Supplementary Material to:

An ab initio investigation of the hydration of lead(II)

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Table S1: Total Energies of Aqualead(II) Species (bold indicates a minimum energy structure)

	HF/CEP-4G (6d)	HF/CEP-31G*(6d)	HF/CEP-121G* (6d)
Pb^{2+} K_h	**-2.6207713**	**-2.6207713**	**-2.6207713**
$Pb(H_2O)^{2+}$ C_{2v}	**-19.5093600**	**-19.5721795**	**-19.5757397**
$Pb(H_2O)_2^{2+}$ D_{2d}	-36.3530035	-36.4953929	-36.5025292
$Pb(H_2O)_2^{2+}$ C_s	-36.3828241	-36.5106573	-36.5181191
$Pb(H_2O)_2^{2+}$ C_2	**-36.3831323**	**-36.5107561**	**-36.5181916**
$Pb(H_2O)_2^{2+}$ [1+1] C_s	**-36.3447126**	**-36.4732710**	**[2+0]**
$PbOH^+ + H_3O^+$ C_s	[1+1] C_s	**-36.4733896**	**-36.4808476**
$Pb(H_2O)_3^{2+}$ D_{3h} #1	-53.2066526	-53.4196530	-53.4304256
$Pb(H_2O)_3^{2+}$ D_{3h} #2	-53.2085268	-53.4199874	-53.4306811
$Pb(H_2O)_3^{2+}$ D_3	-53.2086640	-53.4206853	-53.4314642
$Pb(H_2O)_3^{2+}$ C_{3v} #1	-53.2421161	-53.4347928	-53.4462281
$Pb(H_2O)_3^{2+}$ C_{3v} #2	-53.2387273	-53.4330348	-53.4444359
$Pb(H_2O)_3^{2+}$ C_3	**-53.2447267**	**-53.4389643**	**-53.4507597**
$Pb(H_2O)_3^{2+}$ [2+1] C_{2v}	-53.2092375	**-53.4125913**	**-53.4237681**
$Pb(H_2O)_3^{2+}$ [2+1] C_s	**-53.2093732**	n/a	n/a
$Pb(H_2O)_4^{2+}$ D_{2d} #1	-70.0505490	-70.3342016	-70.3486791
$Pb(H_2O)_4^{2+}$ D_{2d} #2	-70.0504947	-70.3341320	-70.3486195
$Pb(H_2O)_4^{2+}$ D_2	D_{2d} #1	D_{2d} #1	-70.3486859
$Pb(H_2O)_4^{2+}$ S_4	-70.0511256	-70.3348934	-70.3494801
$Pb(H_2O)_4^{2+}$ C_{2v} #1	-70.0723991	-70.3422919	-70.3576265
$Pb(H_2O)_4^{2+}$ C_{2v} #2	-70.0731749	-70.3415197	-70.3569000
$Pb(H_2O)_4^{2+}$ C_{2v} #3	-70.0778703	-70.3470735	-70.3624767
$Pb(H_2O)_4^{2+}$ C_2	**-70.0778735**	**-70.3471305**	**-70.3626094**
$Pb(H_2O)_4^{2+}$ [3+1] C_s #1	-70.0624406	-70.3333486	-70.3489047
$Pb(H_2O)_4^{2+}$ [3+1] C_s #2	**-70.0633465**	**-70.3342043**	**-70.3497255**
$Pb(H_2O)_5^{2+}$ C_{2v} #1	-86.8925626	-87.2401416	-87.2590576
$Pb(H_2O)_5^{2+}$ C_{2v} #2	-86.8961871	-87.2407041	-87.2596039
$Pb(H_2O)_5^{2+}$ C_{2v} #3	**-86.9020034**	**-87.2497854**	**-87.2692500**
$Pb(H_2O)_5^{2+}$ C_{2v} #4	-86.8938026	-87.2401481	-87.2590426
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #1	-86.8893604	-87.2360576	-87.2553831
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #2	-86.8881546	-87.2352296	-87.2546249
$Pb(H_2O)_5^{2+}$ [4+1] C_2 #1	n/a	-87.2364803	-87.2559090
$Pb(H_2O)_5^{2+}$ [4+1] C_s #1	-86.8893643	-87.2365676	-87.2557860
$Pb(H_2O)_5^{2+}$ [4+1] C_s #4	**-86.8900136**	**-87.2371606**	**-87.2566787**
$Pb(H_2O)_6^{2+}$ T_h	-103.6987899	-104.1346017	-104.1572252
$Pb(H_2O)_6^{2+}$ C_3	**-103.7114259**	**-104.1404202**	**-104.1634506**
$Pb(H_2O)_6^{2+}$ [5+1] C_s #1	**-103.7123498**	**-104.1376960**	**-104.1609020**

