

**Supplementary Information: An ab initio investigation of the hydration of tin(II)**

Cory C. Pye\* and C. Mahesh Gunasekara

**Table S1: Total Energies of Aquatin(II) Species** (Hartrees, bold indicates a minimum energy structure)

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sn}^{2+} K_h$	<b>-2.4976820</b>	<b>-2.4976820</b>	<b>-2.4976820</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_{2v}$	<b>-19.3834241</b>	<b>-19.4471757</b>	<b>-19.451076</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} D_{2d}$	-36.2134449	-36.3617869	-36.3691509
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_s$	-36.2513972	-36.3811994	-36.3891625
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_2$	<b>-36.2519717</b>	<b>-36.3814073</b>	<b>-36.3893273</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$
$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	<b>-36.2314652</b>	<b>-36.3665039</b>	<b>-36.3745943</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#1$	-53.0535749	-53.2749324	-53.2859914
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#2$	-53.0552289	-53.2749108	-53.2858423
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_3$	-53.0554227	-53.2758017	-53.2868508
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#1$	-53.1041536	-53.2985224	-53.3101763
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#2$	-53.0985720	-53.2954865	-53.3071799
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_3$	<b>-53.1066883</b>	<b>-53.3034407</b>	<b>-53.3155297</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_{2v}$	-53.0831007	<b>-53.2870511</b>	<b>-53.2985935</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_s$	<b>-53.0852889</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-69.8854387	-70.1788927	-70.1934987
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-69.8853439	-70.1787422	-70.1933516
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	-70.1790514	-70.1936992
$\text{Sn}(\text{H}_2\text{O})_4^{2+} S_4$	-69.8859666	-70.1796809	-70.1943981
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-69.9222323	-70.1969552	-70.2123090
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-69.9233806	-70.1958500	-70.2111450
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-69.9285829	-70.2020357	-70.2175340
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_2$	<b>-69.9286022</b>	<b>-70.2021062</b>	<b>-70.2176852</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#1$	-69.9274818	-70.2000827	<b>-70.2158847</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#2$	-69.9286969	<b>-70.2009104</b>	<b>-70.2166196</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_I \#2$	<b>-69.9318203</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#1$	-86.7405151	-87.0953573	-87.1145853
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	-86.7305692	-87.0853187	-87.1041995
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	-86.7341384	-87.0852413	-87.1038539
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$	-86.7311648	-87.0842526	-87.1029393
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#1$	[4+1]	<b>-87.0953722</b>	<b>-87.1146106</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	-86.7431707	-87.0929515	-87.1121303
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	-86.7414078	-87.0920399	-87.1113562
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$	n/a	-87.0932092	-87.1125601
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	<b>-86.7432960</b>	-87.0929977	-87.1121727
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#2$	-86.7437804	<b>-87.0945197</b>	<b>-87.1139350</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_I \#2$	<b>-86.7480007</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s [4+1]$	<b>-86.7496935</b>	<b>-87.0949666</b>	<b>-87.1142566</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 2\text{H}_2\text{O} C_s \#1$	<b>-86.7431609</b>	<b>-87.0907782</b>	<b>-87.1103930</b>

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	-103.5184256	-103.9659040	-103.9883122
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3$	[3+3]	<b>-103.9781668</b>	<b>-104.0012817</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	-103.5514850	-103.9787634	-104.0012949
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-103.5541494</b>	<b>-103.9844125</b>	<b>-104.0072757</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	-103.5480427	-103.9798195	-104.0023692
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_2 \#1$	-103.5630470	<b>-103.9890809</b>	<b>-104.0122594</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$	-103.5583146	<b>-103.9816992</b>	-104.0047619
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#2$	-103.5587732	<b>-103.9849344</b>	<b>-104.0081441</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_{3v} \#1$	-103.5464789	<b>-103.9758716</b>	<b>-103.9997380</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_3 \#1$	-103.5583515	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3 [3+3]$	<b>-103.5678612</b>	<b>-103.9794553</b>	<b>-104.0023033</b>
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3$	[5+2]	[5+2]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#5$	-120.3150449	-120.8314501	-120.8573659
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#6$	-120.3190256	-120.8367818	-120.8627180
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#7$	-120.3147157	-120.8305532	-120.8562555
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#8$	-120.3278412	-120.8438312	-120.8703080
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10$	[5+2]	-120.8333056	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11$	[4+3]	[6+1]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#13$	[4+3]	-120.8426599	-120.8692813
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#14$	[4+3]	-120.8424404	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#15$	[4+3]	-120.8447408	-120.8714230
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#16$	[5+2]	-120.8452330	-120.8714987
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1 [5+2]$	-120.3507532	-120.8609829	-120.8876534
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2 [5+2]$	-120.3433698	-120.8511482	-120.8773714
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3 [5+2]$	-120.3433635	-120.8494953	120.8755932
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4 [5+2]$	-120.3451163	-120.8510203	-120.8771806
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9 [5+2]$	-120.3499502	-120.8590936	-120.8856083
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10 [5+2]$	-120.3420870	-120.8485514	-120.8745535
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11 [5+2]$			
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12 [5+2]$	-120.3431742	-120.8474987	-120.8734204
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#5$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#6$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#7$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#8$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#10$	n/a	-120.8462544	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#13$	n/a	$C_2 \#15$	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#14$	n/a	$C_2 \#15$	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#15$	n/a	-120.8473088	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#16$	n/a	[5+2]	[5+2]

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4h} \#1$	-137.0916423	-137.6920082	-137.7207007
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4h} \#2$	-137.0917640	-137.6921976	-137.7209488
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4d} \#1$	-137.1069771	-137.7109686	-137.7403521
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4d} \#2$	-137.1055061	-137.7097560	-137.7386785
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#1$	$D_4 \#2$	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#2$	-137.1128956	-137.7200850	-137.7502337
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#3$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#4$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4h} \#1$	-137.1082453	-137.7171293	-137.7474312
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#1$	-137.1175902	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#2$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#3$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#4$	-137.0930142	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_8 \#1$	-137.1161257	-137.7236543	-137.7533251
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_8 \#2$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#1$	-137.1021904	-137.7073334	-137.7368372
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#2$	-137.1033734	-137.7059272	-137.7348490
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#3$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#4$	-137.1037657	-137.7062567	-137.7356012
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#5$	-137.1121360	-137.7194401	-137.7493279
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#1$	$D_{4h} \#2$	$D_{4h} \#2$	$D_{4h} \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#3$	-137.1062596	-137.7127311	-137.7423831
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#4$	$D_{2h} \#3$	$D_{2h} \#3$	$D_{2h} \#3$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#1$	[4+4]	-137.7172126	-137.7468867
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#2$	[4+4]	$C_{2v} \#1$	$C_{2v} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#3$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#4$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#5$	[6+2]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#6$	[6+2]	[6+2]	[6+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#1$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#2$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#3$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#1$	-137.1121360	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#2$	-137.1120004	-137.7188204	-137.7489013
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#3$	$S_4 \#2$	$S_4 \#2$	$S_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#4$	$S_4 \#2$	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#1$	-137.1136552	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#2$	$D_2 \#1$	-137.7196880	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#3$	$D_2 \#1$	$D_2 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#4$	$D_2 \#1$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#5$	$D_2 \#1$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#7$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$

$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#1$	n/a	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#6$	[4+2+2]	[4+4]	[6+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#8$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#9$	n/a	[4+4]	n/a
	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#1$	-153.8970798	-154.5809886	-154.6141191
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#2$	-153.8825396	-154.5599663	-154.5925006
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#3$	-153.8869544	-154.5676578	-154.6008449
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#4$	-153.8990692	-154.5839746	-154.6171675
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#1$	-153.9043313	-154.5920425	-154.6256192
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#3$	$D_3 \#1$	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 [6+3]$	-153.9216208	-154.6141129	-154.6480905
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#1$	-153.9012495	-154.5883577	-154.6218005
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#2$	-153.9014039	-154.5868623	-154.6200976
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1$	[6+3]	$D_{3h} \#1$	$D_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4$	-153.9099261	-154.5839750	-154.6172324
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2 [6+3]$	-153.9438890	-154.5981505	-154.6314686
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3 [6+3]$	-153.9259339	-154.5981562	-154.6329234
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1$	[6+3], then [3+3+3]	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2$	[6+3], then [3+3+3]	$C_3 \#1 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3$	[3+3+3]	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#4$	n/a	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#5$	[6+3], then [3+3+3]	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1 [6+3]$	n/a	<b>-154.6117308</b>	<b>-154.6461228</b>
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3 [6+3]$	n/a	<b>-154.6017287</b>	<b>-154.6369464</b>
$\text{Sn}(\text{H}_2\text{O})_{18}^{2+} T [6+12]$	-305.0353548	-306.4668456	-306.5371867

