

Supplementary Information

The Mulliken atomic charge of an arbitrary atom A is defined as:

$$q_A = Z_A - \sum_i n_{i,A} = Z_A - \sum_i \eta_i \sum_{a \in A} \Theta_{i,a} \quad (\text{S1})$$

where Z_A is the number of nuclear charges of atom A , $n_{i,A}$ is the contribution of atom A to occupation number of orbital i , $\Theta_{i,a}$ is the population of basis function a in orbital i , and η is the orbital occupation number.

The Mayer bond order between atoms A and B is defined as:

$$I_{AB} = \sum_{a \in A} \sum_{b \in B} [(PS)_{ba}(PS)_{ab} + (P^S S)_{ba}(P^S S)_{ab}] \quad (\text{S2})$$

where \mathbf{P} , \mathbf{P}^S , and \mathbf{S} are the total density matrix, spin density matrix, and overlap matrix, respectively, while a and b are basis functions.

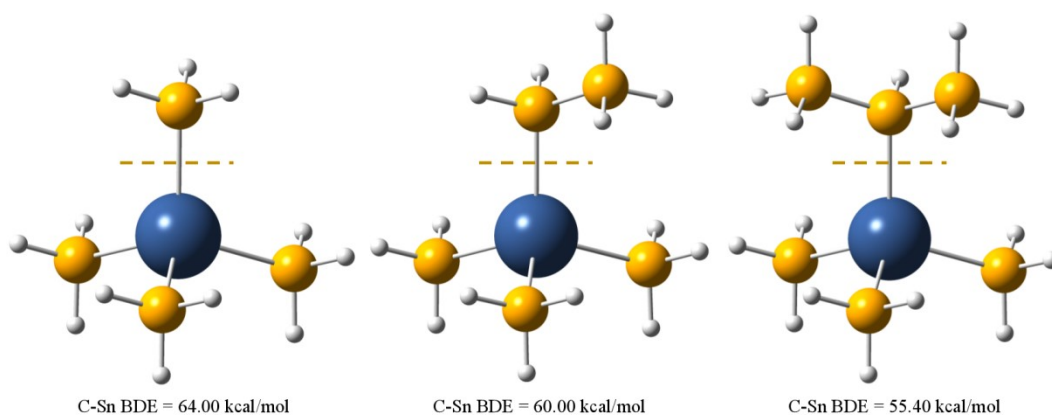
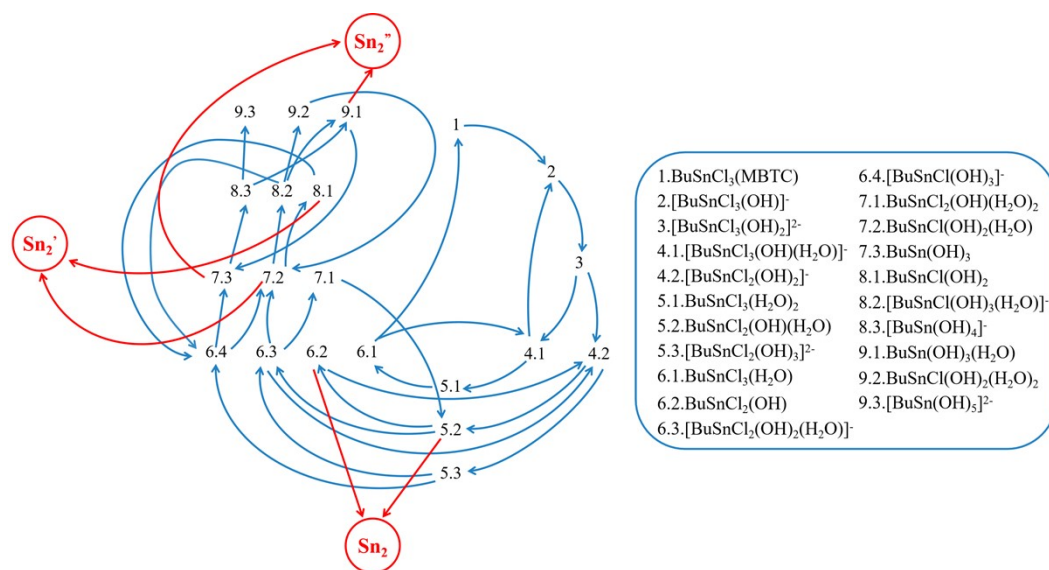
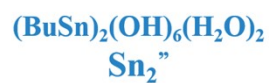
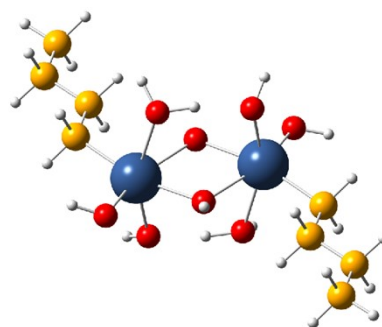
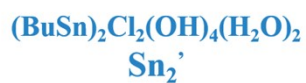
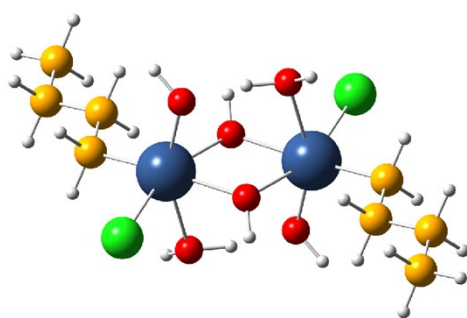