$Pb(H_2O)_7^{2+}$ C_{2v} #1	-120.5091447	-121.0217847	-121.0483867
$Pb(H_2O)_7^{2+}$ C_{2v} #2	-120.5052153	-121.0168375	-121.0430594
$Pb(H_2O)_7^{2+}$ C_{2v} #3	-120.5023879	-121.0152635	-121.0413014
$Pb(H_2O)_7^{2+}$ C_{2v} #4	[5+2]	-121.0151514	-121.0413933
$Pb(H_2O)_7^{2+}$ C_{2v} #5	-120.4947241	-121.0040033	-121.0296727
$Pb(H_2O)_7^{2+}$ C_{2v} #6	-120.4985435	-121.0104912	-121.0364285
$Pb(H_2O)_7^{2+}$ C_{2v} #7	-120.4955065	-121.0045365	-121.0304676
$Pb(H_2O)_7^{2+}$ C_{2v} #8	-120.5040168	-121.0162731	-121.0426799
$Pb(H_2O)_7^{2+}$ C_{2v} #9	-120.5030413	-121.0168077	-121.0431632
$Pb(H_2O)_7^{2+}$ C_{2v} #10	-120.4963264	-121.0069876	-121.0324854
$Pb(H_2O)_7^{2+}$ C_{2v} #11	-120.5025805	-121.0127195	-121.0386317
$Pb(H_2O)_7^{2+}$ C_{2v} #12	-120.4972729	-121.0069881	-121.0324908
$Pb(H_2O)_7^{2+}$ C_{2v} #13	-120.5028241	-121.0140964	-121.0402449
$Pb(H_2O)_7^{2+}$ C_{2v} #14	-120.5026395	-121.0153577	-121.0414440
$Pb(H_2O)_7^{2+}$ C_{2v} #15	-120.5046976	-121.0167712	-121.0431131
$Pb(H_2O)_7^{2+}$ C_{2v} #16	-120.5059453	-121.0208016	-121.0471797
$Pb(H_2O)_7^{2+}$ C_2 #1	-120.5101543	-121.0234646	-121.0498471
$Pb(H_2O)_7^{2+}$ C_s #1	-120.5131606	-121.0231207	-121.0499083
$Pb(H_2O)_7^{2+}$ C_s #16	-120.5106872	-121.0216786	-121.0481856
$Pb(H_2O)_7^{2+}$ C_1 #1	**-120.5132479**	**-121.0243706**	**-121.0508913**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #1	-120.5001090	-121.0016677	-121.0280573
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #2	-120.5175461	-121.0208691	-121.0477669
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #3	-120.5069239	[7+0] C_{2v} #4	[7+0] C_{2v} #4
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #4	-120.5024305	-121.0034257	-121.0299846
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #5	-120.5043997	-121.0040281	-121.0305379
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #6	-120.5090258	-121.0131792	-121.0403186
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #7	**-120.5114449**	**-121.0146044**	**-121.0416801**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #8	-120.5147543	-121.0201555	-121.0470152
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #9	-120.5057900	[7+0] C_{2v} #2	[7+0] C_{2v} #2
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #10	-120.5109209	-121.0179834	-121.0449407
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #11	**-120.5114234**	-121.0186204	-121.0458130
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #12	-120.5101474	-121.0116390	-121.0385440
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #2	**-120.5175621**	-121.0214864	-121.0485256
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #3	**-120.5107927**	n/a	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #10	n/a	[5+2] C_{2v} #11	-121.0449913
$Pb(H_2O)_7^{2+}$ [5+2] C_s #15	-120.5064008	n/a	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_s #17	-120.5123414	-121.0191966	-121.0460402
$Pb(H_2O)_7^{2+}$ [5+2] C_s #18	n/a	**-121.0188718**	**-121.0463581**
$Pb(H_2O)_7^{2+}$ [5+2] C_s #21	-120.5169725	**-121.0221484**	**-121.0491832**
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #1	-120.5111658	-121.0168538	-121.0430398
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #2	-120.5151924	-121.0229314	-121.0497643
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #3	-120.5114161	-121.0175239	-121.0438247
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #4	-120.5127694	-121.0197146	-121.0463202
$Pb(H_2O)_7^{2+}$ [6+1] C_2 #2	-120.5152071	-121.0233179	-121.0501454
$Pb(H_2O)_7^{2+}$ [6+1] C_s #3	-120.5160050	-121.0232055	-121.0500335