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sn}^{2+} K_h$	<b>-2.4626155</b>	<b>-2.4628587</b>	<b>-2.4725025</b>
$\text{Sn}(\text{H}_2\text{O})^{2+} C_{2v}$	<b>-77.5834802</b>	<b>-78.5957448</b>	<b>-78.5989430</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} D_{2d}$	-152.6316254	-154.6805982	-154.6821858
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_s$	-152.6845504	-154.7068436	-154.7051774
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_2$	(i.p. $C_{2v}$ ) <b>-152.6868650</b>	<b>-154.7070937</b>	<b>-154.7053064</b>
$\text{Sn}(\text{H}_2\text{O})^{2+} + \text{H}_2\text{O} C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$
$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	<b>-152.6554919</b>	<b>154.6931148</b>	<b>-154.6904362</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#1$	-227.6866932	-230.7632816	-230.7636386
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#2$	-227.6954459	-230.7631326	-230.7636101
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_3$	$D_{3h} \#2$	-230.7643214	-230.7646327
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#1$	-227.7731084	-230.7973847	-230.7918660
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#2$	-227.7623134	-230.7923859	-230.7880092
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_3$	<b>-227.7731643</b>	<b>-230.8021235</b>	<b>-230.7965443</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_{2v}$	<b>-227.7455791</b>	<b>-230.7870719</b>	<b>-230.7832017</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-302.7381288	-306.8338578	-306.8337552
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-302.7380715	-306.8337348	-306.8336536
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	-306.8341441	-306.8338267
$\text{Sn}(\text{H}_2\text{O})_4^{2+} S_4$	-302.7386944	-306.8349177	-306.8346022
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-302.8057711	-306.8603573	-306.8547402
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-302.8146823	-306.8608890	-306.8547556
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-302.8161753	<b>-306.8679144</b>	-306.8612116
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_2$	-302.8166961	n/a	<b>-306.8612335</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_s$	<b>-302.8178253</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#1$	-302.8155723	-306.8707698	-306.8638543
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-302.8187704</b>	<b>-306.8722193</b>	<b>-306.8651379</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#1$	-377.8435705	-382.9252031	-382.9187846
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	-377.8279961	-382.9116388	-382.9069352
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	-377.8425752	-382.9143048	-382.9081495
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$	-377.8328574	-382.9118302	-382.9065311
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#1$	n/a	[4+1]	[4+1]
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_2$	$C_{2v}$ <b>-377.8437618</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	<b>-377.8531250</b>	-382.9294848	-382.9218655
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	-377.8471287	-382.9273404	-382.9202837
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$	n/a	n/a	-382.9218892
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	n/a	-382.9294932	-392.9219212
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#2$	-377.8509902	<b>-382.9305530</b>	<b>-392.9229099</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_I \#2$	<b>-377.8531250</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s [4+1]$	<b>-377.8542952</b>	<b>-382.9331753</b>	<b>-382.9249897</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 2\text{H}_2\text{O} C_s \#1$	<b>-377.8431471</b>	<b>-382.9309163</b>	<b>-382.9231226</b>

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	-452.7838912	-458.9487651	-458.9477675
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3$	-452.8439257	[3+3]	[3+3]
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	-452.8758478	-458.9789543	-458.9714842
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-452.8759277</b>	<b>-458.9847079</b>	<b>-458.9771795</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	-452.8749358	-458.9857764	-458.9786397
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_2 \#1$	<b>-452.8843354</b>	<b>-458.9964446</b>	<b>-458.9874922</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$	-452.8761688	-458.9871596	-458.9786425
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#2$	<b>-452.8776668</b>	<b>-458.9912546</b>	<b>-458.9826880</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_{3v} \#1$	-452.8532537	458.9822721	-458.9729986
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_3 \#1$	<b>-452.8786065</b>	-458.9862080	-458.9766731
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3 [3+3]$	<b>-452.8874055</b>	<b>-458.9955291</b>	<b>-458.9853491</b>
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1$	[6+1]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2$	[6+1]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3$	[6+1] -527.8032887	[6+1]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#5$	[5+2]	-534.9755149	-534.9739495
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#6$	[5+2]	-534.9808923	-534.9797286
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#7$	[5+2]	-534.9779544	-534.9753134
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#8$	[5+2]	[5+2]	-534.9881490
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10$	[6+1] -527.8000604	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11$	[6+1] -527.8061942	[4+3] -535.0096029	[4+3] -535.0025721
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12$	[6+1] -527.8048504	[5+2] -535.0159890	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#13$	[4+3]	[4+3]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#14$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#15$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#16$	[5+2]	-534.9915126	-534.9892702
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1 [5+2]$	-527.8799308	-535.0300659	-535.0222504
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2 [5+2]$	-527.8717812	-535.0183830	-535.0115350
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3 [5+2]$	-527.8779058	-535.0172752	-535.0098693
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4 [5+2]$	-527.8786727	-535.0191211	-535.0115904
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9 [5+2]$	-527.8806916	-535.0285143	-535.0203857
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10 [5+2]$	-527.8718080	-535.0162755	-535.0090377
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11 [5+2]$			
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12 [5+2]$	-527.8787610	-535.0159894	-535.0080829
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#5$	n/a	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#6$	n/a	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#7$	n/a	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#8$	n/a	n/a	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#16$	n/a	[5+2]	[5+2]

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4h} \#1$	-602.7629056	-610.9908991	-610.9927169
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4h} \#2$	-602.7630829	-610.9910799	-610.9928801
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4d} \#1$	-602.7758593	-611.0141986	-611.0145752
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{4d} \#2$	-602.7752269	-611.0110672	-611.0116444
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#1$	$D_4 \#2$	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#2$	-602.7810916	-611.0260888	-611.0261437
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#3$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \#4$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4h} \#1$	-602.7757305	-611.0236917	-611.0241601
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#1$	-602.8062907	-611.0178104	-611.0152471
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#2$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#3$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \#4$	-602.7697254	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_8 \#1$	-602.7836074	-611.0285336	-611.0282437
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_8 \#2$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#1$	-602.7709485	-611.0089524	-611.0098318
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#2$	-602.7724245	-611.0074649	-611.0080770
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#3$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#4$	-602.7753969	-611.0073923	-611.0080452
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \#5$	-602.7798527	-611.0250322	-611.0251432
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#1$	$D_{4h} \#2$	$D_{4h} \#2$	$D_{4h} \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#3$	-602.7734770	-611.0155752	-611.0160446
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \#4$	$D_{2h} \#3$	$D_{2h} \#3$	$D_{2h} \#3$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#1$	[4+4]	[4+4]	-611.0239684
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#2$	[4+4]	[4+4]	$C_{2v} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#3$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#4$	[6+2]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#5$	[6+2]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2v} \#6$	[6+2]	[6+2]	[6+2] -611.0485412
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#1$	[4+4]	[4+4]	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#2$	[4+4]	-611.0287362	-611.0274035
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_4 \#3$	[4+4]	-611.0287589	-611.0276042
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#1$	-602.7799271	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#2$	-602.7805989	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#3$	$S_4 \#2$	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#4$	$S_4 \#1$	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_4 \#5$	$S_4 \#1$	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#1$	-602.7817719	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#2$	$D_2 \#1$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#3$	$D_2 \#1$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#4$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#5$	$D_2 \#1$	$D_4 \#2$	$D_4 \#2$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_2 \#7$	$D_4 \#2$	$D_4 \#2$	$D_4 \#2$



