

# Supplementary Information: An Ab Initio Investigation of the Hydration of Antimony(III).

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**Table S1: Total Energies of Aquaantimony(III) Species** (bold indicates a minimum energy structure)

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{H}_3\text{O}^+ D_{3h}$	<b>-17.0486214</b>	-17.1252753	-17.1290991
$\text{H}_3\text{O}^+ C_{3v}$	n/a	<b>-17.1275085</b>	<b>-17.1323143</b>
$\text{Sb}^{3+} K_h$	<b>-3.4762496</b>	<b>-3.4762496</b>	<b>-3.4762496</b>
$\text{SbOH}^{2+} D_{\infty h}$	<b>-20.6563325</b>	<b>-20.7103708</b>	<b>-20.7141462</b>
$\text{Sb}(\text{H}_2\text{O})^{3+} C_{2v}$	<b>-20.4826249</b>	<b>-20.5417161</b>	<b>-20.5458060</b>
$\text{SbOH}(\text{H}_2\text{O})^{2+} C_s$	<b>-37.5499634</b>	<b>-37.6753198</b>	<b>-37.6836438</b>
$\text{Sb}(\text{H}_2\text{O})_2^{3+} D_{2d}$	-37.3751683	-37.5219139	-37.5294757
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_s$	-37.4443460	-37.5663403	-37.5749714
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_2$	<b>-37.4462008</b>	<b>-37.5674707</b>	<b>-37.5758881</b>
$\text{SbOH}(\text{H}_2\text{O})_2^{2+} C_s$	<b>-54.4242920</b>	<b>-54.6198097</b>	<b>-54.6322133</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#1$	-54.2844838	-54.5009855	-54.5129646
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#2$	-54.2917744	-54.5041550	-54.5157755
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_3$	$D_{3h} \#2$	-54.5047843	-54.5166096
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#1$	-54.3746885	-54.5583507	-54.5711588
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#2$	-54.3662263	-54.5523839	-54.5653978
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_3$	<b>-54.3768748</b>	<b>-54.5630440</b>	<b>-54.5764300</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} [2+1] C_{2v}$	-54.3257103	-54.5154795	-54.5272602
$\text{SbOH}(\text{H}_2\text{O})_3^{2+} C_s$	<b>-71.2585117</b>	<b>-71.5331581</b>	<b>-71.5495815</b>
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-71.1803759	-71.4637620	-71.4795455
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-71.1801967	-71.4633302	-71.4791900
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_4^{2+} S_4$	-71.1812395	-71.4646732	-71.4807505
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-71.2344609	-71.5016110	-71.5185979
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-71.2387458	-71.5016485	-71.5186063
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-71.2444081	-71.5092625	-71.5263612
$\text{Sb}(\text{H}_2\text{O})_4^{3+} C_2$	<b>-71.2444568</b>	<b>-71.5092710</b>	<b>-71.5264308</b>
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#1$	-71.2352972	-71.4934221	-71.5103093
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#2$	-71.2375140	-71.4950052	-71.5116544
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$	-88.0803085	-88.4345760	-88.4548117
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#2$	-88.0800451	<b>-88.4353704</b>	<b>-88.4558451</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#1$	<b>-88.0941515</b>	<b>-88.4425395</b>	<b>-88.4637426</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	-88.0795728	-88.4272295	-88.4477447
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	-88.0867086	-88.4301978	-88.4507269
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$	-88.0824944	-88.4282714	-88.4487756
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#1$	-88.0914865	-88.4296413	<b>-88.4502480</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#2$	-88.0886469	-88.4276694	-88.4485326
$\text{Sb}(\text{H}_2\text{O})_6^{3+} T_h$	-104.8956760	-105.3379058	-105.3623182

$\text{Sb}(\text{H}_2\text{O})_6^{3+} C_3$	<b>-104.9219182</b>	<b>-105.3517838</b>	<b>-105.3764974</b>
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#1$	-104.9490286	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#2$	-104.9518421	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$	<b>-105.3833131</b>

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#1$	[5+2]	-122.2475806	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#2$	[5+2]	-122.2375976	-122.2659968
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#3$	[5+2]	-122.2353167	-122.2630926
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#5$	-121.7086953	-122.2206201	-122.2476558
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#6$	-121.7130477	-122.2282238	-122.2554739
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#7$	-121.7095213	-122.2205447	-122.2475929
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#8$	-121.7236779	-122.2374469	-122.2656049
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#9$	[5+2]	-122.2370848	-122.2649705
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#10$	[5+2]	-122.2243392	-122.2514131
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#11$	-121.7213951	-122.2323546	-122.2600577
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#12$	[5+2]	-122.2246965	-122.2519432
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#13$	-121.7220690	-122.2340395	-122.2619568
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#14$	-121.7212963	-122.2353536	-122.2630145
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#15$	[4+3]	-122.2370808	-122.2652176
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#16$	-121.7245293	-122.2424034	-122.2701447
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#1$	n/a	$C_2 \#16$	n/a
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#2$	n/a	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#3$	n/a	$C_2 \#11$	$C_2 \#11$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#5$	[5+2]	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#6$	[5+2]	-122.2453026	[5+2] -122.2833765
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#7$	[5+2]	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#8$	[5+2]	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#9$	n/a	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#10$	n/a	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#11$	-121.7264112	-122.2418089	-122.2697162
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#12$	n/a	$C_2 \#16$	$C_2 \#16$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#13$	proton transfer	$C_2 \#16$	-122.2700461
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#14$	[4+3]	$C_2 \#16$	$C_2 \#13$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#15$	n/a	$C_2 \#16$	$C_2 \#13$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#16$	[5+2]	-122.2484785	-122.2769974

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #1	n/a	C <sub>s</sub> #5	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #2	n/a	C <sub>s</sub> #7	-122.2675004
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #3	n/a	[6+1]	[6+1]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #4	n/a	C <sub>2v</sub> #1	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #5	[5+2]	-122.2504088	-122.2789821
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #6	C <sub>2v</sub> #7 -121.7117839	C <sub>2v</sub> #7 -122.2222878	C <sub>2v</sub> #7 -122.2500144
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #7	[5+2]	-122.2415134	-122.2694821
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #8	[6+1], then H <sup>+</sup> xfer.	-122.2374944	-122.2656758
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #9	C <sub>s</sub> #6	C <sub>s</sub> #6	C <sub>s</sub> #6
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #10	-121.7312127	-122.2381134	-122.2657843
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #11	[5+2]	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #12	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	C <sub>s</sub> #8	C <sub>s</sub> #8
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #13	n/a	C <sub>s</sub> #5	C <sub>s</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #14	n/a	C <sub>s</sub> #7	-122.2677631
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #15	n/a	C <sub>2v</sub> #12	C <sub>2v</sub> #12
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #16	[5+2]	C <sub>s</sub> #24	C <sub>s</sub> #24
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #17	[5+2]	-122.2348951	-122.2626663
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #18	n/a	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #20	-121.7349682	-122.2462497	-122.2747963
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #21	proton transfer	-122.2388738	[6+1] -122.2686634
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #22	-121.7284199	C <sub>s</sub> #7	[6+1] C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #23	[5+2], proton xfer	-122.2445392	-122.2729014
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #24	n/a	-122.2416956	-122.2697563
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #25	n/a	C <sub>s</sub> #21	[6+1] C <sub>s</sub> #21
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #26	[5+2]	-122.2467913	-122.2748006
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #27	[5+2]	C <sub>s</sub> #23	C <sub>s</sub> #23
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #3 [6+1]		-122.2536627	
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> [5+2]	<b>-121.7631138</b>	<b>-122.2556125</b>	<b>-122.2832656</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #2	n/a	C <sub>1</sub> #3	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #3	[5+2]	<b>-122.2509160</b>	<b>-122.2793177</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #4	n/a	n/a	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #5	n/a	C <sub>1</sub> #3	<b>-122.2790016</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #6	n/a	n/a	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #8	n/a	C <sub>1</sub> #3	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #9	[5+2]	C <sub>1</sub> #3	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #10	n/a	<b>-122.2500300</b>	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #11	n/a	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #12	[5+2]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #14	n/a	n/a	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #15	n/a	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #16	[4+3]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #17	n/a	C <sub>1</sub> #3	<b>[6+1] -122.2885896</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #18	[5+2]	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #19	n/a	C <sub>1</sub> #3	C <sub>1</sub> #3

$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #20	n/a	$C_1$ #3	$C_1$ #5
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #21	n/a	$C_1$ #3	$C_1$ #3

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #1	-138.4997016	-139.0947187	-139.1241154
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #2	-138.4999385	-139.0951166	-139.1246325
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #1	-138.5271959	-139.1269536	-139.1569001
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #2	-138.5248620	-139.1254032	-139.1550032
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #1	-138.5419223	<b>-139.1480934</b>	<b>-139.1786542</b>
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #2	$S_8$ #1	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #1	-138.5340490	-139.1380305	-139.1688739
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #2	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #3	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #4	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4v}$ #1	-138.5346266	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4v}$ #2	-138.5273438	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4v}$ #3	[4+4] -138.6015318	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4v}$ #4	-138.5000098	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #1	-138.5222261	-139.1261677	-139.1571780
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #2	$C_{4h}$ #1	$C_{4h}$ #1	$C_{4h}$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #1	$D_{4h}$ #2	$D_{4h}$ #2	$D_{4h}$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #1	-138.5149496	-139.1159871	-139.1465949
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #2	-138.5204309	-139.1195411	-139.1494837
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #3	$D_{2d}$ #1	$D_{2d}$ #1	$D_{2d}$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #4	-138.5209727	-139.1190224	-139.1492629
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #5	-138.5336386	-139.1378483	-139.1687129
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_4$ #1	[4+4] -138.6148825	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_4$ #2	$C_4$ #1	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_4$ #3	$C_4$ #1	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_4$ #4	$C_4$ #1	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #1	$D_{2d}$ #5	$D_{2d}$ #5	$D_{2d}$ #5
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #2	-138.5343663	-139.1377112	-139.1684921
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #3	$S_4$ #2	$S_4$ #2	$S_4$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #4	$S_4$ #2	$S_4$ #2	$S_4$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #1	-138.5380416	-139.1418500	-139.1723727
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #2	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #3	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #4	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #5	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #1	[4+4] -138.6052835	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #2	[6+2] -138.5621521	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #3	-138.5222450	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #4	[6+2] -138.5715331	n/a	n/a

$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#5$	-138.5388209	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#6$	-138.5275564	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#7$	-138.5450388	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#8$	$C_{2v} \#3$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#9$	$C_{2v} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#1$	[4+4] <b>-138.6227814</b>	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#2$	$C_2 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#1$	-138.5214224	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#2$	-138.5216694	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#1$	[6+2] -138.5242148	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#3$	-138.5664317	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#4$	-138.5220627	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#6$	[4+4] -138.6122626	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#1$	[4+4] -138.5934634	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#2$	[5+3] -138.5845022	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#3$	[4+4] -138.6071528	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_1 \#1$	$\text{Sb}(\text{H}_2\text{O})_3(\text{OH})_2^+ + 2\text{H}_3\text{O}^+ + \text{H}_2\text{O}$		n/a

