H 0.160495 5.139975 6.082509
H 0.901368 0.763147 8.221696
H -0.484039 1.764546 8.708819
H 1.169573 2.267914 9.136206
```

4.5 Model compound $(Sn_{10}(SiMe_3)_5Cl)_2$

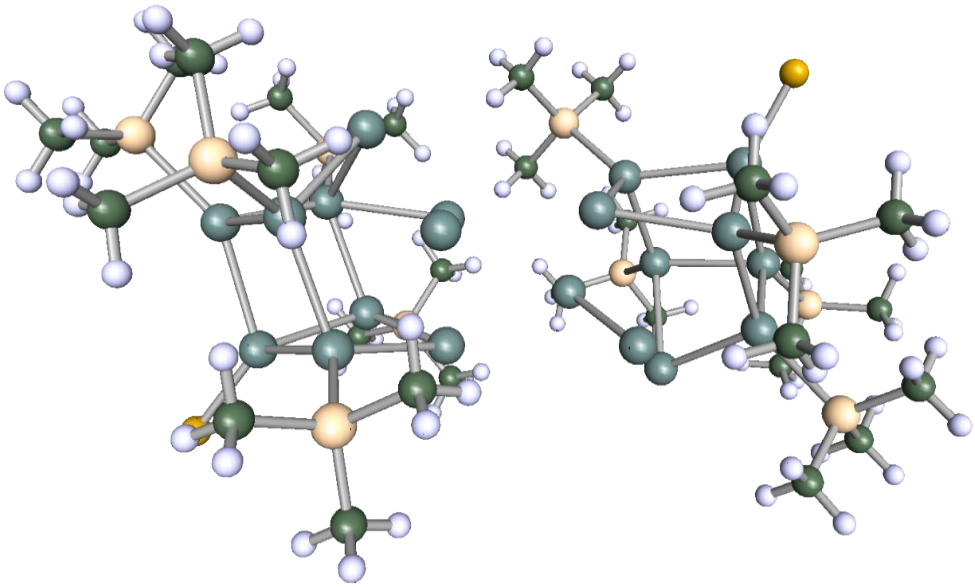

Figure S13: Optimized structure of $(Sn_{10}(SiMe_3)_5Cl)_2$

Point group used: C_1

Total energy: -5083.63069771691 Hartree

HOMO-LUMO-gap: 1.502 eV

XYZ positions of all atoms