Figure S1. Schematic diagrams of the structures of organotin compounds with the known experimental BDEs of the C-Sn bond.



(a)



(b)

Figure S2. (a) All species and feasible reactions considered in the present work. The species are labeled as numbers for convenience, and the corresponding relationship is also shown in the figure.

Sn₂' and Sn₂'' are hydrolysis products of Sn₂. (b) The molecular structures and formulas of Sn₂' and

Sn₂''.

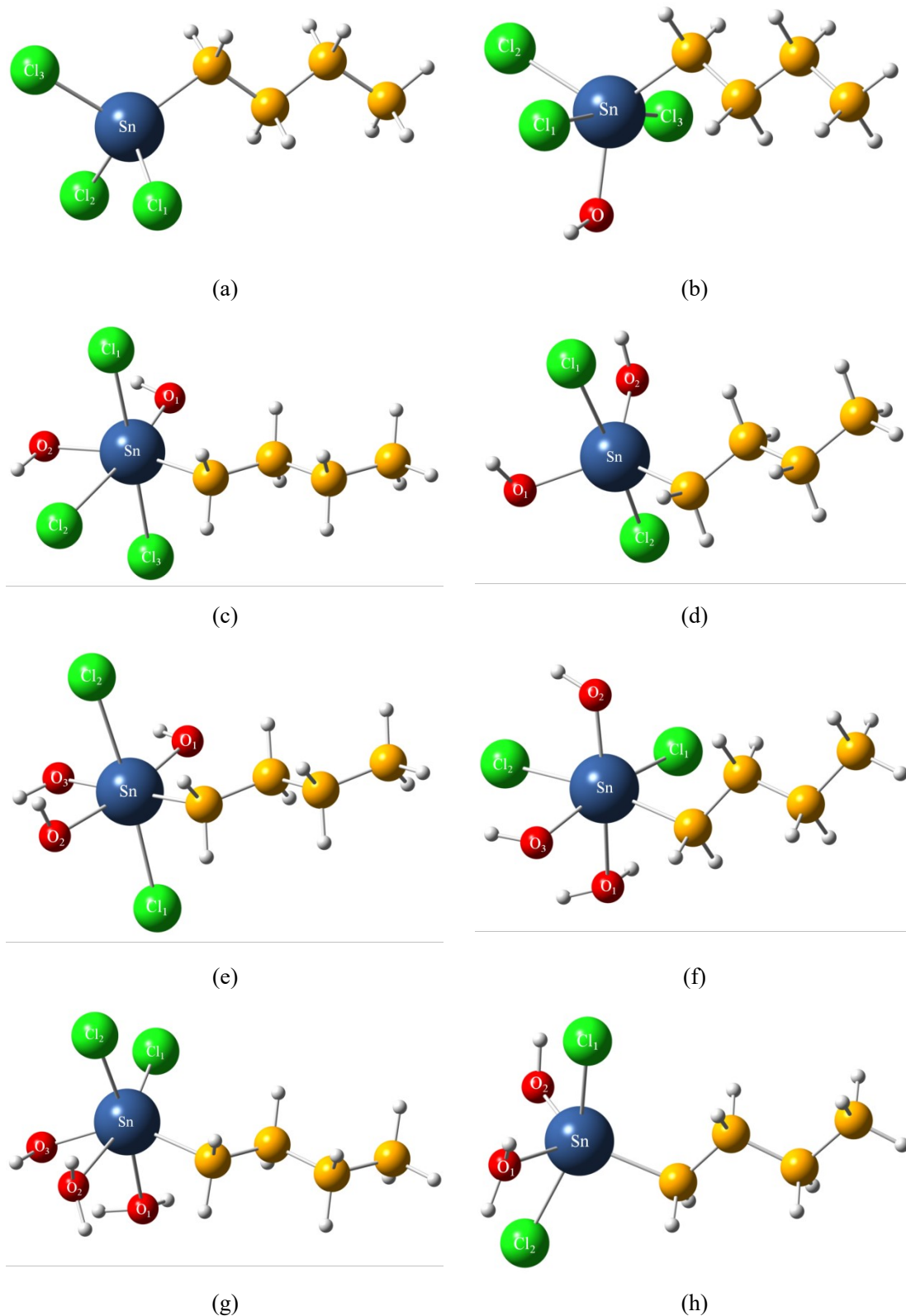


Figure S3. The molecular structures and atomic labels of (a) BuSnCl_3 (b) $[\text{BuSnCl}_3(\text{OH})]^-$ (c) $[\text{BuSnCl}_3(\text{OH})_2]^{2-}$ (d) $[\text{BuSnCl}_2(\text{OH})_2]^-$ (e) $[\text{BuSnCl}_2(\text{OH})_3]^{2-}$ (f) $[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^-$ (g) $\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2$ (h) $\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})$.

Table S1. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 4.1.

Step 4.1	
Reaction	ΔG
$[\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^- \rightarrow [\text{BuSnCl}_3(\text{OH})]^- + \text{H}_2\text{O}$	-6.17
$[\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^- \rightarrow \text{BuSnCl}_3(\text{H}_2\text{O}) + \text{OH}^-$	44.55
$[\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^- \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{Cl}^-$	2.76
$[\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSnCl}_3(\text{H}_2\text{O})_2$	-2.15
