| SnF ₂ | 1 |
|-------------------------------------|----|
| SnCl ₂ | 2 |
| SnBr ₂ | 3 |
| SnI ₂ | 4 |
| SnHF | 5 |
| SnHCl | 6 |
| SnHBr | 7 |
| SnHI | 8 |
| SnFCl | 9 |
| SnFBr | 10 |
| SnFI | 11 |
| SnClBr | 12 |
| SnCII | 13 |
| SnBrI | 14 |
| HSnCH ₃ | 15 |
| FSnCH ₃ | 16 |
| ClSnCH ₃ | 17 |
| BrSnCH ₃ | 18 |
| ISnCH ₃ | 19 |
| HSnSiH ₃ | 20 |
| FSnSiH ₃ | 21 |
| ClSnSiH ₃ | 22 |
| BrSnSiH ₃ | 23 |
| ISnSiH ₃ | 24 |
| HSnGeH ₃ | 25 |
| FSnGeH ₃ | 26 |
| ClSnGeH ₃ | 27 |
| BrSnGeH ₃ | 28 |
| ISnGeH ₃ | 29 |
| FSnSnH ₃ | 30 |
| ClSnSnH ₃ | 31 |
| BrSnSnH ₃ | 32 |
| ISnSnH ₃ | 33 |
| Sn(SiH ₃) ₂ | 34 |
| Sn(GeH ₃) ₂ | 35 |
| Sn(SnH ₃) ₂ | 36 |
| CH ₃ SnSiH ₃ | 37 |
| CH ₃ SnGeH ₃ | 38 |
| CH ₃ SnSnH ₃ | |
| SiH ₃ SnGeH ₃ | 40 |
| GeH ₃ SnSnH ₃ | 42 |

Table of Contents



Figure S1. Equilibrium geometries for the ${}^{1}A_{1}$ ground state of SnF_{2} , ${}^{2}B_{1}$ ground state of the SnF_{2}^{-} anion, ${}^{2}A_{1}$ ground state of the SnF_{2}^{+} cation, and ${}^{3}B_{1}$ excited state of neutral SnF_{2} .



Figure S2. Equilibrium geometries for the ¹A₁ ground state of SnCl₂, ²B₁ ground state of the SnCl₂⁻ anion, ²A₁ ground state of the SnCl₂⁺ cation, and ³B₁ excited state of neutral SnCl₂.



Figure S3. Equilibrium geometries for the ${}^{1}A_{1}$ ground state of $SnBr_{2}$, ${}^{2}B_{1}$ ground state of the $SnBr_{2}^{-}$ anion, ${}^{2}A_{1}$ ground state of the $SnBr_{2}^{+}$ cation, and ${}^{3}B_{1}$ excited state of neutral $SnBr_{2}$.



Figure S4. Equilibrium geometries for the ${}^{1}A_{1}$ ground state of SnI₂, ${}^{2}B_{1}$ ground state of the SnI₂⁻ anion, ${}^{2}A_{1}$ ground state of the SnI₂⁺ cation, and ${}^{3}B_{1}$ excited state of neutral SnI₂.



Figure S5. Equilibrium geometries for the ¹A' ground state of SnHF, ²A" ground state of the SnHF⁻ anion, ²A' ground state of the SnHF⁺ cation, and ³A" excited state of neutral SnHF.



Figure S6. Equilibrium geometries for the ¹A' ground state of SnHCl, ²A" ground state of the SnHCl⁻ anion, ²A' ground state of the SnHCl⁺ cation, and ³A" excited state of neutral SnHCl.



Figure S7. Equilibrium geometries for the ¹A' ground state of SnHBr, ²A" ground state of the SnHBr⁻ anion, ²A' ground state of the SnHBr⁺ cation, and ³A" excited state of neutral SnHBr.



Figure S8. Equilibrium geometries for the ¹A' ground state of SnHI, ²A" ground state of the SnHI⁻ anion, ²A' ground state of the SnHI⁺ cation, and ³A" excited state of neutral SnHI.



Figure S9. Equilibrium geometries for the ¹A' ground state of SnFCl, ²A" ground state of the SnFCl⁻ anion, ²A' ground state of the SnFCl⁺ cation, and ³A" excited state of neutral SnFCl.



Figure S10. Equilibrium geometries for the ¹A' ground state of SnFBr, ²A" ground state of the SnFBr⁻ anion, ²A' ground state of the SnFBr⁺ cation, and ³A" excited state of neutral SnFBr.