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#1$	-155.3341515	-156.0150549	-156.0486198
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#2$	-155.3128517	-155.9848206	-156.0173720
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#3$	-155.3188315	-155.9937787	-156.0280233
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#4$	-155.3384285	-156.0215053	-156.0556499
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#1$	-155.3461587	-156.0330630	-156.0673199
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#3$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#1$	-155.3399432	-156.0248754	-156.0590968
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#2$	-155.3405223	-156.0241243	-156.0580805
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#1$	-155.3411975	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#2$	[6+3] -155.4069179	[6+3] -156.0325104	[6+3] -156.0661119
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#3$	[6+3] -155.3574872	[6+3] -156.0206759	[6+3] -156.0567885
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#4$	-155.3429399	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$	[6+3]	n/a	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$	[6+3]	$D_3 \#1$	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#3$	[6+3]	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#4$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#5$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1 [6+3]$	-155.3684014	<b>-156.0376705</b>	<b>-156.0732980</b>

$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 [6+3]$	-155.3607954	-156.0455158	-156.0810718
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2 [6+3]$	<b>-155.4311137</b>	<b>-156.0669511</b>	<b>-156.1019455</b>
$\text{Sb}(\text{H}_2\text{O})_{18}^{3+} T [6+12]$	-306.5774910	-307.9928904	

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{H}_3\text{O}^+ D_{3h}$	-75.3283916	<b>-76.3001624</b>	<b>-76.3002241</b>
$\text{H}_3\text{O}^+ C_{3v}$	<b>-75.3304394</b>	n/a	n/a
$\text{Sb}^{3+} K_h$	<b>-3.4308101</b>	<b>-3.4315119</b>	<b>-3.4560761</b>
$\text{SbOH}^{2+} D_{\infty h}$	<b>-78.8073115</b>	<b>-79.8488980</b>	<b>-79.8667449</b>
$\text{Sb}(\text{H}_2\text{O})^{3+} C_{2v}$	<b>-78.6765203</b>	<b>-79.6848633</b>	<b>-79.7084775</b>
$\text{SbOH}(\text{H}_2\text{O})^{2+} C_s$	<b>-153.9263384</b>	<b>-155.9884499</b>	<b>-156.0074347</b>
$\text{Sb}(\text{H}_2\text{O})_2^{3+} D_{2d}$	-153.8077302	-155.8432825	-155.8666983
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_s$	-153.8759971	-155.8901543	-155.9136122
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_2$	(i.p. $C_{2v}$ ) <b>-153.8806852</b>	<b>-155.8910252</b>	<b>-155.9145084</b>
$\text{SbOH}(\text{H}_2\text{O})_2^{2+} C_s$	<b>-229.0233050</b>	<b>-232.1073381</b>	<b>-232.1272457</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#1$	-228.9303700	-231.9989186	-232.0234625
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#2$	-228.9524878	-232.0014927	-232.0262880
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_3$	$D_{3h} \#2$	-232.0023796	-232.0270944
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#1$	-229.0443588	-232.0590695	-232.0824046
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#2$	-229.0316799	-232.0525031	-232.0760822
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_3$	<b>-229.0444609</b>	<b>-232.0633633</b>	<b>-232.0866836</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} [2+1] C_{2v}$	-229.0022030	-232.0139063	-232.0367272
$\text{SbOH}(\text{H}_2\text{O})_3^{2+} C_s$	<b>-304.0778370</b>	<b>-308.1922429</b>	<b>-308.2124882</b>
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-304.0558112	-308.1339580	-308.1595600
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-304.0557053	-308.1336481	-308.1592623
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_4^{2+} S_4$	-304.0567238	-308.1351317	-308.1607281
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-304.1253271	-308.1730727	-308.1964933
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-304.1376393	-308.1750249	-308.1982379
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-304.1395722	-308.1820987	<b>-308.2053243</b>
$\text{Sb}(\text{H}_2\text{O})_4^{3+} C_2$	-304.1401384	<b>-308.1820988</b>	n/a
$\text{Sb}(\text{H}_2\text{O})_4^{3+} C_s \#1$	-304.1367597	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_4^{3+} C_s \#2$	<b>-304.1411865</b>	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#1$	-304.1373279	-308.1672284	-308.1901526
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#2$	-304.1411966	-308.1692527	-308.1921417
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$	-379.1111971	-384.2628689	-384.2835074
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#2$	-379.1081140	-384.2614891	-384.2825255
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#1$	-379.2104952	<b>-384.2854213</b>	<b>-384.3088769</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	-379.1916587	-384.2683449	-384.2922034
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	-379.2087904	-384.2733625	-384.2967893
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$	-379.1980813	-384.2709364	-384.2946646
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_2 \#1$	-379.2106800	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_s \#3$	-379.2104952	n/a	n/a

$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_s \#3$	-379.2047006	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_s \#3$	-379.2105012	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_i \#1$	<b>-379.2107065</b>	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#1$	<b>-379.2190566</b>	-384.2753106	-384.2981787
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#2$	-379.2113037	-384.2724642	-384.2954102

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sb}(\text{H}_2\text{O})_6^{3+} T_h$	-454.1877578	-460.3454156	-460.3712631
$\text{Sb}(\text{H}_2\text{O})_6^{3+} C_3$	<b>-454.2370958</b>	<b>-460.3610939</b>	<b>-460.3850775</b>
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#1$	-454.2832656	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#2$	-454.2831948	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} + \text{H}_3\text{O}^+$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#3$	-529.2187231	-536.4082125	-536.4334248
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#5$	-529.2075847	-536.3912294	-536.4167306
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#6$	-529.2119779	-536.3992397	-536.4249231
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#7$	-529.2083711	-536.3912637	-536.4167972
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#8$	-529.2230971	-536.4090304	-536.4342430
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#9$	[5+2]	-536.4086953	-536.4337520
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#10$	[5+2]	-536.3947251	-536.4199511
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#11$	-529.2191491	-536.4052468	-536.4304408
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#12$	[5+2]	[5+2]	-536.4205675
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#13$	-529.2201580	-536.4066358	-536.4317663
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#14$	-529.2186058	-536.4078128	-536.4331852
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#15$	[4+3]	-536.4102484	-536.4353688
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#16$	-529.2235352	-536.4150972	-536.4407213
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#3$	[4+3]	$C_2 \#11$	$C_2 \#11$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#5$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#6$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#7$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#8$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#9$	n/a	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#10$	n/a	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#11$	[4+3]	-536.4148656	-536.4401363
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#12$	n/a	n/a	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#13$	[4+3]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#14$	[4+3]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#15$	n/a	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#16$	[5+2]	[5+2]	[5+2]

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #3	[6+1]	[5+2]	[6+1]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #4	[6+1]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #5	[6+1] -529.2935001	[6+1], [4+3] + H xfer	-536.4495732
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #6	C <sub>2v</sub> #7 -529.2099142	C <sub>2v</sub> #7 -536.3924318	C <sub>2v</sub> #7 -536.4177339
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #7	-529.2417160	-536.4140719	-536.4390867
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #8	C <sub>2v</sub> #8	-536.4091746	-536.4342985
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #9	C <sub>s</sub> #6	C <sub>s</sub> #6	C <sub>s</sub> #6
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #10	-529.2462820	-536.4115233	-536.4359166
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #11	C <sub>s</sub> #26	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #12	n/a	C <sub>s</sub> #8	C <sub>s</sub> #8
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #13	n/a	[6+1]	C <sub>s</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #14	n/a	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #15	n/a	[5+2]	C <sub>2v</sub> #12
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #16	[5+2]	C <sub>s</sub> #24	C <sub>s</sub> #24
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #17	[5+2]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #18	n/a	n/a	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #20	[6+1]	-536.4196485	-536.4440177
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #21	[5+2]	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #22	[6+1]	C <sub>s</sub> #7	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #23	[5+2]	[6+1]	-536.4430575
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #24	n/a	-536.4151306	-536.4398922
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #25	n/a	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #26	-529.2516503	-536.4201602	-536.4448687
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #27	[5+2]	[5+2]	C <sub>s</sub> #23
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> #1 [5+2]	-529.3220144	<b>-536.4456976</b>	<b>-536.4684603</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> #10 [5+2]	-529.3095202		
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> #12 [5+2]	-529.3160224	-536.4285056	-536.4511615
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #3	n/a	<b>-536.4254643</b>	<b>-536.4499689</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #8	n/a	n/a	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #9	[6+1]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #10	[6+1]	[6+1]	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #11	n/a	C <sub>I</sub> #3	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #12	[5+2]	C <sub>I</sub> #3	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #16	n/a	[6+1]	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #19	n/a	n/a	C <sub>I</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #20	n/a	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #21	[5+2]	C <sub>I</sub> #3	C <sub>I</sub> #3



	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{4h} \#1$	-604.2064771	-612.4265230	-612.4520348
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{4h} \#2$	-604.2067691	-612.4268093	-612.4523146
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{4d} \#1$	-604.2293060	-612.4628223	-612.4883421
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{4d} \#2$	-604.2274667	-612.4596069	-612.4852455
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_8 \#1$	-604.2413486	<b>-612.4857484</b>	<b>-612.5114638</b>
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_8 \#2$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_4 \#1$	-604.2353365	-612.4746846	-612.5004146
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_4 \#2$	$D_4 \#1$	$D_4 \#1$	$D_4 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_4 \#3$	$D_4 \#1$	$D_4 \#1$	$D_4 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_4 \#4$	$D_4 \#1$	$D_4 \#1$	$D_4 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4v} \#1$	-604.2414582	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4v} \#2$	-604.2338174	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4h} \#1$	-604.2248509	-612.4628577	-612.4885145
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4h} \#2$	$C_{4h} \#1$	$C_{4h} \#1$	$C_{4h} \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#1$	$D_{4h} \#2$	$D_{4h} \#2$	$D_{4h} \#2$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#1$	-604.2182495	-612.4494804	-612.4750850
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#2$	-604.2226973	-612.4531356	-612.4787760
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#3$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#4$	-604.2262881	-612.4523923	-612.4779644
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#5$	-604.2342995	-612.4744367	-612.5001684
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#1$	[4+4] -604.3909089	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#2$	$C_4 \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#3$	$C_4 \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#4$	$C_4 \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#1$	$D_{2d} \#5$	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#2$	-604.2346901	-612.4736941	-612.4993978
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#3$	$S_4 \#2$	$S_4 \#2$	$S_4 \#2$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#4$	$S_4 \#2$	$S_4 \#2$	$S_4 \#2$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#1$	-604.2379545	-612.4784528	-612.5041682
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#2$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#3$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#4$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#5$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#1$	[4+4] -604.3869861	[4+4] -612.5078578	[4+4] -612.5296362
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#2$	-604.2231784	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#4$	[6+2] -604.3190986	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#5$	-604.2519474	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#6$	-604.2611095	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#7$	-604.2338180	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#1$	[4+4] <b>-604.3930643</b>	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#2$	$C_2 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#1$	-604.2224575	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#2$	-604.2231666	n/a	n/a