$[\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{HCl}$	6.89

Table S2. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 4.2.

Step 4.2	
Reaction	ΔG
$[\text{BuSnCl}_2(\text{OH})_2]^- \rightarrow \text{BuSnCl}_2(\text{OH}) + \text{OH}^-$	46.35
$[\text{BuSnCl}_2(\text{OH})_2]^- \rightarrow \text{BuSnCl}(\text{OH})_2 + \text{Cl}^-$	6.23
$[\text{BuSnCl}_2(\text{OH})_2]^- + \text{H}^+ \rightarrow \text{BuSnCl}(\text{OH})_2 + \text{HCl}$	10.36
$[\text{BuSnCl}_2(\text{OH})_2]^- + \text{H}^+ \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})$	-6.69
$[\text{BuSnCl}_2(\text{OH})_2]^- + \text{OH}^- \rightarrow [\text{BuSnCl}_2(\text{OH})_3]^{2-}$	-18.48
$[\text{BuSnCl}_2(\text{OH})_2]^- + \text{H}_2\text{O} \rightarrow [\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^-$	12.95
$2[\text{BuSnCl}_2(\text{OH})_2]^- \rightarrow [(\text{BuSn})_2\text{Cl}_4(\text{OH})_4]^{2-}$	12.01

Table S3. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 5.1.

Step 5.1	
Reaction	ΔG
$\text{BuSnCl}_3(\text{H}_2\text{O})_2 \rightarrow \text{BuSnCl}_3(\text{H}_2\text{O}) + \text{H}_2\text{O}$	-9.23
$\text{BuSnCl}_3(\text{H}_2\text{O})_2 \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})_2]^+ + \text{Cl}^-$	14.30
$\text{BuSnCl}_3(\text{H}_2\text{O})_2 + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})_2]^+ + \text{HCl}$	18.43

Table S4. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 5.2.