$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#1$	n/a	n/a	[4+4]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#4$	n/a	[4+2+2]	[6+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#5$	n/a	[4+2+2]	[6+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#6$	[4+2+2]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#8$	[4+4]	n/a	n/a
	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#1$	-677.7659303	-687.0436706	-687.0445328
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#2$	-677.7567919	-687.0185417	-687.0207191
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#3$	-677.7557639	-687.0306811	-687.0305720
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#4$	-677.7669325	-687.0457065	-687.0465128
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#1$	-677.7717322	[6+3]	-687.0565025
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#2$	$D_3 \#1$	[6+3]	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#3$	$D_3 \#1$	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#4$	$D_3 \#1$	[6+3]	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 [6+3]$	-677.8122748	-687.0997880	-687.0982714
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#1$	-677.7699489	-687.0513492	-687.0522836
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#2$	-677.7679599	-687.0514534	-687.0523265
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3$	$C_{3h} \#1$	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4$	$C_{3h} \#2$	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3 [6+3]$		-687.0655164	-687.0641968
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4 [6+3]$		-687.0964117	-687.0951859
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1$	[6+3]	-687.0480445	-687.0458295
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4$	[6+3]	-687.0506703	-687.0478828
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1 [6+3]$	-677.8875289		
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2 [6+3]$	-677.8752448	-687.0914505	-687.0844896
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3 [6+3]$	-677.8061296	-687.0822411	-687.0779010
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4 [6+3]$	-677.8111663		
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1$	[6+3], then [3+3+3]	n/a	[6+3], then [3+3+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2$	$C_3 \#2 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3$	$C_3 \#3 [6+3]$	[3+3+3]	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#4$	n/a	[3+3+3]	[3+3+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#5$	n/a	[3+3+3]	[3+3+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2 [6+3]$	<b>-677.8955091</b>	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3 [6+3]$	<b>-677.8925007</b>	-687.0923185	-687.0848568
$\text{Sn}(\text{H}_2\text{O})_{18}^{2+} T [6+12]$	-1352.7603230	-1371.4460182	-1371.4444249

	MP2/CEP-31G*	MP2/CEP-121G*	MP2/gen (5d) M: CEP-121G* OH: 6-31G*	MP2/gen (5d) M: CEP-121G* OH: 6-31+G*
$\text{Sn}^{2+} K_h$	<b>-2.5167184</b>	<b>-2.5167184</b>	<b>-2.5167184</b>	<b>-2.5167184</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_{2v}$	<b>-19.6540746</b>	<b>-19.6698782</b>	<b>-78.8235443</b>	<b>-78.8292647</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} D_{2d}$	-36.7558913	-36.7872336	-155.0888630	-155.1031358
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_s$	-36.7742112	-36.8061781	-155.1111468	-155.1231046
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_2$	<b>-36.7744271</b>	<b>-36.8063047</b>	<b>-155.1112802</b>	<b>-155.1232946</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$
$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	<b>-36.7648087</b>	<b>-36.7962511</b>	<b>-155.1005517</b>	<b>-155.1161746</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#1$	-53.8550190	-53.9023358	-231.3541460	-231.3757110
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#2$	-53.8551131	-53.9020189	-231.3533533	-231.3756406
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_3$	-53.8561844	-53.9033956	-231.3549609	-231.3769215
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#1$	-53.8759476	-53.9236103	-231.3791796	-231.3991269
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#2$	-53.8730658	-53.9208078	-231.3761524	-231.3960019
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_3$	<b>-53.8819903</b>	<b>-53.9303315</b>	<b>-231.3853827</b>	<b>-231.4050646</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_{2v}$	<b>-53.8708551</b>	<b>-53.9176792</b>	<b>-231.3747520</b>	<b>-231.3941638</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-70.9442561	-71.0070795	-307.6075985	-307.6398960
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-70.9440391	-71.0068474	-307.6074914	-307.6397588
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_2$	-70.9443738	-71.0072629	$D_{2d} \#1$	-307.6399012
$\text{Sn}(\text{H}_2\text{O})_4^{2+} S_4$	-70.9450923	-71.0081099	-307.6083927	-307.6409923
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-70.9600414	-71.0236551	-307.6273204	-307.6564798
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-70.9581895	-71.0216036	-307.6244786	-307.6547945
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-70.9657754	-71.0296173	-307.6331990	-307.6625141
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_2$	<b>-70.9660317</b>	<b>-71.0301991</b>	<b>-307.6337727</b>	<b>-307.6629445</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#1$	<b>-70.9676161</b>	<b>-71.0312429</b>	-307.6373867	<b>-307.6651269</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-70.9683594</b>	<b>-71.0316288</b>	<b>-307.6379641</b>	<b>-307.6657735</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#1$	-88.0448420	-88.1248411	-383.8745675	-383.9157711
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	-88.0332257	-88.1126254	-383.8628047	-383.9039197
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	-88.0325006	88.1112474	-383.8624118	-383.9032234
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$	-88.0315241	-88.1104893	-383.8604384	-383.9025321
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_2$	n/a	n/a	-383.8746235	n/a
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#1$	<b>-88.0449020</b>	<b>-88.1249398</b>	<b>-383.8753704</b>	<b>-383.9159029</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#2$	n/a	n/a	-383.8745677	n/a
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	-88.0442260	-88.1230951	-383.8765091	-383.9155685
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	-88.0437062	-88.1230097	-383.8766242	-383.9150198
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$	-88.0452154	-88.1248338	-383.8786596	-383.9169395
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	-88.0444629	-88.1233260	-383.8767711	-383.9157711
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#2$	-88.0464965	-88.1260150	-383.8794501	-383.9179260
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_l \#2$	<b>-88.0464992</b>	<b>-88.1261893</b>	<b>-383.8800403</b>	<b>-383.9180171</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s [4+1]$	<b>-88.0464646</b>	<b>-88.1257151</b>	<b>-383.8778419</b>	<b>-383.9170463</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 2\text{H}_2\text{O} C_s \#1$	<b>-88.0463078</b>	<b>-88.1254686</b>	<b>-383.8826452</b>	<b>-383.9185739</b>

	MP2/CEP-31G*	MP2/CEP-121G*	MP2/gen (5d) M: CEP-121G* OH: 6-31G*	MP2/gen (5d) M: CEP-121G* OH: 6-31+G*
$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	-105.0998234	-105.1950030	-460.0872358	-460.1464384
$\text{Sn}(\text{H}_2\text{O})_6^{2+} S_6$	n/a	n/a	-460.0885222	n/a
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3$	<b>-105.1128911</b>	-105.2090915	[3+3]	-460.1584960
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	-105.1145549	-105.2089004	-460.1101352	-460.1599624
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-105.1220925</b>	<b>-105.2171871</b>	<b>-460.1182637</b>	<b>-460.1676422</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	-105.1209405	-105.2148016	-460.1196755	-460.1658292
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_2 \#1$	<b>-105.1300427</b>	<b>-105.2248808</b>	<b>-460.1290800</b>	<b>-460.1755889</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$	-105.1208933	-105.2157921	-460.1201502	-460.1664532
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#2$	<b>-105.1254209</b>	<b>-105.2204533</b>	<b>-460.1247914</b>	<b>-460.1710329</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_{3v} \#1$	<b>-105.1158160</b>	<b>-105.2122038</b>	<b>-460.1191138</b>	<b>-460.1636853</b>
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3 [3+3]$	<b>-105.1200335</b>	<b>-105.2135731</b>	<b>-460.1164441</b>	<b>-460.1645166</b>
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3$	[6+1]	[6+1]	[6+1]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#5$	-122.1466977	-122.2576220	-536.3019035	-536.3670074
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#6$	-122.1541133	-122.2648606	-536.3067786	-536.3744048
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#7$	-122.1503047	-122.2620385	-536.3071092	-536.3709942
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#8$	-122.1621089	-122.2738236	-536.3174359	-536.3824650
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9$	-122.1610826	-122.2722681	[5+2]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10$	-122.1492798	-122.2589951	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11$	[4+3]	[4+3]	[4+3]	[4+3]
	-122.1622854	-122.2717312	-536.3173541	-536.3814919
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12$	-122.1493804	[5+2]	-536.3020924	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#13$	-122.1605101	[4+3]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#14$	[4+3]	[5+2]	[5+2]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#15$	-122.1634274	-122.2749151	[5+2]	-536.3842153
			-536.3216623	[5+2]
				-536.3858208
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#16$	-122.1637137	-122.2750229	-536.3159358	-536.3858338
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1 [5+2]$	-122.1832342	-122.2940842	-536.3401952	-536.4025476
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2 [5+2]$	-122.1711558	-122.2812292	-536.3278935	-536.3908497
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3 [5+2]$	-122.1691414	-122.2787901	-536.3265558	-536.3884279
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4 [5+2]$	-122.1708561	-122.2806541	-536.3286509	-536.3902309
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9 [5+2]$	-122.1807966	-122.2912013	-536.3376788	-536.4001543
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10 [5+2]$	-122.1677760	-122.2771905	-536.3242955	-536.3872004
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11 [5+2]$				
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12 [5+2]$	-122.1662762	-122.2754472	-536.3238739	-536.3853546
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#5$	[5+2]	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#6$	[5+2]	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#7$	[4+3]	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#8$	[5+2]	[5+2]	[5+2]	[5+2]