Figure S11. Equilibrium geometries for the ¹A' ground state of SnFI, ²A" ground state of the SnFI⁻ anion, ²A' ground state of the SnFI⁺ cation, and ³A" excited state of neutral SnFI.





SnClBr⁻ Anion (²A")

Figure S12. Equilibrium geometries for the ¹A' ground state of SnClBr, ²A" ground state of the SnClBr⁻ anion, ²A' ground state of the SnClBr⁺ cation, and ³A" excited state of neutral SnClBr.

119.9°



Figure S13. Equilibrium geometries for the ¹A' ground state of SnClI, ²A" ground state of the SnClI⁻ anion, ²A' ground state of the SnClI⁺ cation, and ³A" excited state of neutral SnClI.



Figure S14. Equilibrium geometries for the ¹A' ground state of SnBrI, ²A" ground state of the SnBrI⁻ anion, ²A' ground state of the SnBrI⁺ cation, and ³A" excited state of neutral SnBrI.

HSnCH₃



Figure S15. Equilibrium geometries for the ¹A' ground state of HSnCH₃, ²A" ground state of the HSnCH₃⁻ anion, ²A" ground state of the HSnCH₃⁺ cation, and ³A" excited state of neutral HSnCH₃.



Figure S16. Equilibrium geometries for the ¹A' ground state of FSnCH₃, ²A" ground state of the FSnCH₃⁻ anion, ²A" ground state of the FSnCH₃⁺ cation, and ³A" excited state of neutral FSnCH₃.

ClSnCH₃



Figure S17. Equilibrium geometries for the ¹A' ground state of ClSnCH₃, ²A" ground state of the ClSnCH₃⁻ anion, ²A" ground state of the ClSnCH₃⁺ cation, and ³A" excited state of neutral ClSnCH₃.

BrSnCH₃



Figure S18. Equilibrium geometries for the ¹A' ground state of BrSnCH₃, ²A" ground state of the BrSnCH₃⁻ anion, ²A" ground state of the BrSnCH₃⁺ cation, and ³A" excited state of neutral BrSnCH₃.



Figure S19. Equilibrium geometries for the ¹A' ground state of ISnCH₃, ²A" ground state of the ISnCH₃⁻ anion, ²A" ground state of the ISnCH₃⁺ cation, and ³A" excited state of neutral ISnCH₃.

HSnSiH₃



Figure S20. Equilibrium geometries for the ¹A' ground state of HSnSiH₃, ²A" ground state of the HSnSiH₃⁻ anion, ²A" ground state of the HSnSiH₃⁺ cation, and ³A" excited state of neutral HSnSiH₃.





Figure S21. Equilibrium geometries for the ¹A' ground state of FSnSiH₃, ²A" ground state of the FSnSiH₃⁻ anion, ²A" ground state of the FSnSiH₃⁺ cation, and ³A" excited state of neutral FSnSiH₃.

ClSnSiH₃



Figure S22. Equilibrium geometries for the ¹A' ground state of ClSnSiH₃, ²A" ground state of the ClSnSiH₃⁻ anion, ²A" ground state of the ClSnSiH₃⁺ cation, and ³A" excited state of neutral ClSnSiH₃.

BrSnSiH₃



Figure S23. Equilibrium geometries for the ¹A' ground state of BrSnSiH₃, ²A" ground state of the BrSnSiH₃⁻ anion, ²A" ground state of the BrSnSiH₃⁺ cation, and ³A" excited state of neutral BrSnSiH₃.





Figure S24. Equilibrium geometries for the ¹A' ground state of $ISnSiH_3$, ²A" ground state of the $ISnSiH_3^-$ anion, ²A" ground state of the $ISnSiH_3^+$ cation, and ³A" excited state of neutral $ISnSiH_3$.

HSnGeH₃



Figure S25. Equilibrium geometries for the ¹A' ground state of HSnGeH₃, ²A" ground state of the HSnGeH₃⁻ anion, ²A" ground state of the HSnGeH₃⁺ cation, and ³A" excited state of neutral HSnGeH₃.

FSnGeH₃



Figure S26. Equilibrium geometries for the ¹A' ground state of FSnGeH₃, ²A" ground state of the FSnGeH₃⁻ anion, ²A" ground state of the FSnGeH₃⁺ cation, and ³A" excited state of neutral FSnGeH₃.





Figure S27. Equilibrium geometries for the ¹A' ground state of ClSnGeH₃, ²A" ground state of the ClSnGeH₃⁻ anion, ²A" ground state of the ClSnGeH₃⁺ cation, and ³A" excited state of neutral ClSnGeH₃.