Step 5.2	
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Reaction	ΔG
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) \rightarrow \text{BuSnCl}_2(\text{OH}) + \text{H}_2\text{O}$	-2.89
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})]^+ + \text{OH}^-$	71.25
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})]^+ + \text{Cl}^-$	27.65
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})_2]^+$	9.39
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})]^+ + \text{HCl}$	31.78
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{OH}^- \rightarrow [\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^-$	-36.28
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{H}_2\text{O} \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2$	3.68
$2\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) \rightarrow (\text{BuSn})_2\text{Cl}_4(\text{OH})_2(\text{H}_2\text{O})_2$	-11.86

Table S5. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 5.3.

Step 5.3	
Reaction	ΔG
$[\text{BuSnCl}_2(\text{OH})_3]^{2-} \rightarrow [\text{BuSnCl}_2(\text{OH})_2]^- + \text{OH}^-$	18.48
$[\text{BuSnCl}_2(\text{OH})_3]^{2-} \rightarrow [\text{BuSnCl}(\text{OH})_3]^- + \text{Cl}^-$	-15.01
$[\text{BuSnCl}_2(\text{OH})_3]^{2-} + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^-$	-24.49
$[\text{BuSnCl}_2(\text{OH})_3]^{2-} + \text{H}^+ \rightarrow [\text{BuSnCl}(\text{OH})_3]^- + \text{HCl}$	-10.88

Table S6. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 6.1.

Step 6.1	
Reaction	ΔG
$\text{BuSnCl}_3(\text{H}_2\text{O}) + \text{OH}^- \rightarrow [\text{BuSnCl}_3(\text{OH})(\text{H}_2\text{O})]^-$	-44.55
$\text{BuSnCl}_3(\text{H}_2\text{O}) + \text{H}_2\text{O} \rightarrow \text{BuSnCl}_3(\text{H}_2\text{O})_2$	9.23
$\text{BuSnCl}_3(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})]^+ + \text{HCl}$	33.59
$\text{BuSnCl}_3(\text{H}_2\text{O}) \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})]^+ + \text{Cl}^-$	29.46
$\text{BuSnCl}_3(\text{H}_2\text{O}) \rightarrow \text{BuSnCl}_3 + \text{H}_2\text{O}$	-4.09

Table S7. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 6.2.

Step 6.2	
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Reaction	ΔG
$\text{BuSnCl}_2(\text{OH}) + \text{OH}^- \rightarrow [\text{BuSnCl}_2(\text{OH})_2]^-$	-46.35
$\text{BuSnCl}_2(\text{OH}) + \text{H}_2\text{O} \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})$	2.89
$\text{BuSnCl}_2(\text{OH}) + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})]^+$	18.21
$2\text{BuSnCl}_2(\text{OH}) \rightarrow (\text{BuSn})_2\text{Cl}_4(\text{OH})_2$	-8.64
$(\text{BuSn})_2\text{Cl}_4(\text{OH})_2 + 2\text{OH}^- \rightarrow [(\text{BuSn})_2\text{Cl}_4(\text{OH})_4]^{2-}$	-72.04
$[(\text{BuSn})_2\text{Cl}_4(\text{OH})_4]^{2-} + 2\text{H}^+ \rightarrow (\text{BuSn})_2\text{Cl}_4(\text{OH})_2(\text{H}_2\text{O})_2$	-37.25

Table S8. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 6.3.

Step 6.3	
Reaction	ΔG
$[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^- \rightarrow [\text{BuSnCl}_2(\text{OH})_2]^- + \text{H}_2\text{O}$	-12.95
$[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^- \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{OH}^-$	36.28
$[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^- \rightarrow \text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{Cl}^-$	-5.98
$[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{HCl}$	-1.85
$[\text{BuSnCl}_2(\text{OH})_2(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2$	-15.97

Table S9. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 6.4.