$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#9$	[5+2]	[5+2]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#10$	[6+1]	[6+1]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#12$	[5+2]	n/a	[6+1]	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#13$	[4+3]	n/a	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#15$	[4+3]	[4+3]	n/a	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#16$	[5+2]	[5+2]	[5+2]	[4+3]

	MP2/CEP-31G*	MP2/CEP-121G*	MP2/gen (5d) M: CEP-121G* OH: 6-31G*	MP2/gen (5d) M: CEP-121G* OH: 6-31+G*
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #1	-139.1899651	-139.3151683	-612.5068117	-612.5850668
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #2	-139.1903160	-139.3157341	-612.5074275	-612.5853035
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #1	-139.2124287	-139.3396504	-612.5279764	-612.6078220
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #2	-139.2116219	-139.3375183	-612.5251916	-612.6069587
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #1	-139.2124288*	-139.3396941	-612.5284151	-612.6078463
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #2	-139.2270820	-139.3554088	-612.5459720	-612.6241169
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #1	-139.2247492	-139.3533155	-612.5438270	-612.6217057
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #2	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #1	n/a	n/a	-612.5283028	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #2	n/a	-139.3378893	[4+4]	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #1	-139.2283462	-139.3568124	-612.5452691	-612.6250077
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #2	<i>S</i> <sub>8</sub> #1 -139.2278620	<i>S</i> <sub>8</sub> #1 -139.3561942	<i>S</i> <sub>8</sub> #1 -612.5460669	<i>S</i> <sub>8</sub> #1 -612.6250219
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #1	-139.2103157	-139.3372680	-612.5269562	-612.6058790
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #2	-139.2069033	-139.3323566	-612.5218283	-612.6026542
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #3	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #4	-139.2077505	-139.3346638	-612.5259344	-612.6036306
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #5	-139.2245461	-139.3521339	-612.5409272	-612.6218308
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #1	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #2	-139.1910699	-139.3178215	-612.5098950	-612.5868288
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #3	-139.2160513	-139.3432206	-612.5319117	-612.6124419
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #4	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #1	-139.2197112	-139.3469296	-612.5366690	-612.6160677
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #2	-139.2196464	-139.3465075	<i>C</i> <sub>2v</sub> #1	<i>C</i> <sub>2v</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #3	[4+4]	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #6	[6+2]	[6+2]	[6+2]	[6+2]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #1	[4+4]	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #2	n/a	n/a	-612.5460811	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #3	<i>S</i> <sub>8</sub> #2	<i>S</i> <sub>8</sub> #2	-612.5461289	-612.6250219
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #2	-139.2244835	-139.3526430	-612.5433776	612.6218317
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #3	<i>S</i> <sub>4</sub> #5	<i>S</i> <sub>4</sub> #2	<i>S</i> <sub>4</sub> #2	<i>S</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #4	<i>S</i> <sub>4</sub> #2	-139.3526812	-612.5435486	<i>S</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #5	-139.2246084	<i>S</i> <sub>4</sub> #2	<i>S</i> <sub>4</sub> #2	<i>S</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #5	<i>D</i> <sub>4</sub> #2	-139.3554087	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #6	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>2</sub> #5	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #7	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>2</sub> #5	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1

$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{2h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#1$	[4+4]	[4+4]	[4+2+2]	[4+2+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#2$	[4+4]	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#6$	[4+4]	[6+2]	[4+2+2]	[6+2]
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#7$	n/a	n/a	[4+2+2]	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#10$	n/a	[6+2]	n/a	n/a
	MP2/CEP-31G*	MP2/CEP-121G*	MP2/gen (5d) M: CEP-121G* OH: 6-31G*	MP2/gen (5d) M: CEP-121G* OH: 6-31+G*
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#1$	-156.2662794	156.4091563	-688.7445207	-688.8391740
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#2$	156.2410392	-156.3830509	-688.7207277	-688.8121788
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#3$	-156.2505175	-156.3933783	-688.7306496	-688.8235196
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#4$	-156.2712296	-156.4140620	-688.7492059	-688.8432813
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#1$	-156.2801652	-156.4239790	-688.7592218	-688.8533523
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#2$	$D_3 \#1$	-156.4238043	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#3$	[6+3]	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	[6+3]	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 [6+3]$	-156.3114007	-156.4531152	-688.7947135	-688.8819366
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#1$	-156.2792308	-156.4230212	-688.7597329	-688.8512464
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#2$	-156.2765182	-156.4206692	-688.7577908	-688.8495496
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4$	-156.2743044	-156.4179850	-688.7527138	-688.8477433
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1$	$D_{3h} \#1$	$D_{3h} \#1$	-688.7447753	$D_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2$	[6+3]	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3$	[6+3]	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4$	-156.2712922	-156.4142206	-688.7502038	-688.8432914
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2 [6+3]$	-156.2838724	-156.4254644	-688.7686107	-688.8538609
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3 [6+3]$	-156.2894899	-156.4329061	-688.7687221	-688.8537569
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#4$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#5$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1 [6+3]$	-156.3038864	-156.4470389	<b>-688.7899471</b>	-688.8734770
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3 [6+3]$	<b>-156.2989000</b>	<b>-156.4432958</b>	<b>-688.7894818</b>	<b>-688.8708052</b>

	HF/gen (5d) M: CEP-121G* OH: 6-31G*	HF/gen (5d) M: LANL2DZ OH: 6-31G*	HF/gen (5d) M: SDD OH: 6-31G*
$\text{Sn}^{2+} K_h$	<b>-2.4976820</b>	<b>-2.4628587</b>	<b>-2.4725025</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_{2v}$	<b>-78.6112981</b>	<b>-78.5822197</b>	<b>-78.5856492</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} D_{2d}$	-154.6844694	-154.6561475	-154.6581328
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_s$	-154.7077973	-154.6813850	-154.6803524
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_2$	<b>-154.7079465</b>	<b>-154.6815799</b>	<b>-154.6804476</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$
$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	<b>-154.6925861</b>	<b>-154.6681461</b>	<b>-154.6643350</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#1$	-230.7585184	-230.7306753	-230.7312716
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#2$	-230.7578208	-230.7298397	-230.7307192
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_3$	-230.7591167	-230.7312491	-230.7318750
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#1$	-230.7866025	-230.7616359	-230.7572787
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#2$	-230.7832867	-230.7578270	-230.7542790
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_3$	<b>-230.7917260</b>	<b>-230.7666933</b>	<b>-230.7621929</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_{2v}$	<b>-230.7769536</b>	<b>-230.7516944</b>	<b>-230.7485694</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-306.8219853	-306.7939497	-306.7939928
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-306.8219090	-306.7938756	-306.7939224
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sn}(\text{H}_2\text{O})_4^{2+} S_4$	-306.8226755	-306.7946605	-306.7946393
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-306.8444100	-306.8193055	-306.8144601
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-306.8427195	-306.8179706	-306.8130096
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-306.8499170	-306.8253020	-306.8197822
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_2$	<b>-306.8500601</b>	<b>-306.8253687</b>	<b>-306.8199417</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#1$	-306.8510849	-306.8266512	-306.8208356
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-306.8518165</b>	<b>-306.8274239</b>	<b>-306.8215566</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#1$	-382.9014525	-382.8765821	-382.8710536
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	-382.8909851	-382.8652901	-382.8610975
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	-382.8910309	-382.8660930	-382.8610184
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$	-382.8893169	-382.8639376	-382.8594786
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#1$	<b>-382.9020192</b>	<b>-382.8771113</b>	<b>-382.8715255</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	-382.9023499	-382.8781321	-382.8717812
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	-382.9018315	-382.8773238	-382.8712348
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$	-382.9030632	-382.8785857	-382.8724359
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	-382.9023949	-382.8781412	-382.8718450
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#2$	-382.9043422	<b>-382.8800856</b>	-382.8735706
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_I \#2$	<b>-382.9043448</b>	n/a	<b>-382.8735706</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s [4+1]$	<b>-382.9036049</b>	<b>-382.8792872</b>	<b>-382.8724747</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 2\text{H}_2\text{O} C_s \#1$	<b>-382.9042930</b>	<b>-382.8800374</b>	<b>-382.8734552</b>