$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#1$	[6+2] -604.2565870	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#3$	-604.2267693	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#1$	[4+4] -604.3909088	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#1$	[5+3] -604.3592495	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#2$	[6+2] -604.3389899	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#3$	[4+4] -604.3869861	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_I \#1$	[6+2] <b>-604.3382108</b>	n/a	n/a

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#1$	-679.2392122	-688.5134387	-688.5388794
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#2$	-679.2252417	-688.4794014	-688.5046403
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#3$	-679.2226456	-688.4888448	-688.5143900
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#4$	-679.2405066	-688.5192176	-688.5447768
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#1$	-679.2482891	-688.5332665	-688.5588150
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#3$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#1$	-679.2440199	-688.5225732	-688.5481255
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#2$	-679.2421220	-688.5232999	-688.5488116
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#1$	-679.2432649	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#2$	[6+3] -679.3596403	[6+3] -688.5529638	[6+3] -688.5764421
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#3$	-679.2274133	[6+3] -688.5316995	[6+3] -688.5564487
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#4$	-679.2412617	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#3$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#4$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#5$	[6+3]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1 [6+3]$	-679.3265562	<b>-688.5591255</b>	<b>-688.5831920</b>
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 [6+3]$	-679.3022021	-688.5644005	-688.5903519
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2 [6+3]$	<b>-679.3876817</b>	<b>-688.5869110</b>	<b>-688.6104140</b>
$\text{Sb}(\text{H}_2\text{O})_{18}^{3+} T [6+12]$	-1354.3684678	-1373.0133805	-1373.0401422

	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*
$\text{H}_3\text{O}^+ D_{3h}$	-17.3009663	-17.3164953	-76.4676869	-76.4701581
$\text{H}_3\text{O}^+ C_{3v}$	<b>-17.3045552</b>	<b>-17.3209842</b>	<b>-76.4717194</b>	<b>-76.4743392</b>
$\text{Sb}^{3+} K_h$	<b>-3.4964312</b>	<b>-3.4964312</b>	<b>-3.4964312</b>	<b>-3.4964312</b>
$\text{SbOH}^{2+} D_{\infty h}$	<b>-20.9435204</b>	<b>-20.9585048</b>	<b>-80.1130636</b>	<b>-80.1230272</b>

$\text{Sb}(\text{H}_2\text{O})^{3+} C_{2v}$	<b>-20.7571370</b>	<b>-20.7726419</b>	<b>-79.9290012</b>	<b>-79.9337746</b>
$\text{SbOH}(\text{H}_2\text{O})^{2+} C_s$	<b>-38.0872104</b>	<b>-38.1186372</b>	<b>-156.4265649</b>	<b>-156.4404073</b>
$\text{Sb}(\text{H}_2\text{O})_2^{3+} D_{2d}$	-37.9336966	-37.9644968	-156.2717081	-156.2829469
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_s$	-37.9693745	-38.0013761	-156.3110386	-156.3210818
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_2$	<b>-37.9709592</b>	<b>-38.0024894</b>	<b>-156.3124674</b>	<b>-156.3223744</b>
$\text{SbOH}(\text{H}_2\text{O})_2^{2+} C_s$	<b>-55.2105186</b>	<b>-55.2584800</b>	<b>-232.7176413</b>	<b>-232.7385692</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#1$	-55.0989191	-55.1466896	-232.6055112	-232.6230454
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#2$	-55.1055719	-55.1523555	-232.6109096	-232.6280864
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_3$	-55.1060480	-55.1531705	-232.6116715	-232.6292563
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#1$	-55.1453289	-55.1934091	-232.6554103	-232.6733489
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#2$	-55.1399828	-55.1883826	-232.6499947	-232.6674829
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_3$	<b>-55.1508887</b>	<b>-55.1997688</b>	<b>-232.6607978</b>	<b>-232.6783981</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} [2+1] C_{2v}$	-55.1179253	-55.1636858	-232.6275422	-232.6428930
$\text{SbOH}(\text{H}_2\text{O})_3^{2+} C_s$	<b>-72.3078482</b>	-72.3721115	-308.9795080	<b>-309.0095545</b>
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-72.2508891	-72.3142722	-308.9225195	-308.9502967
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-72.2502258	-72.3135957	-308.9221204	-308.9498671
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_4^{2+} S_4$	-72.2517022	-72.3155032	-308.9235799	-308.9520893
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-72.2763389	-72.3407410	-308.9515722	-308.9759379
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-72.2751641	-72.3394405	308.9498719	-308.9749658
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	-72.2839881	-72.3485326	<b>-308.9596893</b>	<b>-308.9843712</b>
$\text{Sb}(\text{H}_2\text{O})_4^{3+} C_2$	<b>-72.2839895</b>	<b>-72.3486911</b>	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#1$	-72.2756445	-72.3391781	-308.9533524	-308.9765831
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#2$	-72.2772101	-72.3402691	-308.9548471	-308.9782294
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$	-89.3944172	-89.4746922	-385.2305473	-385.2700447
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#2$	<b>-89.3964223</b>	<b>-89.4773526</b>	<b>-385.2332807</b>	<b>-385.2723336</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#1$	<b>-89.4053322</b>	<b>-89.4866013</b>	<b>-385.2441383</b>	<b>-385.2778438</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	-89.3891732	-89.4696320	-385.2278362	-385.2613205
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	-89.3905152	-89.4702866	-385.2296401	-385.2625615
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$	-89.3893617	-89.4694423	-385.2274210	-385.2618034
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#1$	-89.3959385	-89.4751802	-385.2377412	-385.2697490
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#2$	-89.3943659	-89.4742035	-385.2365906	-385.2678048
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_2 \#1$	-89.3959517	-89.4755194	-385.2379309	-385.2698176

	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*
Sb(H <sub>2</sub> O) <sub>6</sub> <sup>3+</sup> <i>T<sub>h</sub></i>	-106.4926475	-106.5891811	-461.4880920	-461.5407216
Sb(H <sub>2</sub> O) <sub>6</sub> <sup>3+</sup> <i>C<sub>3</sub></i>	<b>-106.5016567</b>	<b>-106.5988702</b>	<b>-461.5041846</b>	<b>-461.5475308</b>
Sb(H <sub>2</sub> O) <sub>6</sub> <sup>3+</sup> [5+1] <i>C<sub>s</sub></i> #1	proton transfer	proton transfer	proton transfer	proton transfer
Sb(H <sub>2</sub> O) <sub>6</sub> <sup>3+</sup> [5+1] <i>C<sub>s</sub></i> #2	proton transfer	proton transfer	proton transfer	proton transfer
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #1	-123.5854377	[5+2]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #2	-123.5758369	-123.6876824	[5+2]	-537.7966813
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #3	-123.5728450	-123.6845110	[4+3]	[6+1]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #4	[5+2]	[5+2]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #5	-123.5555450	-123.6667451	-537.7179437	-537.7758286
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #6	-123.5660883	-123.6777953	-537.7278686	-537.7862877
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #7	-123.5568248	-123.6692822	-537.7214384	-537.7779005
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #8	-123.5747636	-123.6874493	-537.7375120	-537.7951939
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #9	-123.5756813	-123.6874032	-537.7376952	-537.7952493
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #10	-123.5619762	-123.6718650	-537.7221767	-537.7813129
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #11	-123.5692633	-123.6803848	-537.7316463	-537.7898408
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #12	-123.5619760	-123.6718648	-537.7218688	-537.7813115
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #13	-123.5714460	-123.6834061	-537.7339083	-537.7918490
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #14	-123.5733052	-123.6848870	-537.7352021	-537.7934037
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #15	-123.5751298	-123.6873303	-537.7372133	-537.7956465
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2v</sub></i> #16	-123.5819987	-123.6939889	-537.7422039	-537.8026076
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #1	<i>C<sub>2</sub></i> #16	n/a	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #2	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	n/a	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #3	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #5	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #6	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #6	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	-537.7430786	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #7	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #13	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #8	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	[5+2]	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #9	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	[5+2]	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #10	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #6	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #11	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	-537.7431704	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #12	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	[5+2]	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #13	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	-537.7433431	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #14	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #13	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #15	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #16	<i>C<sub>2</sub></i> #13	<i>C<sub>2</sub></i> #16
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> <i>C<sub>2</sub></i> #16	-123.5865535	-123.6993311	[5+2]	-537.8068390

	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*
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #1	C <sub>s</sub> #5	n/a	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #2	C <sub>s</sub> #7	C <sub>s</sub> #7	n/a	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #3	C <sub>s</sub> #10	C <sub>s</sub> #10	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #4	C <sub>2v</sub> #1	[5+2]	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #5	-123.5870918	-123.7004156	-537.7493664	-537.8069848
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #6	C <sub>2v</sub> #7	C <sub>2v</sub> #7	C <sub>2v</sub> #7	C <sub>2v</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #7	-123.5798424	-123.6923281	-537.7440619	-537.8003498
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #8	-123.5747708	-123.6875172	-537.7383005	C <sub>2v</sub> #8
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #10	-123.5787751	-123.6906842	-537.7412480	-537.7993227
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #11	C <sub>s</sub> #26	C <sub>s</sub> #26	[5+2]	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #12	C <sub>s</sub> #8	C <sub>s</sub> #8	C <sub>s</sub> #8	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #13	C <sub>s</sub> #5	C <sub>s</sub> #5	[6+1]	C <sub>s</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #14	C <sub>s</sub> #7	C <sub>s</sub> #7	C <sub>s</sub> #7	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #15	C <sub>2v</sub> #10	C <sub>2v</sub> #10	C <sub>2v</sub> #10	C <sub>2v</sub> #10
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #16	C <sub>s</sub> #10	C <sub>s</sub> #10	C <sub>s</sub> #10	C <sub>s</sub> #10
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #17	-123.5756813	-123.6874034	-537.7345858	-537.7952492
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #18	C <sub>s</sub> #26	C <sub>s</sub> #26	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #19	C <sub>s</sub> #15	C <sub>s</sub> #15	C <sub>s</sub> #15	C <sub>s</sub> #15
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #20	-123.5827814	-123.6961636	C <sub>s</sub> #5	-537.8027280
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #21	-123.5767829	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #22	C <sub>s</sub> #7	C <sub>s</sub> #7	C <sub>s</sub> #7	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #23	-123.5831955	-123.6957337	[6+1]	-537.8035883
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #24	C <sub>s</sub> #10	-123.6905657	-537.7424392	C <sub>s</sub> #10
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #25	C <sub>s</sub> #21	[6+1]	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>	SbOHAq <sub>5</sub> <sup>2+</sup> + H <sub>3</sub> O <sup>+</sup>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #26	-123.5835146	-123.6959600	-537.7467739	-537.8031975
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #27	C <sub>s</sub> #23	C <sub>s</sub> #23	[6+1]	C <sub>s</sub> #23
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> [5+2]	-123.5865538	-123.6993312		
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> #12 [5+2]	Sb(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>2</sub> <sup>+</sup> +2H <sub>3</sub> O <sup>+</sup>			
Sb(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>2</sub> <sup>+</sup> +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #1	<b>-123.6047957</b>	Sb(H <sub>2</sub> O) <sub>2</sub> (OH) <sub>2</sub> <sup>+</sup> + H <sub>2</sub> O +2H <sub>3</sub> O <sup>+</sup>		
Sb(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>2</sub> <sup>+</sup> +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #12	-123.5806262	-123.6892007		
Sb(H <sub>2</sub> O) <sub>2</sub> (OH) <sub>2</sub> <sup>+</sup> + H <sub>2</sub> O +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #1		-123.7379707	-537.7958369	-537.8474576
Sb(H <sub>2</sub> O) <sub>2</sub> (OH) <sub>2</sub> <sup>+</sup> + H <sub>2</sub> O +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #12			-537.7755747	-537.8286347
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #2	n/a	n/a	[5+2]	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #3	n/a	n/a	[6+1]	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>I</sub> #4	n/a	n/a	[6+1]	n/a

Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #5	<b>-123.5878549</b>	<b>-123.7008595</b>	n/a	<b>-537.8079765</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #8	C <sub>1</sub> #5	C <sub>1</sub> #5	[5+2]	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #10	C <sub>1</sub> #5	C <sub>1</sub> #5	[5+2]	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #11	C <sub>1</sub> #5	C <sub>1</sub> #5	[5+2]	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #12	C <sub>1</sub> #5	C <sub>1</sub> #5	[5+2]	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #15	C <sub>1</sub> #5	C <sub>1</sub> #5	[5+2]	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #16	C <sub>1</sub> #5	C <sub>1</sub> #5	n/a	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #17	C <sub>1</sub> #5	n/a	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #19	C <sub>1</sub> #5	C <sub>1</sub> #5	n/a	C <sub>1</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #20	n/a	C <sub>1</sub> #5	[5+2]	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #21	C <sub>1</sub> #5	C <sub>1</sub> #5	[6+1]	C <sub>1</sub> #5

	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*
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4h</sub> #1	-140.6137869	-140.7394741	-613.9410372	-614.0073375
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4h</sub> #2	-140.6145080	-140.7404067	-613.9421391	-614.0081562
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4d</sub> #1	-140.6487462	-140.7757898	-613.9744276	-614.0426831
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4d</sub> #2	-140.6483732	-140.7740459	-613.9728677	-614.0429895
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>8</sub> #1	<b>-140.6730119</b>	<b>-140.8006821</b>	<b>-613.9966816</b>	<b>-614.0685084</b>
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>8</sub> #2	S <sub>8</sub> #1	S <sub>8</sub> #1	S <sub>8</sub> #1	S <sub>8</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4</sub> #1	-140.6631590	-140.7910931	-613.9874850	-614.0587759
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4</sub> #2	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4</sub> #3	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>4</sub> #4	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1	D <sub>4</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> C <sub>4h</sub> #1	-140.6515679	-140.7802955	-613.9781802	-614.0472085
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> C <sub>4h</sub> #2	C <sub>4h</sub> #1	C <sub>4h</sub> #1	C <sub>4h</sub> #1	C <sub>4h</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2h</sub> #1	D <sub>4h</sub> #2	D <sub>4h</sub> #2	D <sub>4h</sub> #2	D <sub>4h</sub> #2
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2d</sub> #1	-140.6400765	-140.7678290	-613.9668209	-614.0349750
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2d</sub> #2	-140.6418519	-140.7674762	-613.9664211	-614.0360146
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2d</sub> #3	D <sub>2d</sub> #1	D <sub>2d</sub> #1	D <sub>2d</sub> #1	D <sub>2d</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2d</sub> #4	-140.6413835	-140.7688696	-613.9692782	-614.0367830
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2d</sub> #5	-140.6630477	-140.7909094	-613.9873132	-614.0587531
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> C <sub>4</sub> #1	S <sub>8</sub> #1	S <sub>8</sub> #1	S <sub>8</sub> #1	S <sub>8</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>4</sub> #1	D <sub>2d</sub> #5	D <sub>2d</sub> #5	D <sub>2d</sub> #5	D <sub>2d</sub> #5
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>4</sub> #2	-140.6627869	-140.7907340	-613.9871649	-614.0574488
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>4</sub> #3	S <sub>4</sub> #2	S <sub>4</sub> #2	S <sub>4</sub> #2	S <sub>4</sub> #2
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> S <sub>4</sub> #4	S <sub>4</sub> #2	D <sub>2d</sub> #5	S <sub>4</sub> #2	D <sub>2d</sub> #5
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2</sub> #1	-140.6662559	-140.7938882	-613.9905241	-614.0617473
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2</sub> #2	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2</sub> #3	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2</sub> #4	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1
Sb(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> D <sub>2</sub> #5	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1	D <sub>2</sub> #1

$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#1$	-140.6665393	-140.7943830	-613.9922423	-614.0620472
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#2$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$

	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*
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#1$	-157.7230960	-157.8662428	-690.2117104	-690.2925510
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#2$	-157.6878787	-157.8297544	-690.1775834	-690.2564165
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#3$	-157.6996023	-157.8428207	-690.1895806	-690.2720072
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#4$	-157.7317734	-157.8751617	-690.2199346	-690.3010862
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#1$	<b>-157.7441294</b>	-157.8879753	-690.2315171	-690.3142216
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#3$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#1$	-157.7370466	-157.8807051	-690.2264705	-690.3065951
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#2$	-157.7341023	-157.8777583	-690.2218972	-690.3042632
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#2$	[6+3] -157.7412304	[6+3] -157.8809091	[6+3] -690.2344761	[6+3] -690.3293430
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#3$	[6+3] -157.7345560	[6+3] -157.8793549	[6+3] -690.2354031	[6+3] -690.3066202
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 [6+3]$	-157.7712390	-157.9135715	-690.2668004	-690.3425276
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$	n/a	n/a	[6+3]	n/a
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$	-157.7371339	-157.8810704	$C_3 \#3$	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#3$	$D_3 \#1$	$D_3 \#1$	-690.2269659	-690.3072321
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1 [6+3]$	<b>-157.7536859</b>	<b>-157.8968050</b>	<b>-690.2481182</b>	<b>-690.3206965</b>
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2 [6+3]$	<b>-157.7853989</b>	<b>-157.9271329</b>	<b>-690.2844568</b>	<b>-690.3531483</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*
$\text{H}_3\text{O}^+ D_{3h}$	-76.2843091	n/a	n/a
$\text{H}_3\text{O}^+ C_{3v}$	<b>-76.2872019</b>	n/a	n/a
$\text{Sb}^{3+} K_h$	<b>-3.4762496</b>	<b>-3.4315119</b>	<b>-3.4560761</b>
$\text{SbOH}^{2+} D_{\infty h}$	<b>-79.8738668</b>	<b>-79.8417216</b>	<b>-79.8560540</b>
$\text{Sb}(\text{H}_2\text{O})^{3+} C_{2v}$	<b>-79.7082145</b>	<b>-79.6719322</b>	<b>-79.6948352</b>
$\text{SbOH}(\text{H}_2\text{O})^{2+} C_s$	<b>-156.0048849</b>	<b>-155.9694325</b>	<b>-155.9865546</b>
$\text{Sb}(\text{H}_2\text{O})_2^{3+} D_{2d}$	-155.8497035	-155.8150550	-155.8380937
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_s$	-155.8972125	-155.8632140	-155.8856774
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_2$	<b>-155.8981591</b>	<b>-155.8640722</b>	<b>-155.8865553</b>
$\text{SbOH}(\text{H}_2\text{O})_2^{2+} C_s$	<b>-232.1127771</b>	<b>-232.0756673</b>	<b>-232.0935774</b>

$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#1$	-231.9915204	-231.9583180	-231.9823400
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#2$	-231.9937308	-231.9601123	-231.9844469
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_3$	-231.9946808	-231.9612212	-231.9854379
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#1$	-232.0521690	-232.0180934	-232.0404288
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#2$	-232.0461132	-232.0123872	-232.0349748
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_3$	<b>-232.0569291</b>	<b>-232.0228750</b>	<b>-232.0450968</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} [2+1] C_{2v}$	-232.0106318	-231.9764442	-231.9978215
$\text{SbOH}(\text{H}_2\text{O})_3^{2+} C_s$	<b>-308.1866249</b>	<b>-308.1493814</b>	<b>-308.1677101</b>
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-308.1143408	-308.0813108	-308.1062944
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-308.1140495	-308.0810475	-308.1060293
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_4^{2+} S_4$	-308.1153447	-308.0823508	-308.1073164
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-308.1559670	-308.1221091	-301.1444658
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-308.1557684	-308.1220415	-308.1443602
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	<b>-308.1642251</b>	<b>-308.1302763</b>	<b>-308.1524691</b>
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#1$	-308.1513620	-308.1168815	-308.1384625
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#2$	-308.1528707	-308.1183066	-308.1398996
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$	-384.2482513	-384.2110335	-384.2298286
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#2$	<b>-384.2492581</b>	<b>-384.2118910</b>	<b>-384.2307229</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#1$	<b>-384.2563856</b>	<b>-384.2226327</b>	<b>-384.2450550</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	-384.2406990	-384.2070988	-384.2298966
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	-384.2438141	-384.2104947	-384.2330695
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$	-384.2412830	-384.2079290	-384.2307655
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#1$	<b>-384.2472610</b>	<b>-384.2128990</b>	<b>-384.2346403</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#2$	-384.2455684	-384.2111277	-384.2327898
$\text{Sb}(\text{H}_2\text{O})_6^{3+} T_h$	-460.3038506	-460.2707479	-460.2958606
$\text{Sb}(\text{H}_2\text{O})_6^{3+} C_3$	<b>-460.3251186</b>	<b>-460.2912939</b>	<b>-460.3141284</b>
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#1$	-460.3293950	-460.2953447	-460.3173893
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#2$	<b>-460.3357925</b>	<b>-460.3015281</b>	<b>-460.3234794</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*
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#3$	536.3646000	-536.3318165	-536.3559276
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#5$	-536.3491789	-536.3163585	-536.3408320
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#6$	-536.3552721	-536.3224006	-536.3472173
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#7$	-536.3525701	-536.3195717	-536.3436233
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#8$	-536.3670051	-536.3337782	-536.3578205
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#9$	-536.3665516	-536.3333788	-536.3571553
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#10$	-536.3527630	-536.3200283	-536.3441500