Step 6.4	
Reaction	ΔG
$[\text{BuSnCl}(\text{OH})_3]^- \rightarrow \text{BuSnCl}(\text{OH})_2 + \text{OH}^-$	39.11
$[\text{BuSnCl}(\text{OH})_3]^- \rightarrow \text{BuSn}(\text{OH})_3 + \text{Cl}^-$	-0.67
$[\text{BuSnCl}(\text{OH})_3]^- + \text{H}_2\text{O} \rightarrow [\text{BuSnCl}(\text{OH})_3(\text{H}_2\text{O})]^-$	12.18
$[\text{BuSnCl}(\text{OH})_3]^- + \text{H}^+ \rightarrow \text{BuSn}(\text{OH})_3 + \text{HCl}$	3.45
$[\text{BuSnCl}(\text{OH})_3]^- + \text{H}^+ \rightarrow \text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O})$	-15.46
$2[\text{BuSnCl}(\text{OH})_3]^- \rightarrow [(\text{BuSn})_2\text{Cl}_2(\text{OH})_6]^{2-}$	0.65

Table S10. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 7.1.

Step 7.1	
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Reaction	ΔG
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2 \rightarrow \text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O}) + \text{H}_2\text{O}$	-3.68
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2 \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})_2]^+ + \text{OH}^-$	61.64
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2 \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})_2]^+ + \text{Cl}^-$	17.17
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2 + \text{H}^+ \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})_2]^+ + \text{HCl}$	21.30
$\text{BuSnCl}_2(\text{OH})(\text{H}_2\text{O})_2 + \text{H}^+ \rightarrow [\text{BuSnCl}_2(\text{H}_2\text{O})_3]^+$	9.30

Table S11. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 7.2.

Step 7.2	
Reaction	ΔG
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})]^+ + \text{OH}^-$	69.91
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) \rightarrow \text{BuSnCl}(\text{OH})_2 + \text{H}_2\text{O}$	-1.35
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) \rightarrow [\text{BuSn}(\text{OH})_2(\text{H}_2\text{O})]^+ + \text{Cl}^-$	26.17
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{OH}^- \rightarrow [\text{BuSnCl}(\text{OH})_3(\text{H}_2\text{O})]^-$	-28.28
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{H}_2\text{O} \rightarrow \text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O})_2$	8.67
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSn}(\text{OH})_2(\text{H}_2\text{O})]^+ + \text{HCl}$	30.30
$\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSnCl}(\text{OH})(\text{H}_2\text{O})_2]^+$	7.18
$2\text{BuSnCl}(\text{OH})_2(\text{H}_2\text{O}) \rightarrow (\text{BuSn})_2\text{Cl}_2(\text{OH})_4(\text{H}_2\text{O})_2$	-9.63

Table S12. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 7.3.

Step 7.3	
Reaction	ΔG
$\text{BuSn}(\text{OH})_3 + \text{OH}^- \rightarrow [\text{BuSn}(\text{OH})_4]^-$	-28.73
$\text{BuSn}(\text{OH})_3 + \text{H}_2\text{O} \rightarrow \text{BuSn}(\text{OH})_3(\text{H}_2\text{O})$	3.16
$\text{BuSn}(\text{OH})_3 + \text{H}^+ \rightarrow [\text{BuSn}(\text{OH})_2(\text{H}_2\text{O})]^+$	11.39
$2\text{BuSn}(\text{OH})_3 \rightarrow (\text{BuSn})_2(\text{OH})_6$	-5.73
$(\text{BuSn})_2(\text{OH})_6 + 2\text{OH}^- \rightarrow [(\text{BuSn})_2(\text{OH})_8]^{2-}$	-51.45
$[(\text{BuSn})_2(\text{OH})_8]^{2-} + 2\text{H}^+ \rightarrow (\text{BuSn})_2(\text{OH})_6(\text{H}_2\text{O})_2$	-56.86

Table S13. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 8.1.

Step 8.1	
Reaction	ΔG
$\text{BuSnCl(OH)}_2 + \text{OH}^- \rightarrow [\text{BuSnCl(OH)}_3]^-$	-39.11
$\text{BuSnCl(OH)}_2 + \text{H}_2\text{O} \rightarrow \text{BuSnCl(OH)}_2(\text{H}_2\text{O})$	1.35
$\text{BuSnCl(OH)}_2 + \text{H}^+ \rightarrow [\text{BuSnCl(OH)(H}_2\text{O)}]^+$	15.34
$2\text{BuSnCl(OH)}_2 \rightarrow (\text{BuSn})_2\text{Cl}_2(\text{OH})_4$	-10.09
$(\text{BuSn})_2\text{Cl}_2(\text{OH})_4 + 2\text{OH}^- \rightarrow [(\text{BuSn})_2\text{Cl}_2(\text{OH})_6]^{2-}$	-68.56
$[(\text{BuSn})_2\text{Cl}_2(\text{OH})_6]^{2-} + 2\text{H}^+ \rightarrow (\text{BuSn})_2\text{Cl}_2(\text{OH})_4(\text{H}_2\text{O})_2$	-40.12

Table S14. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 8.2.