	HF/gen (5d) M: CEP-121G* OH: 6-31G*	HF/gen (5d) M: LANL2DZ OH: 6-31G*	HF/gen (5d) M: SDD OH: 6-31G*
$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	n-458.9251621	-458.8966175	-458.8956482
$\text{Sn}(\text{H}_2\text{O})_6^{2+} S_6$	-458.9251693	-458.8968061	-458.8957101
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3$	-458.9442676	-458.9192268	-458.9135830
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	-458.9468911	-458.9224177	-458.9161571
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-458.9530390</b>	<b>-458.9284905</b>	<b>-458.9220996</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	-458.9519831	-458.9275680	-458.9214775
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_2 \#1$	<b>-458.9615350</b>	<b>-458.9376224</b>	<b>-458.9299845</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$	-458.9536329	-458.9294898	-458.9223920
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#2$	<b>-458.9574340</b>	<b>-458.9334129</b>	<b>-458.9261302</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_{3v} \#1$	<b>-458.9509318</b>	<b>-458.9268370</b>	<b>-458.9193977</b>
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3 [3+3]$	<b>-458.9503789</b>	<b>-458.9265914</b>	<b>-458.9182573</b>
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3$	[6+1]	[6+1]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#5$	-534.9535371	-534.9264668	-534.9240631
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#6$	-534.9576228	-534.9302713	-534.9281329
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#7$	-534.9572340	-534.9304144	-534.9272545
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#8$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11$	[6+1] [4+3] -534.9686715	[6+1] -534.9342016 [4+3] -534.9436517	[4+3] -534.9378475
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#13$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#14$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#15$	[5+2] -534.9719362	[5+2] -534.9467909	[5+2] -534.9410932
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#16$	-534.9657419	-534.9385240	-534.9359482
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1 [5+2]$	-534.9876333	-534.9631520	-534.9564404
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2 [5+2]$	-534.9770486	-534.9521860	-534.9463502
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3 [5+2]$	-534.9759371	-534.9514724	-534.9452546
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4 [5+2]$	-534.9776255	-534.9531545	-534.9468560
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9 [5+2]$	-534.9857827	-534.9614882	-534.9546465
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10 [5+2]$	-534.9744169	-534.9497911	-534.9437513
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11 [5+2]$			
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12 [5+2]$	-534.9740862	-534.9498937	-534.9433829
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#5$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#6$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#7$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#16$	[5+2]	[5+2]	[5+2]



	HF/gen (5d) M: CEP-121G* OH: 6-31G*	HF/gen (5d) M: LANL2DZ OH: 6-31G*	HF/gen (5d) M: SDD OH: 6-31G*
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #1	-610.9717840	-610.9427852	-610.9438852
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #2	-610.9720979	-610.9430417	-610.9440865
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #1	-610.9895323	-610.9610768	-610.9609642
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #2	-610.9873896	-610.9589987	-610.9590722
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #2	-611.0002501	-610.9712586	-610.9710045
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #1	-610.9980519	-610.9691900	-610.9692277
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #2	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #1	-610.9904855	-610.9635865	-610.9617527
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #2	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #3	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #1	-611.0014542	-610.9726486	-610.9719091
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #2	<i>S</i> <sub>8</sub> #1	<i>S</i> <sub>8</sub> #1	<i>S</i> <sub>8</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #1	-610.9869206	-610.9580942	-610.9582983
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #2	-610.9842909	-610.9554446	-610.9555170
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #3	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #4	-610.9862435	-610.9573355	-610.9572626
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #5	-610.9989176	-610.9701312	-610.9698607
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #1	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #3	-610.9919901	-610.9633412	-610.9632692
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #4	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #1	-610.9983511	[4+4]	-610.9686482
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #2	<i>C</i> <sub>2v</sub> #1	-610.9722860	<i>C</i> <sub>2v</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #3	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #4	[4+4]	[4+4]	-610.9555672
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #6	[6+2]	[6+2]	[6+2]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #1	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #3	<i>S</i> <sub>8</sub> #1	[4+4]	-610.9721317
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #2	-610.9989261	<i>D</i> <sub>2d</sub> #5	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #3	<i>S</i> <sub>4</sub> #2	<i>D</i> <sub>2d</sub> #5	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #4	-610.9987746	-610.9699202	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #5	<i>S</i> <sub>4</sub> #2	<i>D</i> <sub>2d</sub> #5	-610.9698614
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #5	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #7	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2h</sub> #2	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2</sub> #1	[4+4]	n/a	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2</sub> #2	n/a	[4+4]	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2</sub> #3	n/a	n/a	[4+2+2]

$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#6$	[4+4]	n/a	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#7$	[4+2+2]	[4+2+2]	n/a
	HF/gen (5d) M: CEP-121G* OH: 6-31G*	HF/gen (5d) M: LANL2DZ OH: 6-31G*	HF/gen (5d) M: SDD OH: 6-31G*
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#1$	687.0188543	-686.9903997	-686.9907756
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#2$	-686.9985501	-686.9696936	-686.9713239
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#3$	-687.0059230	-686.9771705	-686.9770349
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#4$	-687.0217424	-686.9928868	-686.9930307
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#1$	-687.0296007	-687.0010788	-687.0010402
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 [6+3]$	-687.0584528	-687.0301581	-687.0281723
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#1$	-687.0273099	-686.9988300	-686.9988503
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#2$	-687.0253427	-686.9968895	-686.9971127
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1$	-687.0194802	-686.9920016	-686.9908228
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4$	-687.0230789	-686.9955808	-686.9938103
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2 [6+3]$	-687.0439978	-687.0193439	-687.0132442
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3 [6+3]$	-687.0464853	-687.0196851	-687.0160018
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#4$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#5$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1 [6+3]$	-687.0575126	-687.0322417	-687.0262950
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3 [6+3]$	<b>-687.0507717</b>	-687.0250467	<b>-687.0189766</b>
$\text{Sn}(\text{H}_2\text{O})_{18}^{2+} T [6+12]$	-1371.3599113	-1371.3311860	-1371.3283559