$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#11$	-536.3615613	-536.3287889	-536.3529939
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#12$	-536.3532351	-536.3205321	-536.3445097
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#13$	-536.3637057	-536.3307402	-536.3548773
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#14$	-536.3642439	-536.3313745	-536.3556364
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#15$	-536.3664403	-536.3334037	-536.3575319
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#16$	-536.3697857	-536.3368261	-536.3612822
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#3$	$C_2 \#11$	$C_2 \#11$	$C_2 \#11$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#5$	$C_2 \#6$	$C_2 \#6$	$C_2 \#6$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#6$	-536.3710953	-536.3381535	-536.3623779
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#7$	$C_2 \#13$	$C_2 \#13$	$C_2 \#13$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#8$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#9$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#10$	$C_2 \#6$	$C_2 \#6$	$C_2 \#11$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#11$	-536.3715725	-536.3386560	-536.3627311
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#12$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#13$	-536.3713118	-536.3381938	-536.3622840
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#14$	$C_2 \#13$	$C_2 \#13$	$C_2 \#13$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#15$	$C_2 \#13$	$C_2 \#13$	$C_2 \#13$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#16$	[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*
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#3$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#4$	-536.3702763	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#5$	-536.3792510	-536.3459046	-536.3690500
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#6$	$C_{2v} \#7$	$C_{2v} \#7$	$C_{2v} \#7$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#7$	-536.3727784	-536.3396272	-536.3632857
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#8$	-536.3676466	-536.3343223	-536.3582214
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#10$	[5+2]	[5+2]	-536.3632369
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#11$	[5+2]	$C_s \#26$	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#12$	$C_s \#8$	$C_s \#8$	$C_s \#8$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#13$	[6+1]	[6+1]	-536.3724480
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#14$	$C_s \#7$	$C_s \#7$	$C_s \#7$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#15$	$C_{2v} \#12$	$C_{2v} \#12$	$C_{2v} \#12$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#16$	[5+2]	[5+2]	-536.3616091
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#17$	[5+2]	[5+2]	-536.3551867
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#18$	$C_s \#26$	$C_s \#26$	$C_s \#26$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#20$	$C_s \#5$	$C_s \#5$	$C_s \#5$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#21$	[6+1] -536.3733301	[6+1] -536.3398453	[6+1] -536.3627192
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#22$	$C_s \#7$	$C_s \#7$	$C_s \#7$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#23$	[6+1] -536.3747167	[6+1]	-536.3651319
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_s \#24$	[6+1]	-536.3399844	$C_s \#10$

$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_s$ #25	[6+1] $C_s$ #21	[6+1] $C_s$ #21	[6+1] $C_s$ #21
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_s$ #26	-536.3773702	-536.3441900	-536.3676973
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_s$ #27	[5+2]	[6+1] -536.3449478	$C_s$ #23
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_{2v}$ [5+2]	<b>-536.3909992</b>	<b>-536.3567103</b>	<b>-536.3783534</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_{2v}$ #4 [5+2]		-536.3452201	
$\text{Sb}(\text{H}_2\text{O})_3(\text{OH})_2^+ + 2\text{H}_3\text{O}^+$ $C_{2v}$ #12	$\text{Sb}(\text{H}_2\text{O})_2(\text{OH})_2^+ +$ $\text{H}_2\text{O} + 2\text{H}_3\text{O}^+$		
$\text{Sb}(\text{H}_2\text{O})_2(\text{OH})_2^+ + \text{H}_2\text{O}$ $+ 2\text{H}_3\text{O}^+$ $C_{2v}$ #1	-536.4289658	-536.3896123	-536.4077793
$\text{Sb}(\text{H}_2\text{O})_2(\text{OH})_2^+ + \text{H}_2\text{O}$ $+ 2\text{H}_3\text{O}^+$ $C_{2v}$ #12	-536.4155443	-536.3762666	-536.3943485
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #2	[5+2]	[5+2]	[6+1]
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #3	[6+1]	[6+1]	<b>-536.3726919</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #4	[6+1]	[5+2]	$C_1$ #3
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #7	[6+1]	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #8	[6+1]	[6+1]	<b>-536.3725069</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #10	[6+1]	[6+1]	<b>-536.3727280</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #11	[5+2]	[5+2]	$C_1$ #3
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #12	n/a	n/a	$C_1$ #8
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #13	n/a	n/a	$C_1$ #8
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #15	n/a	n/a	$C_1$ #3
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #17	[5+2] <b>-536.4047803</b>	[5+2] <b>-536.3701871</b>	[6+1] <b>-536.3846023</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #19	n/a	n/a	$C_1$ #3
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #20	n/a	[6+1]	$C_1$ #8
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #21	[6+1]	[6+1]	$C_1$ #8

	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*
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #1	-612.3830569	-612.3509030	-612.3756662
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #2	-612.3836814	-612.3514345	-612.3761718
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #1	-612.4144491	-612.3824947	-612.4073710
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #2	-612.4124616	-612.3804700	-612.4053554
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #1	-612.4344359	<b>-612.4022153</b>	<b>-612.4271711</b>
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #2	$S_8$ #1	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #1	-612.4246659	-612.3921789	-612.4170549
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #2	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #3	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #4	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #1	-612.4144706	-612.3819718	-612.4067968
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #2	$C_{4h}$ #1	$C_{4h}$ #1	$C_{4h}$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #1	$D_{4h}$ #2	$D_{4h}$ #2	$D_{4h}$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #1	-612.4040018	-612.3715332	-612.3963100
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #2	-612.4062445	-612.3740590	-612.3988966

$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#3$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#4$	-612.4073833	-612.3749382	-612.3998682
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#5$	-612.4245484	-612.3920697	-612.4169245
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_4 \#1$	$S_8 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#1$	$D_{2d} \#5$	$D_{2d} \#5$	$D_{2d} \#5$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#2$	-612.4241453	-612.3917304	-612.4166383
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#3$	$S_4 \#2$	$S_4 \#2$	$S_4 \#2$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} S_4 \#4$	$S_4 \#2$	$S_4 \#2$	$S_4 \#2$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#1$	-612.4283756	-612.3961348	-612.4210916
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#2$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#3$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#4$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#5$	$D_2 \#1$	$D_2 \#1$	$D_2 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#4$	[6+2] -612.4366304	[6+2] -612.4025578	[6+2] -612.4251789
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#1$	[6+2] -612.4534584	[6+2] -612.4197482	-612.4212854
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#2$	[6+2] $C_2 \#1$	$S_8 \#1$	$S_8 \#1$
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#1$	-612.4122877	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#2$			
$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2h} \#3$			
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#1$	$D_{2h} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#2$	-612.4127033	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#3$	$C_{4h} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#1$	$D_{2h} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#3$	-612.4130454	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#1$	[5+3] -612.4548945	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#2$	[5+3] -612.4418756	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_I \#1$	[5+3] <b>-612.4637354</b>	n/a	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*
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#1$	-688.4619802	-688.4305233	-688.4552749
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#2$	-688.4321109	-688.4008712	-688.4256540
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#3$	-688.4411573	-688.4093598	-688.4340665
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#4$	-688.4682575	-688.4364148	-688.4611595
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#1$	-688.4793795	-688.4476761	-688.4724195
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#3$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#1$	-688.4723612	-688.4405385	-688.4652606
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#2$	-688.4705815	-688.4388521	-688.4635939
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$

$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#2$	[6+3] -688.4869972	[6+3] -688.4528532	[6+3] -688.4751221
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#3$	[6+3] -688.4794232	[6+3] -688.4455676	[6+3] -688.4689300
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 [6+3]$	-688.5003254	-688.4671713	-688.4919061
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#3$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1 [6+3]$	<b>-688.4927995</b>	<b>-688.4585890</b>	<b>-688.4810750</b>
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2 [6+3]$	<b>-688.5263099</b>	<b>-688.4915269</b>	<b>-688.5136314</b>
$\text{Sb}(\text{H}_2\text{O})_{18}^{3+} T [6+12]$	-1372.8964389	-1372.8626407	-1372.8872522

	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*
$\text{H}_3\text{O}^+ D_{3h}$	-76.2853334	n/a	n/a
$\text{H}_3\text{O}^+ C_{3v}$	<b>-76.2885707</b>	n/a	n/a
$\text{Sb}^{3+} K_h$	<b>-3.4762496</b>	<b>-3.4315119</b>	<b>-3.4560761</b>
$\text{SbOH}^{2+} D_{\infty h}$	<b>-79.8833686</b>	<b>-79.8536754</b>	<b>-79.8666718</b>
$\text{Sb}(\text{H}_2\text{O})^{3+} C_{2v}$	<b>-79.7114734</b>	<b>-79.6883447</b>	<b>-79.7083461</b>
$\text{SbOH}(\text{H}_2\text{O})^{2+} C_s$	<b>-156.0140947</b>	<b>-155.9821609</b>	<b>-155.9981521</b>
$\text{Sb}(\text{H}_2\text{O})_2^{3+} D_{2d}$	-155.8560438	-155.8315056	-155.8524543
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_s$	-155.9031058	-155.8790365	-155.8997482
$\text{Sb}(\text{H}_2\text{O})_2^{3+} C_2$	<b>-155.9041047</b>	<b>-155.8800516</b>	<b>-155.9007546</b>
$\text{SbOH}(\text{H}_2\text{O})_2^{2+} C_s$	<b>-232.1241567</b>	<b>-232.0894157</b>	<b>-232.1067606</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#1$	-232.0014776	-231.9771757	-231.9995975
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_{3h} \#2$	-232.0033474	-231.9788190	-232.0015029
$\text{Sb}(\text{H}_2\text{O})_3^{3+} D_3$	-232.0045373	-231.9801092	-232.0026555
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#1$	-232.0627718	-232.0332654	-232.0545754
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_{3v} \#2$	-232.0564194	-232.0275340	-232.0491369
$\text{Sb}(\text{H}_2\text{O})_3^{3+} C_3$	<b>-232.0671694</b>	<b>-232.0379276</b>	<b>-232.0592269</b>
$\text{Sb}(\text{H}_2\text{O})_3^{3+} [2+1] C_{2v}$	-232.0195161	-231.9937104	-232.0136147
$\text{SbOH}(\text{H}_2\text{O})_3^{2+} C_s$	<b>-308.2020806</b>	<b>-308.1664721</b>	<b>-308.1844320</b>
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#1$	-308.1311094	-308.1028341	-308.1264230
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_{2d} \#2$	-308.1309421	-308.1025321	-308.1261167
$\text{Sb}(\text{H}_2\text{O})_4^{2+} D_2$	$D_{2d} \#1$	$D_{2d} \#1$	$D_{2d} \#1$
$\text{Sb}(\text{H}_2\text{O})_4^{2+} S_4$	-308.1326371	-308.1040734	-308.1276048
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#1$	-308.1696221	-308.1385172	-308.1602694
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#2$	-308.1694773	-308.1380622	-308.1597040
$\text{Sb}(\text{H}_2\text{O})_4^{2+} C_{2v} \#3$	<b>-308.1781884</b>	<b>-308.1466787</b>	<b>-308.1681518</b>
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#1$	-308.1640916	-308.1337213	-308.1545302
$\text{Sb}(\text{H}_2\text{O})_4^{3+} [3+1] C_s \#2$	-308.1658395	-308.1353648	-308.1561431
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$	-384.2684479	-384.2325542	-384.2511386
$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#2$	<b>-384.2692695</b>	<b>-384.2334031</b>	<b>-384.2519561</b>