```
Sn 4.752185 0.727112 -1.864173
Sn 4.713065 -1.843548 -3.226661
Sn 3.688182 1.911146 -4.376321
Sn 3.111333 -1.810834 -0.546634
Si 6.961012 0.895677 -0.446963
Sn 3.539467 -0.819006 -5.659759
Sn 2.004257 -3.264440 -3.095190
Si 6.747196 -3.496456 -3.210688
Sn 0.970333 1.634938 -3.184978
Cl 4.550381 4.045574 -5.263108
Sn 0.278276 -1.132982 -1.597569
Sn 0.621859 1.185262 2.928983
Sn 2.152547 1.228509 -0.464879
Sn 0.839571 -0.891805 -4.643031
Si 3.781649 -2.367854 -7.786429
Sn -0.384946 -1.716204 2.084447
Si -1.276745 2.964060 -3.532435
Sn -1.542903 0.960331 0.733635
Sn -0.627616 -1.100320 4.999632
Sn -1.717299 3.266256 2.824161
Si -1.265963 -1.676416 -5.990924
Sn -3.363730 -1.378943 1.984870
Sn -1.288740 1.698938 5.405833
Sn -3.570266 -1.596535 4.962483
Si 1.388257 -1.784608 6.546237
Sn -4.133612 1.421998 2.337643
Si -4.451978 -2.393336 -0.188483
Sn -4.147204 1.343901 5.219657
Si -0.268927 3.066645 7.392997
Cl -4.711116 -3.460398 6.106847
Si -5.938141 2.514590 0.784020
Si -5.442315 3.374004 6.302571
C -7.317636 3.156181 6.148579
C -4.946876 3.536038 8.124661
C -4.895891 4.925351 5.361076
C -0.900293 2.377646 9.042184
C -0.829483 4.869269 7.215168
C 1.621732 2.965092 7.324434
C 6.751159 2.207709 0.901882
C 8.415575 1.343750 -1.574408
C 7.266328 -0.796052 0.351638
C 1.583098 -3.668323 6.553562
C 2.949693 -0.977170 5.837050
C 1.107905 -1.162535 8.314604
C -6.707611 3.987382 1.697132
C -5.085975 3.111532 -0.798217
C -7.284853 1.251243 0.356840
C 8.378504 -2.538449 -3.327497
C 6.570244 -4.644924 -4.708920
C 6.702689 -4.515536 -1.615904
C -4.360579 -1.068262 -1.538334
C -6.250886 -2.901181 0.115376
C -3.419927 -3.877553 -0.751997
C -1.877286 -0.298146 -7.139082
C -0.775132 -3.193657 -7.015912
C -2.622534 -2.161868 -4.761755
C 3.254832 -4.111251 -7.264764
C 5.571274 -2.394096 -8.408236
C 2.639780 -1.724022 -9.155800
C -2.703257 1.722966 -3.489684
C -1.511112 4.242712 -2.157343
C -1.223362 3.812015 -5.225880
H -2.159932 4.363737 -5.400353
H -0.389125 4.522688 -5.296561
H -1.106712 3.073022 -6.030620
H -3.664513 2.235846 -3.644514
H -2.739266 1.211699 -2.519008
H -2.589022 0.960590 -4.270779
H -2.458486 4.782616 -2.307926
H -1.550527 3.752699 -1.174255
H -0.694534 4.976680 -2.141324
H 2.219807 -4.117172 -6.898493
H 3.899935 -4.492192 -6.461490
H 3.324785 -4.800700 -8.120448
H 1.604285 -1.633261 -8.800599
H 2.646835 -2.412611 -10.014523
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H 5.660665 -3.071224 -9.271415
H 5.900133 -1.394632 -8.723004
H 6.259420 -2.747362 -7.628383
H 6.568292 3.199827 0.467607
H 7.661049 2.267137 1.518549
H 5.906205 1.963965 1.559906
H 9.348094 1.384841 -0.990838
H 8.543324 0.598884 -2.371313
H 8.265295 2.323528 -2.047563
H 6.430112 -1.081592 1.004052
H 7.377438 -1.577653 -0.411634
H 8.186334 -0.773641 0.955471
H 7.409237 -5.356302 -4.749667
H 5.636322 -5.220243 -4.651071
H 6.560195 -4.076708 -5.648801
H 6.767993 -3.873290 -0.727538
H 7.545695 -5.223052 -1.589955
H 5.769196 -5.090414 -1.546511
H 9.227169 -3.238904 -3.358808
H 8.413266 -1.919913 -4.234449
H 8.516866 -1.877761 -2.461579
H -0.416659 -4.002708 -6.364337
H 0.022449 -2.957335 -7.732269
H -1.641711 -3.568967 -7.581457
H -2.942418 -1.302414 -4.159579
H -2.269934 -2.939244 -4.070445
H -3.501797 -2.550529 -5.298138
H -2.767055 -0.630183 -7.695781
H -1.103059 -0.021988 -7.867907
H -2.146672 0.605127 -6.575057
H 1.945936 -1.463973 8.961858
H 1.040344 -0.066870 8.335584
H 0.181506 -1.568696 8.741837
H 0.689991 -4.160626 6.961122
H 1.749743 -4.052733 5.538208
H 2.445621 -3.955634 7.174344
H 2.854906 0.117039 5.818945
H 3.824435 -1.238015 6.452431
H 3.137877 -1.314721 4.808918
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H -5.814235 3.590447 -1.470718
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H -6.856590 -2.041975 0.433943
H -6.322316 -3.672229 0.894346
H -6.690308 -3.306583 -0.808808
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H -1.925370 4.947960 7.245675
H -0.422358 5.481377 8.034500
H 2.002454 3.361261 6.373402
H 1.966926 1.926587 7.417333
H 2.068347 3.547617 8.144578
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H -7.665608 2.264020 6.686344
H -7.836187 4.032190 6.567413
H -7.616568 3.056131 5.096179
H -5.215204 2.639735 8.699865
H -3.863231 3.689423 8.220042
H -5.453496 4.400184 8.580761