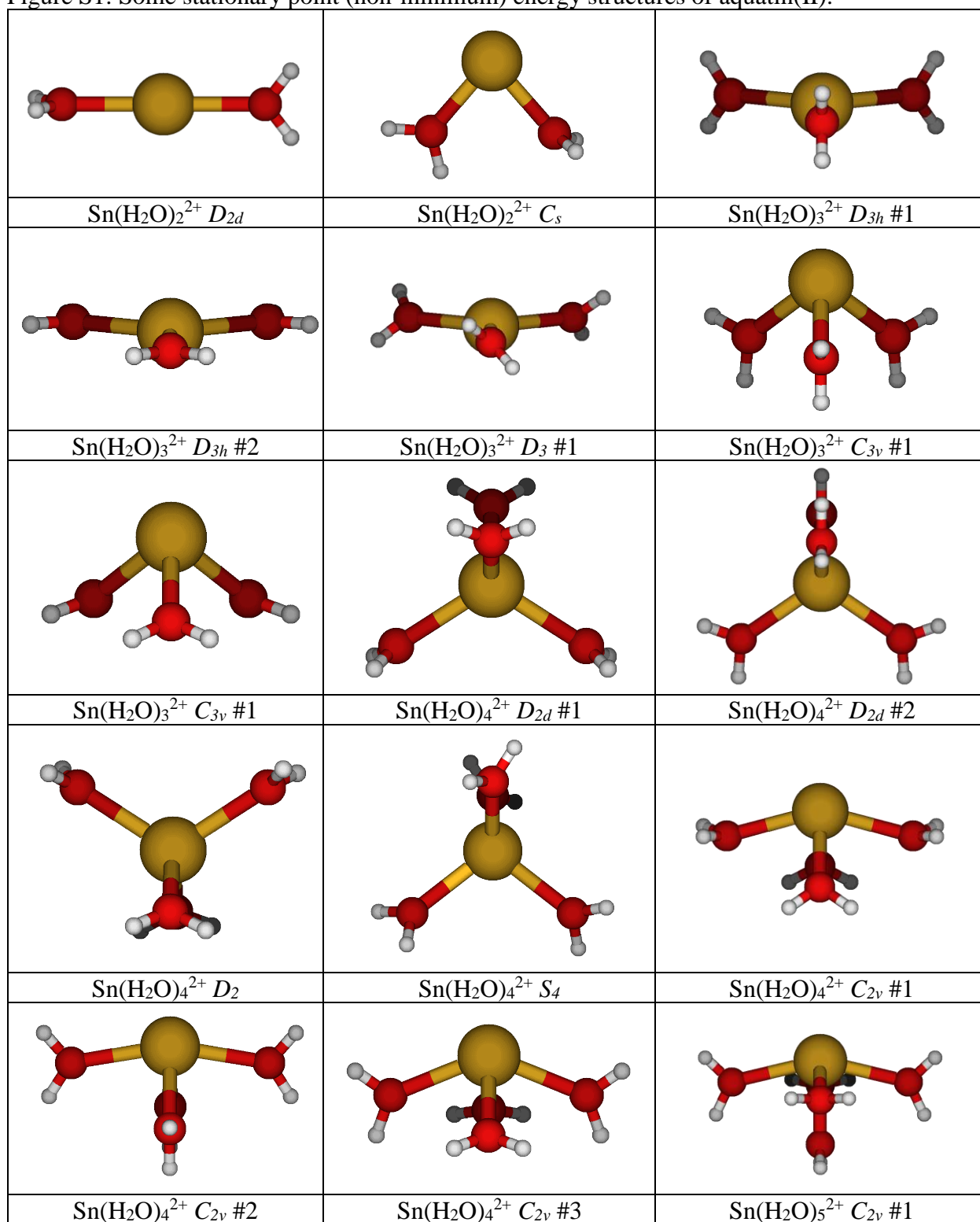
	HF/gen (5d) M: CEP-121G* OH: 6-31+G*	HF/gen (5d) M: LANL2DZ OH: 6-31+G*	HF/gen (5d) M: SDD OH: 6-31+G*
$\text{Sn}^{2+} K_h$	<b>-2.4976820</b>	<b>-2.4628587</b>	<b>-2.4725025</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_{2v}$	<b>-78.6143605</b>	<b>-78.5908722</b>	<b>-78.5934649</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} D_{2d}$	-154.6918891	-154.6690314	-154.6704474
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_s$	-154.7135829	-154.6924351	-154.6912806
$\text{Sn}(\text{H}_2\text{O})_2^{2+} C_2$	<b>-154.7138172</b>	<b>-154.6927306</b>	<b>-154.6914586</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$
$\text{SnOH}^+ + \text{H}_3\text{O}^+ C_s$	<b>-154.7022643</b>	<b>-154.6791322</b>	<b>-154.6752057</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#1$	-230.7698891	-230.7476162	-230.7481216
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_{3h} \#2$	-230.7696542	-230.7472791	-230.7478652
$\text{Sn}(\text{H}_2\text{O})_3^{2+} D_3$	-230.7706780	-230.7484233	-230.7488863
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#1$	-230.7961481	-230.7743712	-230.7704986
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_{3v} \#2$	-230.7928848	-230.7708087	-230.7677221
$\text{Sn}(\text{H}_2\text{O})_3^{2+} C_3$	<b>-230.8010769</b>	<b>-230.7794075</b>	<b>-230.7753601</b>
$\text{Sn}(\text{H}_2\text{O})_2^{2+} + \text{H}_2\text{O} C_{2v}$	<b>-230.7865643</b>	<b>-230.7657369</b>	<b>-230.7626612</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-306.8397366	-306.8155985	-306.8156442
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-306.8396938	-306.8154921	-306.8155494
$\text{Sn}(\text{H}_2\text{O})_4^{2+} D_2$	-306.8397390	-306.8156511	-306.8156510
$\text{Sn}(\text{H}_2\text{O})_4^{2+} S_4$	-306.8405538	-306.8164177	-306.8163866
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-306.8589217	-306.8359758	-306.8318332
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-306.8575859	-306.8346902	-306.8304345
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-306.8644197	<b>-306.8418910</b>	-306.8370052
$\text{Sn}(\text{H}_2\text{O})_4^{2+} C_2$	<b>-306.8644202</b>	n/a	<b>-306.8370222</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#1$	-306.8640430	-306.8425403	-306.8372779
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-306.8650045</b>	<b>-306.8435189</b>	<b>-306.8382200</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#1$	-382.9220253	-382.8983230	-382.8936207
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	-382.9117006	-382.8873648	-382.8839056
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	-382.9120197	-382.8881638	-382.8839382
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$	-382.9108196	-382.8866029	-382.8829158
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s \#1$	<b>-382.9220910</b>	<b>-382.8985032</b>	<b>-382.8936997</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	-382.9213296	-382.8987349	-382.8931747
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	-382.9202418	-382.8974042	-382.8920767
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$	-382.9215737	-382.8988518	-382.8934215
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	-382.9213959	-382.8987810	-382.8933015
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-382.9226809</b>	<b>-382.9001461</b>	<b>-382.8943895</b>
$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_s [4+1]$	<b>-382.9224126</b>	<b>-382.8999833</b>	<b>-382.8939753</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 2\text{H}_2\text{O} C_s \#1$	<b>-382.9211426</b>	<b>-382.8995737</b>	<b>-382.8936227</b>

	HF/gen (5d) M: CEP-121G* OH: 6-31+G*	HF/gen (5d) M: LANL2DZ OH: 6-31+G*	HF/gen (5d) M: SDD OH: 6-31+G*
$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	-458.9577374	-458.9313478	-458.9301383
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3$	-458.9698554	-458.9463441	-458.9414434
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	-458.9717347	-458.9482898	-458.9429658
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#2$	<b>-458.9773796</b>	<b>-458.9539785</b>	<b>-458.9484676</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	-458.9738396	-458.9514764	-458.9462531
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_2 \#1$	<b>-458.9831957</b>	<b>-458.9612049</b>	<b>-458.9544150</b>
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$	-458.9755016	-458.9532637	-458.9469872
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#2$	<b>-458.9791773</b>	<b>-458.9570347</b>	<b>-458.9505256</b>
$\text{Sn}(\text{H}_2\text{O})_3^{2+} + 3\text{H}_2\text{O} C_{3v} \#1$	<b>-458.9716088</b>	<b>-458.9498670</b>	<b>-458.9429896</b>
$\text{Sn}(\text{H}_2\text{O})_6^{2+} C_3 [3+3]$	<b>-458.9733173</b>	<b>-458.9519122</b>	<b>-458.9443719</b>
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3$	[6+1]	[6+1]	[6+1]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#5$	-534.9868134	-534.9612552	-534.9598816
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#6$	-534.9925789	-534.9663938	-534.9654920
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#7$	-534.9895593	-534.9645234	-534.9621255
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#8$	-534.9996800	-534.9745506	-534.9721574
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11$	[6+1] [4+3] -535.0010909	[6+1] [4+3] -534.9773876	[6+1] [4+3] -534.9726580
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#13$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#14$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#15$	[5+2] -535.0042543	[5+2] -534.9805995	-534.9742579 [5+2] -534.9760433
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#16$	-535.0012735	-534.9755810	-534.9740954
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#1 [5+2]$	-535.0182363	-534.9949639	-534.9892807
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#2 [5+2]$	-535.0084745	-534.9847397	-534.9799790
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#3 [5+2]$	-535.0068429	-534.9833732	-534.9782715
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#4 [5+2]$	-534.9850796	-534.9799313	-534.9699017
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#9 [5+2]$	-535.0164925	-534.9933033	-534.9873568
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#10 [5+2]$	-535.0059803	-534.9823485	-534.9772498
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#11 [5+2]$			
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_{2v} \#12 [5+2]$	-535.0050221	-534.9817290	-534.9762500
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#5$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#6$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#7$	[4+3]	[4+3]	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#8$	[5+2]	[5+2]	[5+2]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#15$	n/a	n/a	[4+3]
$\text{Sn}(\text{H}_2\text{O})_7^{2+} C_2 \#16$	[5+2]	[5+2]	[5+2]