$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#1$	<b>-384.2743271</b>	<b>-384.2419957</b>	<b>-384.2640081</b>
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	-384.2584291	-384.2265097	-384.2488065
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	-384.2618900	-384.2296991	-384.2517624
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$	-384.2597493	-384.2277385	-384.2499996
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#1$	<b>-384.2642528</b>	-384.2319209	-384.2531118
$\text{Sb}(\text{H}_2\text{O})_5^{3+} [4+1] C_{2v} \#2$	-384.2618607	-384.2296131	-384.2508352
$\text{Sb}(\text{H}_2\text{O})_6^{3+} T_h$	-460.3339467	-460.3012633	-460.3250792
$\text{Sb}(\text{H}_2\text{O})_6^{3+} C_3$	<b>-460.3472925</b>	<b>-460.3151868</b>	<b>-460.3375715</b>
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#1$	-460.3504723	-460.3175193	-460.3391413
$\text{Sb}(\text{H}_2\text{O})_6^{3+} [5+1] C_s \#2$	<b>-460.3567716</b>	<b>-460.3237836</b>	<b>-460.3453798</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*
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#1$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#2$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#3$	-536.3951651	-536.3632715	-536.3864362
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#4$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#5$	-536.3782585	-536.3463053	-536.3697942
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#6$	-536.3864893	-536.3543396	-536.3779777
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#7$	-536.3813578	-536.3491303	-536.3722130
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#8$	-536.3967005	-536.3643375	-536.3874837
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#9$	-536.3964442	-536.3648741	-536.3879856
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#10$	-536.3837371	-536.3521750	-536.3754627
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#11$	-536.3928380	-536.3607866	-536.3840101
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#12$	-536.3847920	-536.3529838	-536.3761099
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#13$	-536.3934584	-536.3614495	-536.3846254
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#14$	-536.3944141	-536.3627007	-536.3860605
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#15$	-536.3970616	-536.3646313	-536.3878003
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_{2v} \#16$	-536.4014611	-536.3694578	-536.3930181
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#3$	$C_2 \#11$	$C_2 \#11$	$C_2 \#11$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#5$	-536.4008304	-536.3690557	-536.3924571
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#6$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#7$	[5+2]	$C_2 \#13$	<b>[5+2] -536.4052545</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#8$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#9$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#10$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#11$	-536.4012399	-536.3694346	-536.3926353
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#12$	[5+2]	[5+2]	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#13$	[5+2]	-536.3694509	<b>[5+2] -536.4052545</b>
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#14$	<b>[5+2] -536.4166033</b>	$C_2 \#13$	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#15$	[5+2]	$C_2 \#13$	[5+2]
$\text{Sb}(\text{H}_2\text{O})_7^{3+} C_2 \#16$	[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*
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #3	[5+2]	[6+1]	[6+1] -536.4057121
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #4	[5+2]	[5+2]	[5+2]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #5	-536.4056864	-536.3737854	-536.3963769
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #6	C <sub>2v</sub> #7	C <sub>2v</sub> #7	C <sub>2v</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #7	-536.3995196	-536.3687777	-536.3919877
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #8	-536.3967035	-536.3644693	-536.3875698
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #10	[5+2]	-536.3688258	[6+1]
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #11	C <sub>s</sub> #26	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #12	C <sub>s</sub> #8	C <sub>s</sub> #8	C <sub>s</sub> #8
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #13	<b>-536.4100518</b>	-536.3780360	-536.4005494
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #14	C <sub>s</sub> #7	-536.3675953	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #15	C <sub>2v</sub> #12	C <sub>2v</sub> #12	C <sub>2v</sub> #12
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #16	C <sub>s</sub> #24	C <sub>s</sub> #10	C <sub>s</sub> #24
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #17	-536.3951915	-536.3631649	-536.3864537
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #18	C <sub>s</sub> #26	C <sub>s</sub> #26	C <sub>s</sub> #26
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #20	C <sub>s</sub> #5	C <sub>s</sub> #5	C <sub>s</sub> #5
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #21	[6+1] -536.4014856	[6+1] -536.3691532	[6+1] -536.3916869
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #22	-536.4002540	C <sub>s</sub> #7	C <sub>s</sub> #7
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #23	-536.4045862	-536.3726801	-536.3957202
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #24	-536.4010241	C <sub>s</sub> #10	-536.3917842
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #25	[6+1] C <sub>s</sub> #21	[6+1] C <sub>s</sub> #21	[6+1] C <sub>s</sub> #21
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #26	-536.4056095	-536.3736117	-536.3964629
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>s</sub> #27	C <sub>s</sub> #23	C <sub>s</sub> #23	C <sub>s</sub> #23
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> #2 [5+2]	-536.4045515	[5+2]	
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>2v</sub> [5+2]	<b>-536.4166050</b>	<b>-536.3836789</b>	<b>-536.4052556</b>
Sb(H <sub>2</sub> O) <sub>2</sub> (OH) <sub>2</sub> <sup>+</sup> + H <sub>2</sub> O +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #1	-536.4542215	-536.4168223	-536.4348544
Sb(H <sub>2</sub> O) <sub>2</sub> (OH) <sub>2</sub> <sup>+</sup> + H <sub>2</sub> O +2H <sub>3</sub> O <sup>+</sup> C <sub>2v</sub> #12	-536.4419365	-536.4042325	-536.4220360
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #1	[6+1]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #3	[5+2]	<b>-536.3784950</b>	<b>-536.4011801</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #4	n/a	C <sub>1</sub> #3	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #8	<b>-536.4097018</b>	<b>-536.3776262</b>	<b>-536.4000363</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #10	[6+1]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #11	[6+1]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #12	n/a	C <sub>1</sub> #8	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #13	<b>-536.4100521</b>	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #14	n/a	C <sub>1</sub> #3	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #15	[6+1]	C <sub>1</sub> #3	C <sub>1</sub> #3
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #17	[5+2]	[6+1] <b>-536.3891165</b>	[6+1] <b>-536.4110555</b>
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #18	C <sub>1</sub> #8	n/a	n/a
Sb(H <sub>2</sub> O) <sub>7</sub> <sup>3+</sup> C <sub>1</sub> #19	[6+1]	C <sub>1</sub> #3	C <sub>1</sub> #3

$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #20	[6+1]	n/a	[6+1]
$\text{Sb}(\text{H}_2\text{O})_7^{3+}$ $C_1$ #21	[6+1]	$C_1$ #3	$C_1$ #3

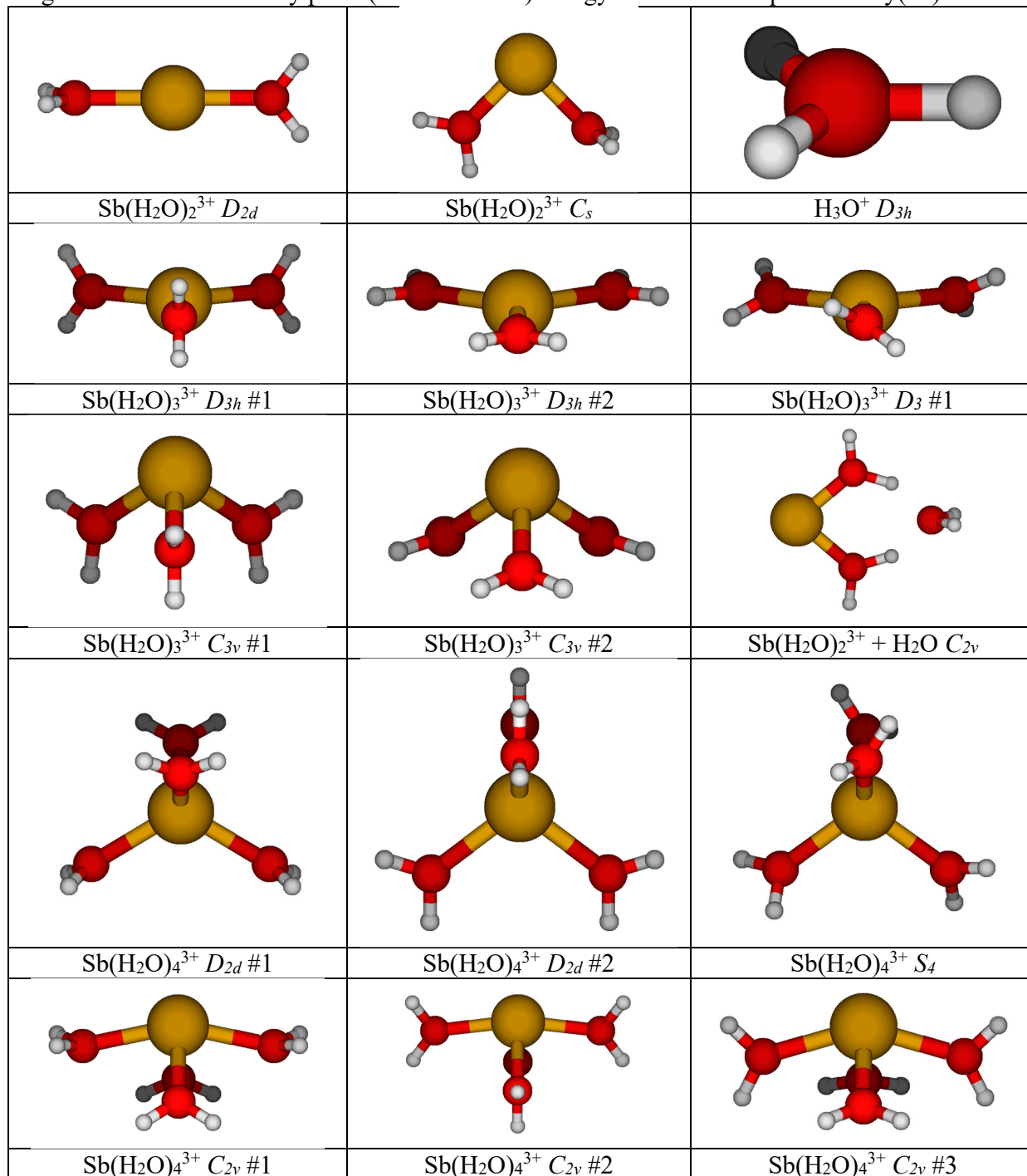
	HF/gen (5d) M: CEP-121G* OH: 6-31+G*	HF/gen (5d) M: LANL2DZ OH: 6-31+G*	HF/gen (5d) M: SDD OH: 6-31+G*
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #1	-612.4161642	-612.3859046	-612.4094348
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4h}$ #2	-612.4166713	-612.3864364	-612.4100136
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #1	-612.4476275	-612.4160099	-612.4393876
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{4d}$ #2	-612.4467945	-612.4153990	-612.4388263
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #1	-612.4703005	<b>-612.4384028</b>	<b>-612.4618398</b>
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_8$ #2	$S_8$ #1	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #1	-612.4604353	-612.4291669	-612.4527303
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #2	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #3	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_4$ #4	$D_4$ #1	$D_4$ #1	$D_4$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #1	-612.4493168	-612.4183706	-612.4418829
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{4h}$ #2	$C_{4h}$ #1	$C_{4h}$ #1	$C_{4h}$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #1	$D_{4h}$ #2	$D_{4h}$ #2	$D_{4h}$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #1	-612.4383633	-612.4077832	-612.4314118
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #2	-612.4415611	-612.4104752	-612.4340180
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #3	$D_{2d}$ #1	$D_{2d}$ #1	$D_{2d}$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #4	-612.4404787	-612.4090142	-612.4326103
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2d}$ #5	-612.4604405	-612.4292609	-612.4528423
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_4$ #1	$S_8$ #1	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #1	$D_{2d}$ #5	$D_{2d}$ #5	$D_{2d}$ #5
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #2	-612.4593490	-612.4276253	-612.4511624
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #3	$S_4$ #2	$S_4$ #2	$S_4$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $S_4$ #4	$S_4$ #2	$S_4$ #2	$S_4$ #2
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #1	-612.4635688	-612.4318345	-612.4553840
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #2	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #3	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #4	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_2$ #5	$D_2$ #1	$D_2$ #1	$D_2$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #2	-612.4418227	-612.4104843	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2v}$ #4	-612.4691752	-612.4367029	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_2$ #1	-612.4637969	-612.4321131	-612.4555685
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_2$ #2	$S_8$ #1	$S_8$ #1	$S_8$ #1
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #1	-612.4475060	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #2			
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $D_{2h}$ #3			
$\text{Sb}(\text{H}_2\text{O})_8^{3+}$ $C_{2h}$ #1	$D_{2h}$ #1	n/a	n/a