Step 8.2	
Reaction	ΔG
$[\text{BuSnCl(OH)}_3(\text{H}_2\text{O})]^- \rightarrow [\text{BuSnCl(OH)}_3]^- + \text{H}_2\text{O}$	-12.18
$[\text{BuSnCl(OH)}_3(\text{H}_2\text{O})]^- \rightarrow \text{BuSnCl(OH)}_2(\text{H}_2\text{O}) + \text{OH}^-$	28.28
$[\text{BuSnCl(OH)}_3(\text{H}_2\text{O})]^- \rightarrow \text{BuSn(OH)}_3(\text{H}_2\text{O}) + \text{Cl}^-$	-9.70
$[\text{BuSnCl(OH)}_3(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSn(OH)}_3(\text{H}_2\text{O}) + \text{HCl}$	-5.57
$[\text{BuSnCl(OH)}_3(\text{H}_2\text{O})]^- + \text{H}^+ \rightarrow \text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2$	-18.98

Table S15. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 8.3.

Step 8.3	
Reaction	ΔG
$[\text{BuSn(OH)}_4]^- \rightarrow \text{BuSn(OH)}_3 + \text{OH}^-$	28.73
$[\text{BuSn(OH)}_4]^- + \text{OH}^- \rightarrow [\text{BuSn(OH)}_5]^{2-}$	-9.27
$[\text{BuSn(OH)}_4]^- + \text{H}^+ \rightarrow \text{BuSn(OH)}_3(\text{H}_2\text{O})$	-24.04
$2[\text{BuSn(OH)}_4]^- \rightarrow [(\text{BuSn})_2(\text{OH})_8]^{2-}$	0.29

Table S16. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 9.1.

Step 9.1	
Reaction	ΔG

$\text{BuSn(OH)}_3(\text{H}_2\text{O}) \rightarrow \text{BuSn(OH)}_3 + \text{H}_2\text{O}$	-3.16
$\text{BuSn(OH)}_3(\text{H}_2\text{O}) \rightarrow [\text{BuSn(OH)}_2(\text{H}_2\text{O})]^+ + \text{OH}^-$	64.15
$\text{BuSn(OH)}_3(\text{H}_2\text{O}) + \text{H}_2\text{O} \rightarrow \text{BuSn(OH)}_3(\text{H}_2\text{O})_2$	16.47
$\text{BuSn(OH)}_3(\text{H}_2\text{O}) + \text{H}^+ \rightarrow [\text{BuSn(OH)}_2(\text{H}_2\text{O})_2]^+$	2.54
$2\text{BuSn(OH)}_3(\text{H}_2\text{O}) \rightarrow (\text{BuSn})_2(\text{OH})_6(\text{H}_2\text{O})_2$	-8.50

Table S17. Possible elementary reactions and corresponding ΔG (kcal/mol) in Step 9.2.

Step 9.2	
Reaction	ΔG
$\text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2 \rightarrow \text{BuSnCl(OH)}_2(\text{H}_2\text{O}) + \text{H}_2\text{O}$	-8.67
$\text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2 \rightarrow [\text{BuSnCl(OH)}(\text{H}_2\text{O})_2]^+ + \text{OH}^-$	54.44
$\text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2 \rightarrow [\text{BuSn(OH)}_2(\text{H}_2\text{O})_2]^+ + \text{Cl}^-$	11.82
$\text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2 + \text{H}^+ \rightarrow [\text{BuSn(OH)}_2(\text{H}_2\text{O})_2]^+ + \text{HCl}$	15.95
$\text{BuSnCl(OH)}_2(\text{H}_2\text{O})_2 + \text{H}^+ \rightarrow [\text{BuSnCl(OH)}(\text{H}_2\text{O})_3]^+$	2.54

Table S18. Possible elementary reaction and corresponding ΔG (kcal/mol) in Step 9.3.