	HF/gen (5d) M: CEP-121G* OH: 6-31+G*	HF/gen (5d) M: LANL2DZ OH: 6-31+G*	HF/gen (5d) M: SDD OH: 6-31+G*
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #1	-611.0118544	-610.9856679	-610.9866285
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4h</sub> #2	-611.0120609	-610.9858379	-610.9867869
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #1	-611.0301936	-611.0041855	-611.0036332
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4d</sub> #2	-611.0292503	-611.0034038	-611.0029194
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #1	<i>D</i> <sub>4</sub> #2	n/a	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #2	-611.0417828	-611.0154656	-611.0147582
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>4</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #1	-611.0390117	-611.0128614	-611.0125798
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4h</sub> #2	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #1	n/a	-611.0043345	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #2	[4+4]	[4+4]	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4v</sub> #3	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #1	-611.0441443	-611.0181132	-611.0169262
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>8</sub> #2	<i>S</i> <sub>8</sub> #1	<i>S</i> <sub>8</sub> #1	<i>S</i> <sub>8</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #1	-611.0278013	-611.0016631	-611.0018115
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #2	-611.0264785	-611.0004108	-611.0001994
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #3	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1	<i>D</i> <sub>2d</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #4	-611.0264062	-610.9999642	-610.9997186
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2d</sub> #5	-611.0407156	-611.0146963	-611.0141323
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #1	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2	<i>D</i> <sub>4h</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #3	-611.0335509	-611.0074859	-611.0072190
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2h</sub> #4	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3	<i>D</i> <sub>2h</sub> #3
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #1	-611.0376513	611.0125362	-611.0104164
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #2	<i>C</i> <sub>2v</sub> #1	<i>C</i> <sub>2v</sub> #1	<i>C</i> <sub>2v</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #3	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #4	-611.0265907	[4+4]	n/a
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2v</sub> #6	[6+2]	[6+2]	[6+2]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #1	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>4</sub> #3	<i>S</i> <sub>8</sub> #1	[4+4]	<i>S</i> <sub>8</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #2	<i>D</i> <sub>2d</sub> #5	-611.0137495	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #3	<i>D</i> <sub>2d</sub> #5	<i>S</i> <sub>4</sub> #2	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>S</i> <sub>4</sub> #4	-611.0400451	<i>S</i> <sub>4</sub> #2	<i>D</i> <sub>2d</sub> #5
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #3	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #4	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #5	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>D</i> <sub>2</sub> #7	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2	<i>D</i> <sub>4</sub> #2
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2h</sub> #2	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1	<i>C</i> <sub>4h</sub> #1
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2</sub> #1	[4+4]	[4+4]	[4+4]
Sn(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> <i>C</i> <sub>2</sub> #3	[4+4]	n/a	n/a

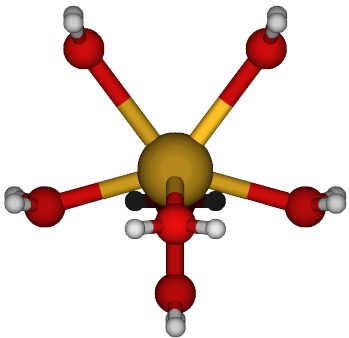
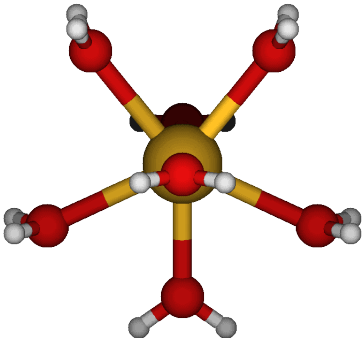
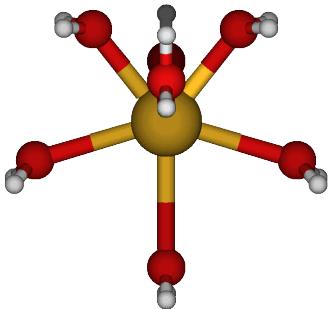
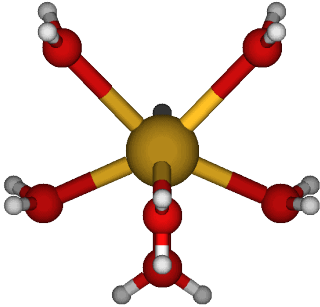
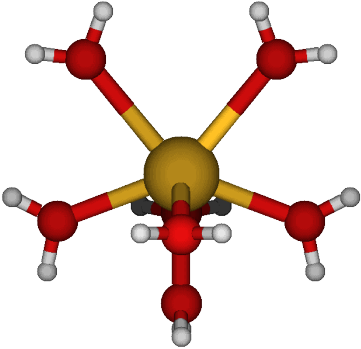
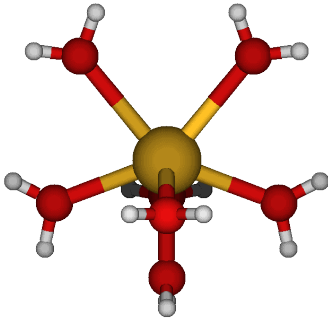
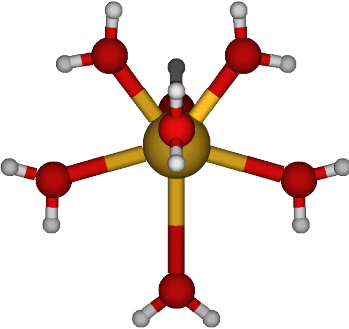
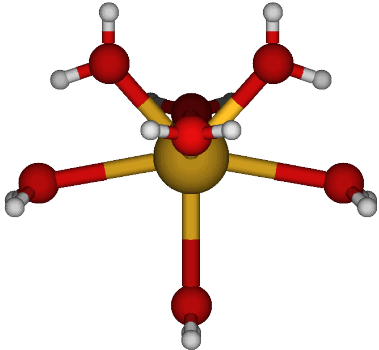
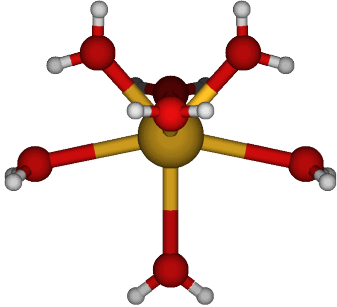
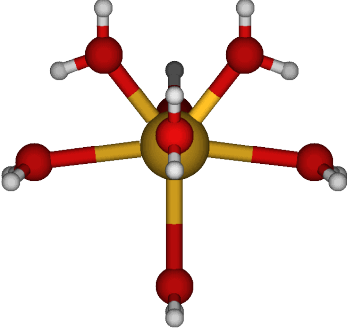
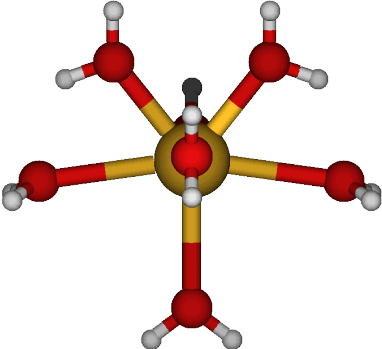
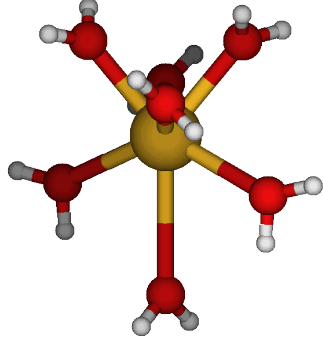
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#6$	n/a	[4+4]	n/a
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_2 \#7$	[4+2+2]	n/a	n/a
	HF/gen (5d) M: CEP-121G* OH: 6-31+G*	HF/gen (5d) M: LANL2DZ OH: 6-31+G*	HF/gen (5d) M: SDD OH: 6-31+G*
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#1$	-687.0656619	-687.0391834	-687.0389503
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#2$	-687.0441565	-687.0173684	-687.0183389
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#3$	-687.0536678	-687.0273827	-687.0266820
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_{3h} \#4$	-687.0692998	-687.0430928	-687.0427101
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#1$	-687.0781885	-687.0520737	-687.0512385
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} D_3 [6+3]$	-687.1036718	-687.0778981	-687.0762446
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#1$	-687.0742064	-687.0482271	-687.0478293
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#2$	-687.0721906	-687.0462267	-687.0454698
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#1$	-687.0658985	-687.0400072	-687.0389565
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3$	[6+3]	[6+3]	[6+3]
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#4$	-687.0694762	-687.0436471	-687.0427902
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#2 [6+3]$	-687.0854922	687.0619449	-687.0568420
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \#3 [6+3]$	-687.0868066	-687.0622692	-687.0593310
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#2$	$C_3 \#1 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$	$C_3 \#3 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#4$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#5$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$	$C_3 \#1 [6+3]$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#1 [6+3]$	-687.0994801	-687.0758798	-687.0708478
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_3 \#3 [6+3]$	<b>-687.0915359</b>	<b>-687.0673880</b>	-687.0623748
$\text{Sn}(\text{H}_2\text{O})_{18}^{2+} T [6+12]$	-1371.4522700	-1371.4266810	-1371.4242523