$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#2$	-612.4480251	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2h} \#3$	$C_{4h} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#1$	$D_{2h} \#1$	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{2v} \#3$	-612.4481269	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#1$	[5+3] -612.4837968	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_s \#2$	[5+3] -612.4721481	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_2 \#1$	[6+2] <b>-612.4829888</b>	n/a	n/a
$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_1 \#1$	<b>-612.4703035</b>	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*
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#1$	-688.4994750	-688.4680299	-688.4912818
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#2$	-688.4685715	-688.4371764	-688.4604079
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#3$	-688.4809815	-688.4492320	-688.4724483
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_{3h} \#4$	-688.5072060	-688.4758140	-688.4991693
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#1$	-688.5195142	-688.4878249	-688.5110906
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#2$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#3$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3 \#4$	$D_3 \#1$	$D_3 \#1$	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#1$	-688.5110529	-688.4798305	-688.5031858
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#2$	-688.5097945	-688.4783259	-688.5016197
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#3$	$C_{3h} \#1$	$C_{3h} \#1$	$C_{3h} \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3h} \#4$	$C_{3h} \#2$	$C_{3h} \#2$	$C_{3h} \#2$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#1$	-688.5003033	-688.4683336	-688.4913337
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#2$	[6+3] -688.5230584	[6+3] -688.4901332	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_{3v} \#3$	[6+3] -688.5137367	[6+3] -688.4822086	[6+3] -688.5048172
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$	[6+3]	[6+3]	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#3$	[6+3]	[6+3]	[6+3]
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#4$	[6+3]	[6+3]	$D_3 \#1$
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#1$ [6+3]	<b>-688.5284002</b>	<b>688.4961909</b>	<b>-688.5185892</b>
$\text{Sb}(\text{H}_2\text{O})_9^{3+} C_3 \#2$ [6+3]	<b>-688.5591671</b>	<b>-688.5261823</b>	<b>-688.5480844</b>
$\text{Sb}(\text{H}_2\text{O})_9^{3+} D_3$ [6+3]	-688.5398128	-688.5082779	-688.5320403

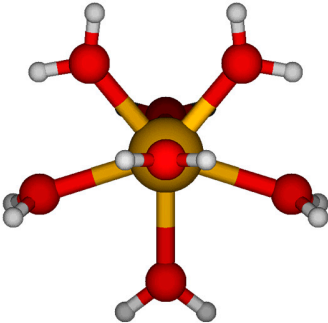
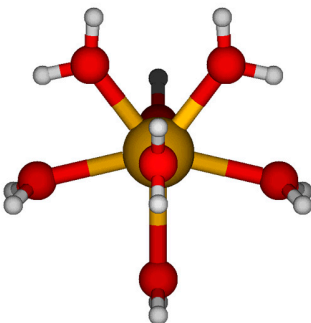
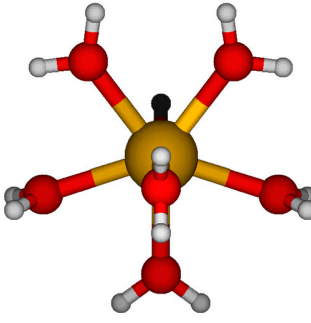
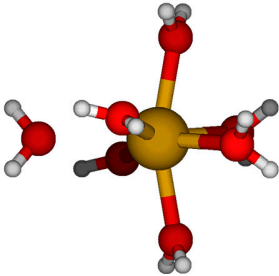
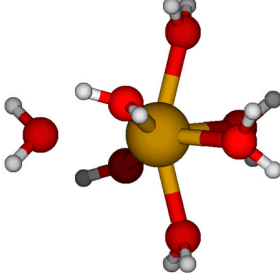
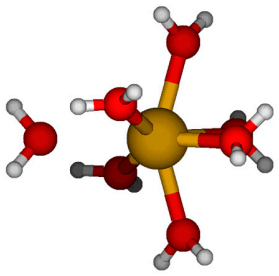
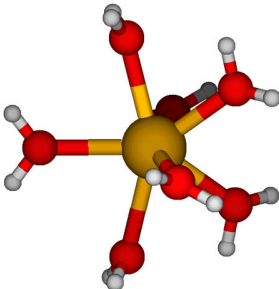
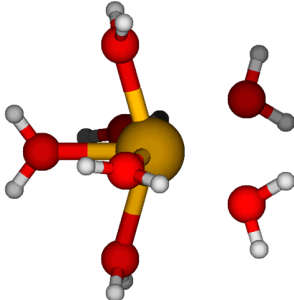
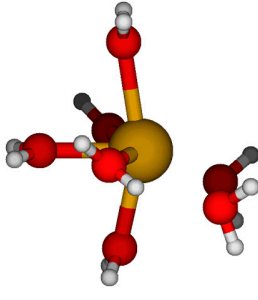
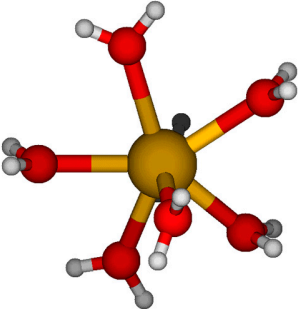
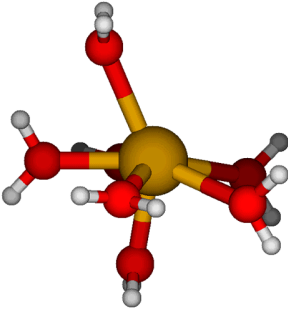
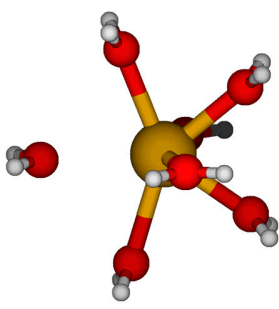


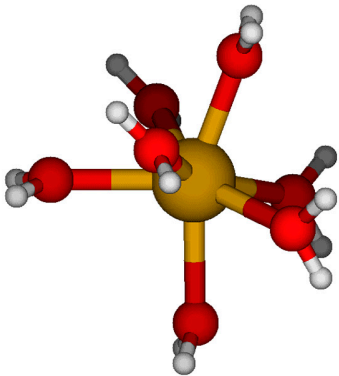
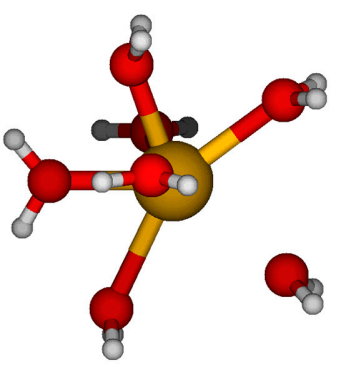
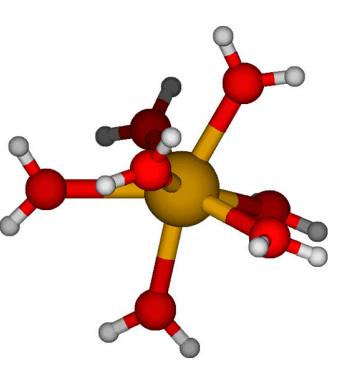
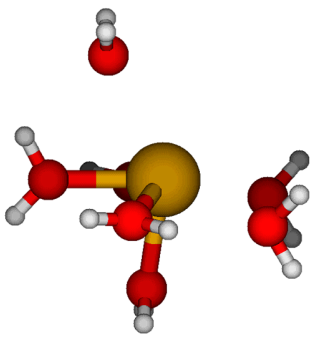
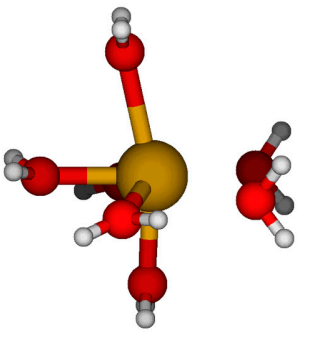
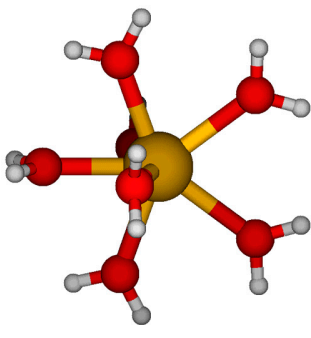
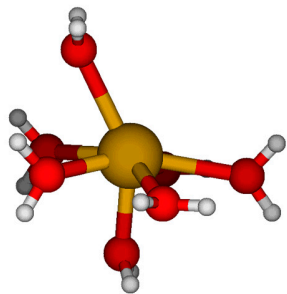
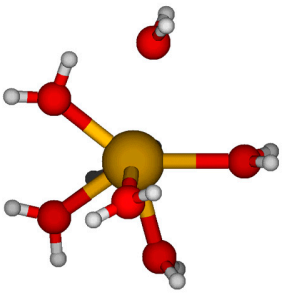
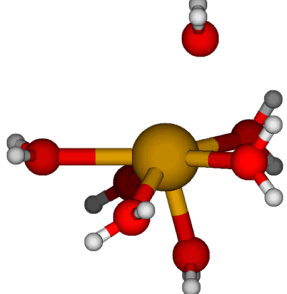
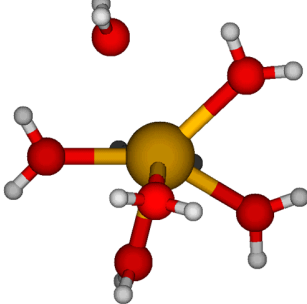
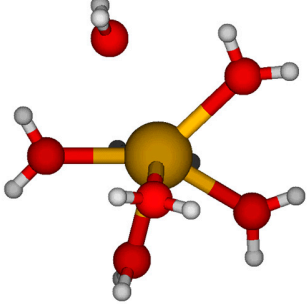
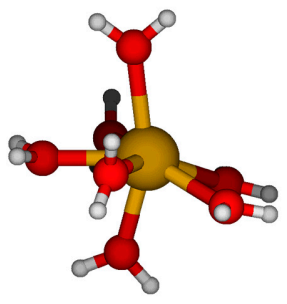
Figure S1: Some stationary point (non-minimum) energy structures of aquaantimony(III).