Step 9.3	
Reaction	ΔG
$[\text{BuSn(OH)}_5]^{2-} \rightarrow [\text{BuSn(OH)}_4]^- + \text{OH}^-$	9.27

Table S19. The Mulliken atomic charge population and Mayer bond order analysis results of

BuSnCl ₃ .	
Atom	Mulliken Atomic Charge
Sn	1.16
Cl ₁	-0.38
Cl ₂	-0.39
Cl ₃	-0.39
Bond	Mayer Bond Order
Sn-Cl ₁	0.90

Sn-Cl ₂	0.89
Sn-Cl ₃	0.89

Table S20. The Mulliken atomic charge population and Mayer bond order analysis results of [BuSnCl₃(OH)]⁻.

Atom	Mulliken Atomic Charge
Sn	1.17
Cl ₁	-0.62
Cl ₂	-0.46
Cl ₃	-0.58
O	-0.73
Bond	Mayer Bond Order
Sn-Cl ₁	0.58
Sn-Cl ₂	0.81
Sn-Cl ₃	0.67
Sn-O	0.84

Table S21. The Mulliken atomic charge population and Mayer bond order analysis results of [BuSnCl₃(OH)₂]²⁻.

Atom	Mulliken Atomic Charge
Sn	1.25
Cl ₁	-0.68
Cl ₂	-0.77
Cl ₃	-0.68
O ₁	-0.81
O ₂	-0.75
Bond	Mayer Bond Order
Sn-Cl ₁	0.53
Sn-Cl ₂	0.32

Sn-Cl ₃	0.52
Sn-O ₁	0.76
Sn-O ₂	0.82

Table S22. The Mulliken atomic charge population and Mayer bond order analysis results of [BuSnCl₂(OH)₂]⁻.

Atom	Mulliken Atomic Charge
Sn	1.26
Cl ₁	-0.66
Cl ₂	-0.59
O ₁	-0.75
O ₂	-0.76
Bond	Mayer Bond Order
Sn-Cl ₁	0.51
Sn-Cl ₂	0.67
Sn-O ₁	0.83
Sn-O ₂	0.81

Table S23. The Mulliken atomic charge population and Mayer bond order analysis results of [BuSnCl₂(OH)₃]²⁻.

Atom	Mulliken Atomic Charge
Sn	1.36
Cl ₁	-0.69
Cl ₂	-0.74
O ₁	-0.84
O ₂	-0.86
O ₃	-0.83
Bond	Mayer Bond Order
Sn-Cl ₁	0.52

Sn-Cl ₂	0.42
Sn-O ₁	0.69
Sn-O ₂	0.61
Sn-O ₃	0.75

Table S24. The Mulliken atomic charge population and Mayer bond order analysis results of [BuSnCl₂(OH)₂(H₂O)]⁻.

Atom	Mulliken Atomic Charge
Sn	1.30
Cl ₁	-0.64
Cl ₂	-0.59
O ₁	-0.62
O ₂	-0.78
O ₃	-0.79
Bond	Mayer Bond Order
Sn-Cl ₁	0.53
Sn-Cl ₂	0.59
Sn-O ₁	0.21
Sn-O ₂	0.79
Sn-O ₃	0.79

Table S25. The Mulliken atomic charge population and Mayer bond order analysis results of BuSnCl₂(OH)(H₂O)₂.

Atom	Mulliken Atomic Charge
Sn	1.26
Cl ₁	-0.48
Cl ₂	-0.50
O ₁	-0.64
O ₂	-0.66

O ₃	-0.74
Bond	Mayer Bond Order
Sn-Cl ₁	0.79
Sn-Cl ₂	0.77
Sn-O ₁	0.20
Sn-O ₂	0.11
Sn-O ₃	0.84

Table S26. The Mulliken atomic charge population and Mayer bond order analysis results of BuSnCl₂(OH)(H₂O).

Atom	Mulliken Atomic Charge
Sn	1.27
Cl ₁	-0.52
Cl ₂	-0.52
O ₁	-0.59
O ₂	-0.70
Bond	Mayer Bond Order
Sn-Cl ₁	0.70
Sn-Cl ₂	0.74
Sn-O ₁	0.31
Sn-O ₂	0.89