4.6 Model compound $Sn_{10}(SiMe_3)_5Cl$

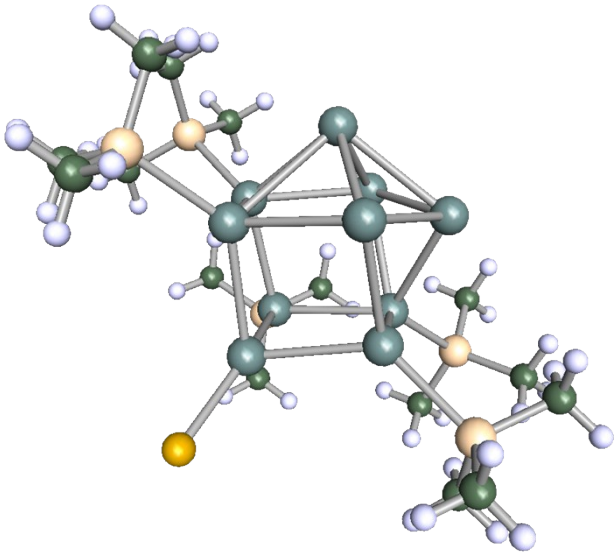

Figure S14: Optimized structure of $Sn_{10}(SiMe_3)_5Cl$

Point group used: C_1

Total energy: -2541.80033551352 Hartree

HOMO-LUMO-gap: 2.121 eV

XYZ positions of all atoms

Sn 0.375076 0.444520 2.134945
Sn -1.004712 -2.204229 1.041692
Sn -2.155229 0.682791 0.357239
Sn -0.570078 -2.057849 4.009834
Sn -1.762022 2.635111 2.778512
Sn -3.901595 -1.748900 1.683837
Sn -0.852654 0.676909 4.967934
Sn -3.476795 -2.342271 4.557302
Si 1.598819 -3.033347 5.135999
Sn -4.352066 1.008957 2.503264
Si -5.881391 -2.368828 0.067837
Sn -3.715462 0.623451 5.289288
Si 0.786405 1.826331 6.663208
Cl -4.361643 -4.459764 5.472082
Si -6.364857 2.534129 1.794136
Si -4.619391 2.590755 6.815932
C -5.758626 4.327183 1.721900
C -7.033672 2.040990 0.093006
C -7.725802 2.357581 3.102602
C 1.562419 -2.605373 6.982672
C 3.106205 -2.230766 4.316178
C 1.666092 -4.913128 4.920297
C -5.733099 -1.319262 -1.501439
C -7.504007 -1.979664 0.969189
C -5.827399 -4.208169 -0.376715
C 0.560803 3.702294 6.519465
C 2.568676 1.367689 6.215382
C 0.393919 1.269787 8.431030
C -3.408574 2.886056 8.244099
C -6.339952 2.177052 7.493090
C -4.726813 4.148001 5.740475
H 2.795474 1.637768 5.175257
H 2.748175 0.291198 6.333558
H 3.271130 1.903687 6.871540
H -0.472065 4.001063 6.743337
H 0.797424 4.047457 5.503931
H 1.227323 4.222020 7.224742
H -0.631702 1.544174 8.711033
H 0.499077 0.182654 8.545973
H 1.082889 1.755923 9.138579
H 3.162146 -2.496853 3.252068
H 3.061578 -1.135825 4.386099
H 4.032243 -2.571027 4.805148
H 1.690822 -5.189020 3.857658
H 0.793669 -5.398514 5.378068
H 2.571736 -5.315750 5.399488
H 1.488634 -1.520545 7.134820
H 0.703073 -3.075287 7.479624
H 2.480638 -2.959666 7.475573
H -4.985802 4.444050 0.949932
H -5.326606 4.647836 2.678856
H -6.593433 5.001640 1.476947
H -7.862151 2.708478 -0.189243
H -6.252290 2.127889 -0.674223
H -7.409999 1.010098 0.082296
H -7.355850 2.632934 4.100012
H -8.575228 3.014650 2.861716
H -8.095483 1.324494 3.153662
H -5.706493 -0.248850 -1.261442
H -4.814921 -1.564346 -2.051949
H -6.592439 -1.503330 -2.164140
H -8.363613 -2.139890 0.300642
H -7.527301 -0.938134 1.317099
H -7.627573 -2.628762 1.846810
H -5.899786 -4.836917 0.520827
H -6.668742 -4.460461 -1.040129
H -4.894313 -4.463023 -0.896953
H -5.052325 5.008922 6.344518
H -5.452185 4.008064 4.927760
H -3.755535 4.388642 5.287151
H -2.408136 3.128412 7.861111
H -3.747000 3.726737 8.868789
H -3.320258 1.998181 8.884556
H -6.318436 1.283460 8.130936
H -7.053319 1.993928 6.678013
H -6.719694 3.016987 8.094799