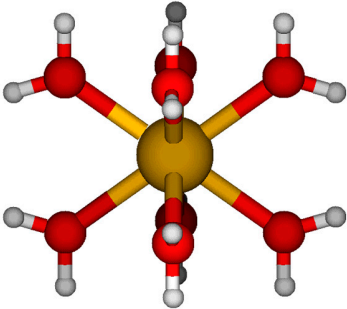
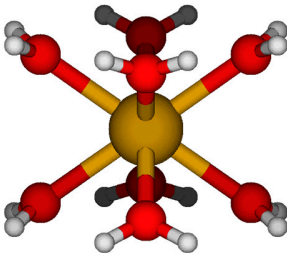
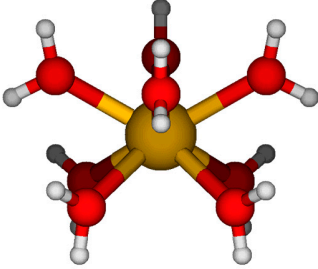
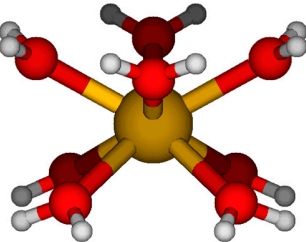
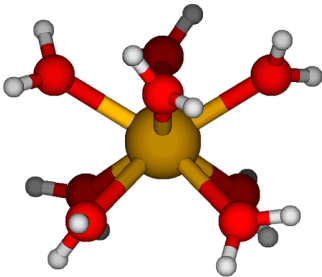
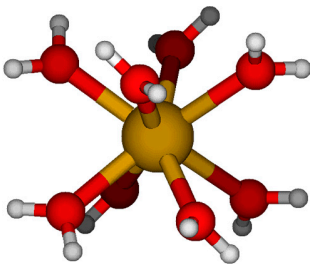
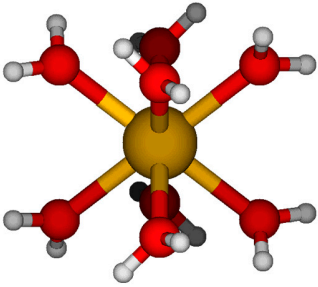
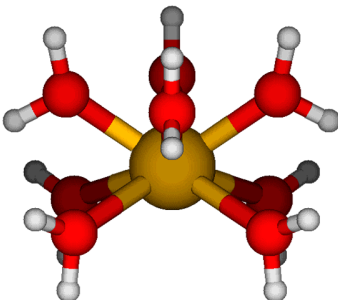
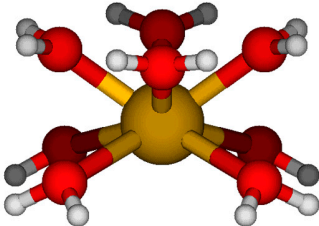
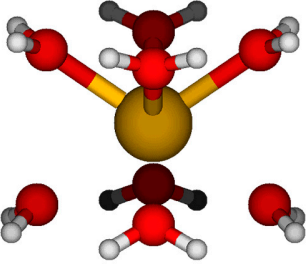
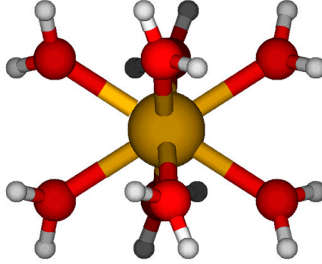
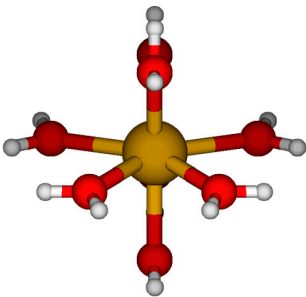


$\text{Sb}(\text{H}_2\text{O})_3^{3+} + \text{H}_2\text{O } C_s \#1$	$\text{Sb}(\text{H}_2\text{O})_3^{3+} + \text{H}_2\text{O } C_s \#2$	$\text{SbOH}(\text{H}_2\text{O})_4^{2+} C_s \#1$
$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#2$	$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#3$	$\text{Sb}(\text{H}_2\text{O})_5^{3+} C_{2v} \#4$
$\text{Sb}(\text{H}_2\text{O})_4^{3+} + \text{H}_2\text{O } C_{2v} \#1$	$\text{Sb}(\text{H}_2\text{O})_4^{3+} + \text{H}_2\text{O } C_{2v} \#2$	$\text{Sb}(\text{H}_2\text{O})_4^{3+} + \text{H}_2\text{O } C_2 \#1$
	$\text{Sb}(\text{H}_2\text{O})_6^{3+} T_h$	$\text{Sb}(\text{H}_2\text{O})_5^{3+} + \text{H}_2\text{O } C_s \#1$

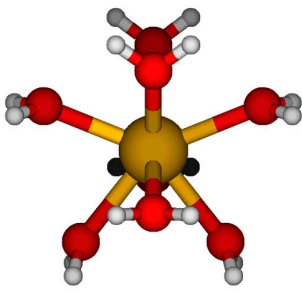
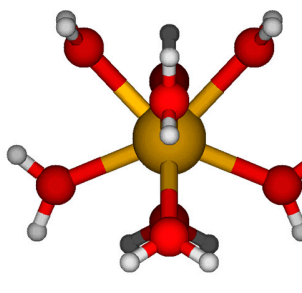
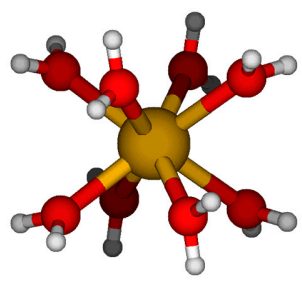
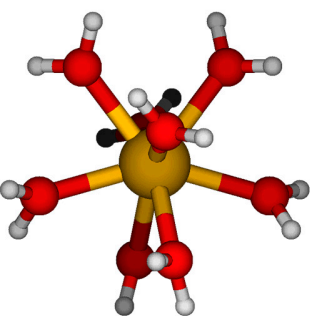
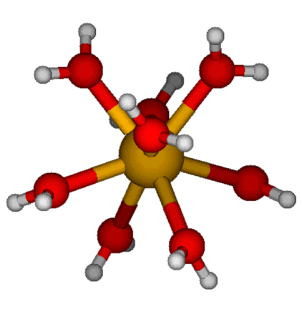
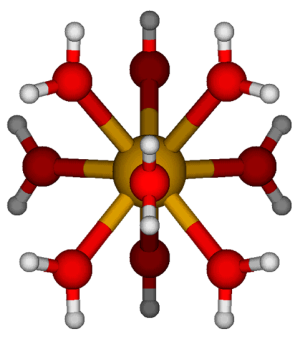
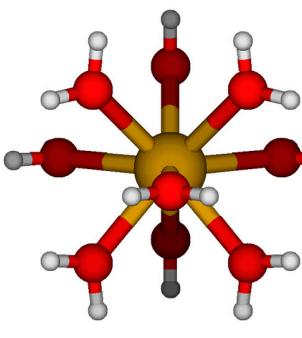
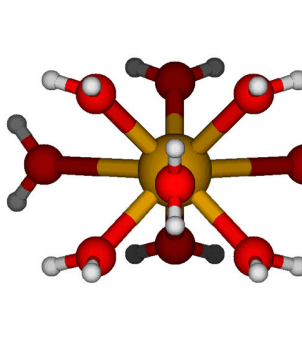
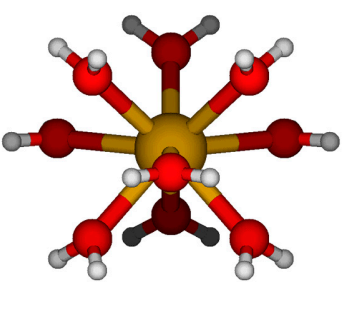
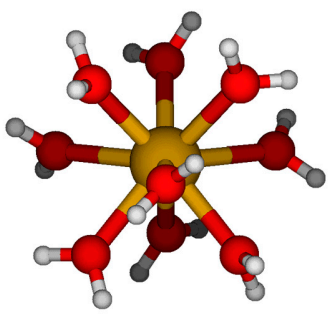
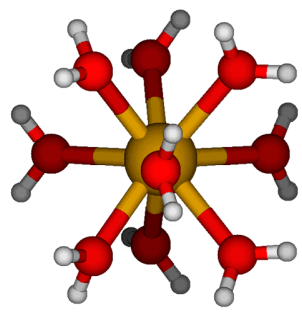
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$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#5}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#6}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#7}$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#8}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#9}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#10}$
$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#11}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#12}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_{2v} \text{ \#13}$

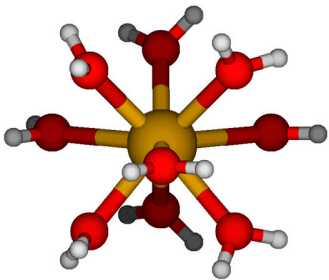
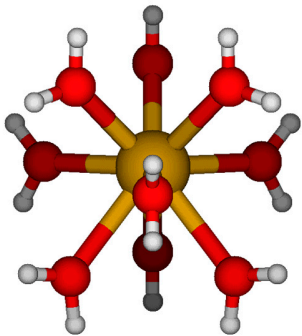
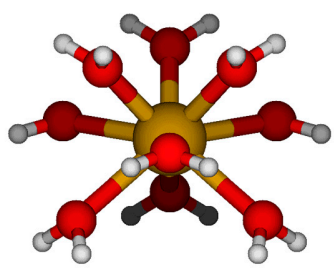
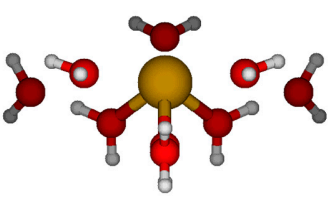
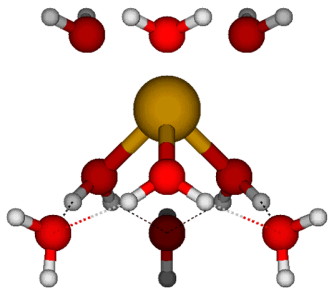
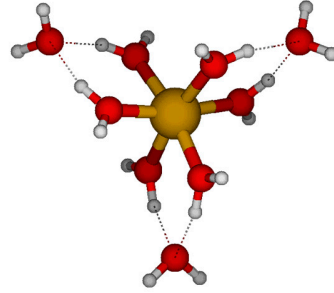
		
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$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_2 \text{ \#13}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_2 \text{ \#16}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#2}$
		
$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#4}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#5}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#6}$

		
$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#7}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#8}$	$\text{Sb}(\text{H}_2\text{O})_7^{3+} \text{ } C_s \text{ \#10}$
		
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$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4h} \#1$	$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4v} \#1$	$\text{Sb}(\text{H}_2\text{O})_8^{3+} C_{4v} \#2$
		
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$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#4$	$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_{2d} \#5$	$\text{Sb}(\text{H}_2\text{O})_8^{3+} D_2 \#1$
		
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$\text{Sb}(\text{H}_2\text{O})_9^{3+} \text{ } C_{3h} \text{ \#2}$	$\text{Sb}(\text{H}_2\text{O})_9^{3+} \text{ } C_{3v} \text{ \#1}$	$\text{Sb}(\text{H}_2\text{O})_9^{3+} \text{ } C_{3v} \text{ \#4}$
		
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