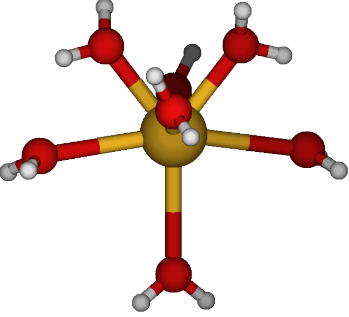
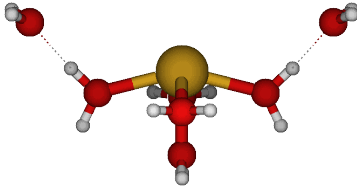
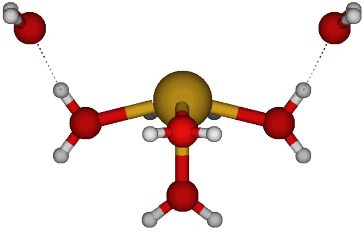
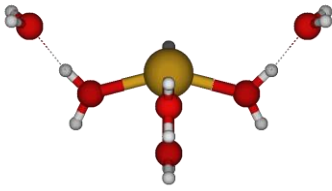
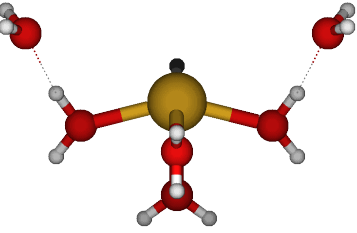
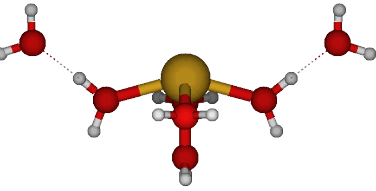
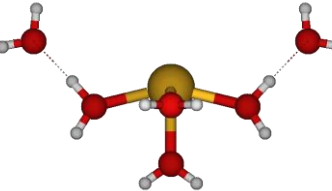
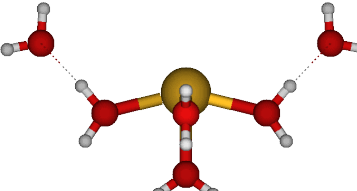
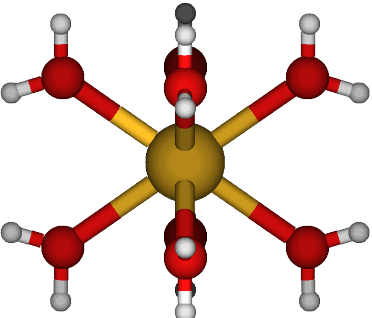
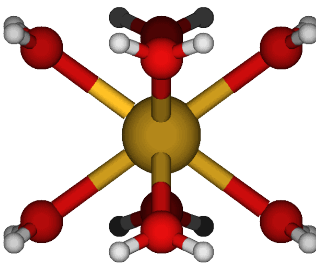
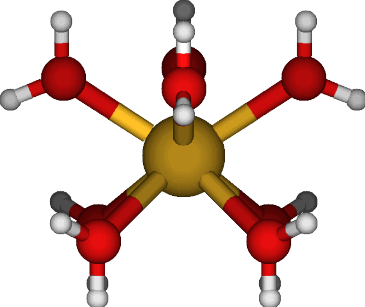
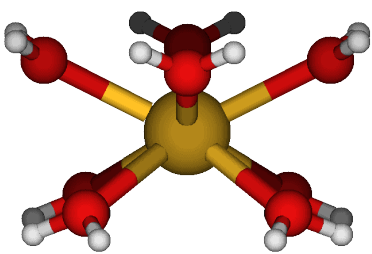
Figure S1: Some stationary point (non-minimum) energy structures of aquatin(II).



$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#2$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#3$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} C_{2v} \#4$
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#1$	$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_{2v} \#2$	$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_2 \#1$
$\text{Sn}(\text{H}_2\text{O})_4^{2+} + \text{H}_2\text{O} C_s \#1$	$\text{Sn}(\text{H}_2\text{O})_6^{2+} T_h$	$\text{Sn}(\text{H}_2\text{O})_6^{2+} S_6$
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + \text{H}_2\text{O} C_s \#1$	$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_{2v} \#1$	$\text{Sn}(\text{H}_2\text{O})_4^{2+} + 2\text{H}_2\text{O} C_s \#1$

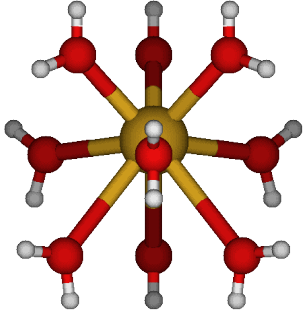
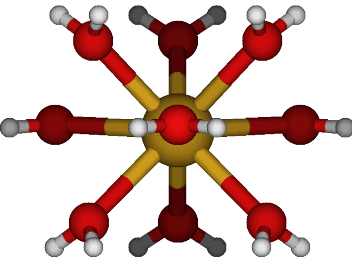
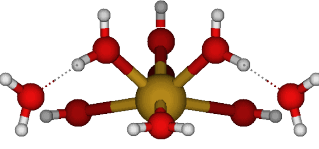
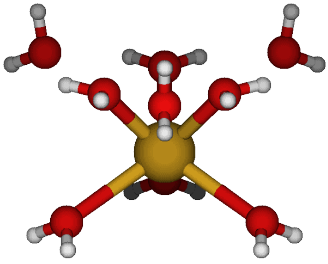
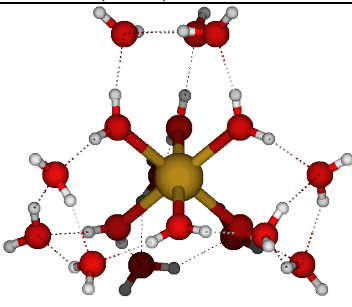


		
$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#5}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#6}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#7}$
		
$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#8}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#9}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#10}$
		
$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#12}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#13}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#14}$
		
$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#15}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_{2v} \text{ \#16}$	$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_2 \text{ \#10}$

		
$\text{Sn}(\text{H}_2\text{O})_7^{2+} \text{ } C_2 \text{ \#15}$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#2}$
		
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#3}$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#4}$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#9}$
		
$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#10}$	$\text{Sn}(\text{H}_2\text{O})_5^{2+} + 2\text{H}_2\text{O} \text{ } C_{2v} \text{ \#12}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } D_{4h} \text{ \#1}$
		
$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } D_{4h} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } D_{4d} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } D_{4d} \text{ \#2}$

$\text{Sn}(\text{H}_2\text{O})_8^{2+} S_8 \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_4 \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \text{ \#1}$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4v} \text{ \#4}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} C_{4h} \text{ \#1}$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2h} \text{ \#3}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \text{ \#1}$
$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \text{ \#4}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} D_{2d} \text{ \#5/S}_4 \text{ \#2}$

$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } C_{2v} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } C_4 \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_8^{2+} \text{ } D_2 \text{ \#1}$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_{3h} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_{3h} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_{3h} \text{ \#3}$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_{3h} \text{ \#4}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_3 \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } D_3 \text{ [6+3]}$
$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } C_{3h} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } C_{3h} \text{ \#2}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} \text{ } C_{3h} \text{ [6+3]}$

		
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \text{ \#1}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \text{ \#4}$	$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \text{ \#2 [6+3]}$
		
$\text{Sn}(\text{H}_2\text{O})_9^{2+} C_{3v} \text{ \#3 [6+3]}$	$\text{Sn}(\text{H}_2\text{O})_{18}^{2+} T \text{ [6+12]}$	