4.7 Model compound Sn_8

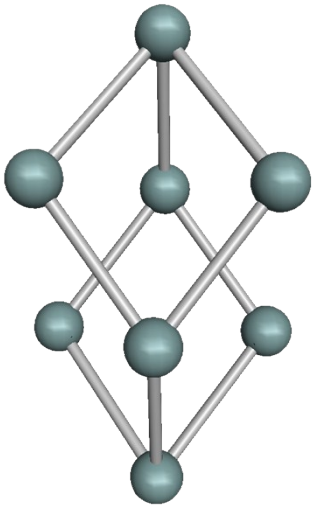

Figure S15: Optimized structure of Sn_8

Point group used: C_1

Total energy: -27.63696554707 Hartree

HOMO-LUMO-gap: 1.004 eV

XYZ positions of all atoms

```
Sn 1.203466 12.884376 20.684912
Sn 0.019765 10.379299 18.623200
Sn -1.502965 12.924438 19.068748
Sn -0.506221 10.648444 21.719745
Sn -0.677937 15.300905 20.372965
Sn -1.331142 8.272297 20.415691
Sn -3.212707 10.688567 20.103614
Sn -2.028897 13.193673 22.165314
```

4.8 Model compound $Sn_6(SiMe_3)_5Cl$

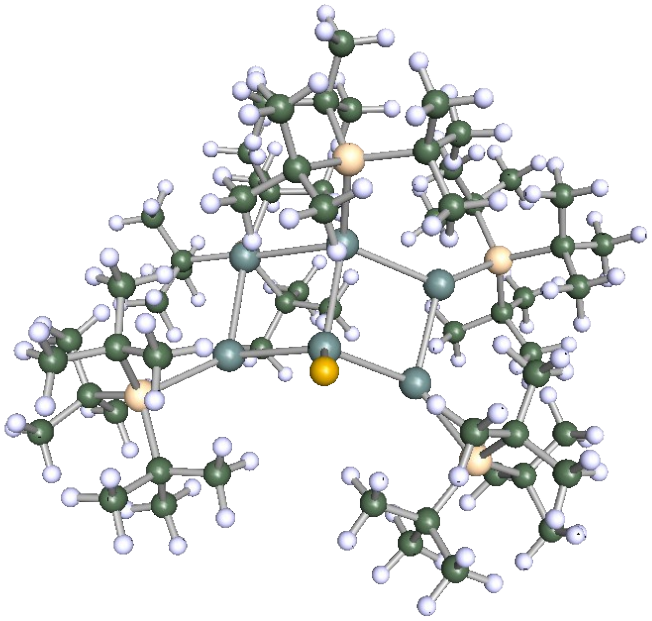

Figure S16: Optimized structure of Sn_6 $(SiMe_3)_5Cl$

Point group used: C_1

Total energy: -4297.69783224413 Hartree

HOMO-LUMO-gap: 0.916 eV

XYZ positions of all atoms

```
Sn -1.674814 10.674442 24.749269
Sn -5.924150 10.860911 22.307239
Sn -2.049902 13.002402 26.155659
Sn -4.515957 10.227306 24.696726
Si -0.153554 8.560031 25.342280
Sn -6.447984 13.414456 23.337921
Si -7.687703 9.068063 21.413948
Sn -4.938335 12.909615 25.763419
Si -0.217039 14.931952 26.532505
H -0.127668 13.768807 23.653909
Cl -5.207586 8.194528 25.906565
C 1.708833 9.153281 25.099315
C -0.519630 8.024239 27.203491
C -0.652714 7.162149 24.047711
Si -5.682379 15.439762 21.776360
C -9.080610 8.856100 22.791985
C -6.664553 7.410493 21.119744
C -8.406338 9.803660 19.734525
Si -6.393240 13.051834 27.993845
C 1.144781 14.813024 25.115201
C 0.520429 14.490569 28.310977
C -1.118870 16.681875 26.537687
C 0.497876 14.670315 23.721276
C 1.866543 10.026634 23.836052
C 2.123544 10.021090 26.302537