Figure S28. Equilibrium geometries for the ¹A' ground state of BrSnGeH₃, ²A" ground state of the BrSnGeH₃⁻ anion, ²A" ground state of the BrSnGeH₃⁺ cation, and ³A" excited state of neutral BrSnGeH₃.





Figure S29. Equilibrium geometries for the ¹A' ground state of ISnGeH₃, ²A" ground state of the ISnGeH₃⁻ anion, ²A" ground state of the ISnGeH₃⁺ cation, and ³A" excited state of neutral ISnGeH₃.





Figure S30. Equilibrium geometries for the ¹A' ground state of FSnSnH₃, ²A" ground state of the FSnSnH₃⁻ anion, ²A" ground state of the FSnSnH₃⁺ cation, and ³A" excited state of neutral FSnSnH₃.





Figure S31. Equilibrium geometries for the ¹A' ground state of $ClSnSnH_3$, ²A" ground state of the $ClSnSnH_3^-$ anion, ²A" ground state of the $ClSnSnH_3^+$ cation, and ³A" excited state of neutral $ClSnSnH_3$.

BrSnSnH₃



Figure S32. Equilibrium geometries for the ¹A' ground state of BrSnSnH₃, ²A" ground state of the BrSnSnH₃⁻ anion, ²A" ground state of the BrSnSnH₃⁺ cation, and ³A" excited state of neutral BrSnSnH₃.





Figure S33. Equilibrium geometries for the ¹A' ground state of ISnSnH₃, ²A" ground state of the ISnSnH₃⁻ anion, ²A" ground state of the ISnSnH₃⁺ cation, and ³A" excited state of neutral ISnSnH₃.

Sn(SiH₃)₂



Figure S34. Equilibrium geometries for the ¹A ground state of $Sn(SiH_3)_2$, ²A ground state of the $Sn(SiH_3)_2^-$ anion, ²A ground state of the $Sn(SiH_3)_2^+$ cation, and ³A excited state of neutral $Sn(SiH_3)_2$.

Sn(GeH₃)₂



Figure S35. Equilibrium geometries for the ¹A ground state of $Sn(GeH_3)_2$, ²A ground state of the $Sn(GeH_3)_2^-$ anion, ²A ground state of the $Sn(GeH_3)_2^+$ cation, and ³A excited state of neutral $Sn(GeH_3)_2$.

$$Sn(SnH_3)_2$$



Figure S36. Equilibrium geometries for the ¹A ground state of $Sn(SnH_3)_2$, ²A ground state of the $Sn(SnH_3)_2^-$ anion, ²A ground state of the $Sn(SnH_3)_2^+$ cation, and ³A excited state of neutral $Sn(SnH_3)_2$.

CH₃SnSiH₃



Figure S37. Equilibrium geometries for the ¹A ground state of CH_3SnSiH_3 , ²A ground state of the $CH_3SnSiH_3^-$ anion, ²A ground state of the $CH_3SnSiH_3^+$ cation, and ³A excited state of neutral CH_3SnSiH_3 .

CH₃SnGeH₃



Figure S38. Equilibrium geometries for the ¹A ground state of CH₃SnGeH₃, ²A ground state of the CH₃SnGeH₃⁻ anion, ²A ground state of the CH₃SnGeH₃⁺ cation, and ³A excited state of neutral CH₃SnGeH₃.

CH₃SnSnH₃



Figure S39. Equilibrium geometries for the ¹A ground state of CH₃SnSnH₃, ²A ground state of the CH₃SnSnH₃⁻ anion, ²A ground state of the CH₃SnSnH₃⁺ cation, and ³A excited state of neutral CH₃SnSnH₃.

SiH₃SnGeH₃



Figure S40. Equilibrium geometries for the ¹A ground state of SiH₃SnGeH₃, ²A ground state of the SiH₃SnGeH₃⁻ anion, ²A ground state of the SiH₃SnGeH₃⁺ cation, and ³A excited state of neutral SiH₃SnGeH₃.



Figure S41. Equilibrium geometries for the ¹A ground state of SiH₃SnSnH₃, ²A ground state of the SiH₃SnSnH₃⁻ anion, ²A ground state of the SiH₃SnSnH₃⁺ cation, and ³A excited state of neutral SiH₃SnSnH₃.



Figure S42. Equilibrium geometries for the ¹A ground state of GeH₃SnSnH₃, ²A ground state of the GeH₃SnSnH₃⁻ anion, ²A ground state of the GeH₃SnSnH₃⁺ cation, and ³A excited state of neutral GeH₃SnSnH₃.