C 2.690442 7.968068 24.991186
C -0.620208 9.238732 28.150338
C 0.584194 7.082958 27.732103
C -1.870702 7.289840 27.287065
C -0.110309 5.783643 24.482583
C -2.183083 7.054708 23.878842
C -0.079608 7.490091 22.654149
C -6.940502 15.526807 20.265230
C -3.831973 15.106546 21.175335
C -5.817330 17.033440 22.928885
C -10.308077 8.106657 22.229848
C -9.559608 10.214444 23.343463
C -8.520592 8.064102 23.989723
C -5.807839 7.521625 19.842851
C -5.686771 7.129376 22.281140
C -7.605251 6.196330 20.969064
C -9.116454 8.722631 18.892362
C -9.421020 10.924388 20.038587
C -7.288322 10.434520 18.877241
C -7.759733 11.638263 27.940845
C -7.190101 14.856368 27.920497
C -5.180132 12.838351 29.527095
C 2.069716 16.047837 25.110459
C 2.008624 13.557376 25.326189
C -0.503159 14.847704 29.406933
C 1.830786 15.253955 28.592115
C 0.805593 12.980357 28.454887
C -2.507390 16.587986 27.203375
C -1.354211 17.150358 25.090585
C -0.291774 17.763024 27.262961
H -0.122878 15.527077 23.439596
H 1.292954 14.575484 22.961269
H 1.221242 10.916925 23.862600
H 2.908441 10.383725 23.768486
H 1.643396 9.485100 22.910446
H 2.217674 9.441306 27.228539
H 3.103693 10.488356 26.105372
H 1.406054 10.830248 26.487841
H 2.520862 7.368404 24.087744
H 3.723943 8.351761 24.935707
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4.9 Overall dissociation mechanism

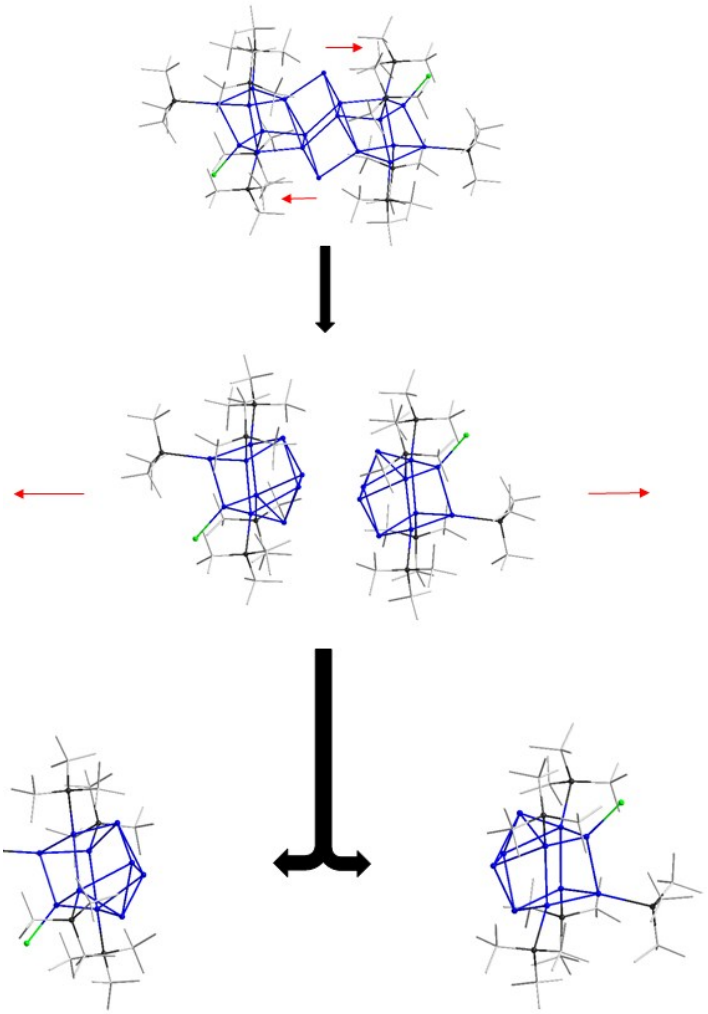

Figure S17 : Assumed reaction mechanism of the dissociation of $Sn_{20}(Si^tBu_3)_{10}Cl_2$

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