$Pb(H_2O)_7^{2+}$ [6+1] C_s #4	-120.5152786	-121.0234028	-121.0503023
$Pb(H_2O)_7^{2+}$ [6+1] C_s #5	[6+1] C_s #7	[6+1] C_s #7	-121.0467843
$Pb(H_2O)_7^{2+}$ [6+1] C_s #6	-120.5114860	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #7	-120.5140886	-121.0208417	-121.0475434
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #2	**-120.5166648**	**-121.0243713**	**-121.0505445**
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #4	[6+1] C_1 #2	[6+1] C_1 #2	**-121.0511438**

$Pb(H_2O)_8^{2+}$ D_{4h} #1	-137.2821617	-137.8693711	-137.8981547
$Pb(H_2O)_8^{2+}$ D_{4h} #2	-137.2823240	-137.8696235	-137.8985174
$Pb(H_2O)_8^{2+}$ D_{4d} #1	-137.3016211	-137.8916182	-137.9211175
$Pb(H_2O)_8^{2+}$ D_{4d} #2	-137.3001577	-137.8903343	-137.9193747
$Pb(H_2O)_8^{2+}$ D_4 #1	-137.3084343	**-137.9024949**	**-137.9328205**
$Pb(H_2O)_8^{2+}$ C_{4h} #1	-137.3011938	-137.8978229	-137.9283336
$Pb(H_2O)_8^{2+}$ S_8 #1	**-137.3120883**	**-137.9063486**	**-137.9362783**
$Pb(H_2O)_8^{2+}$ D_{2d} #1	-137.2947479	-137.8871870	-137.9168934
$Pb(H_2O)_8^{2+}$ D_{2d} #2	-137.2978679	-137.8869655	-137.9160717
$Pb(H_2O)_8^{2+}$ D_{2d} #4	-137.2977594	-137.8862084	-137.9157069
$Pb(H_2O)_8^{2+}$ D_{2d} #5	-137.3074086	-137.9016053	-137.9317067
$Pb(H_2O)_8^{2+}$ D_{2h} #2	-137.2993445	-137.8932865	-137.9231914
$Pb(H_2O)_8^{2+}$ D_2 #3	-137.3092729	-137.9017929	D_4 #1
$Pb(H_2O)_8^{2+}$ S_4 #3	-137.3072848	-137.9007907	-137.9310032
$Pb(H_2O)_8^{2+}$ S_4 #4	-137.3075163	D_{2d} #5	D_{2d} #5
$Pb(H_2O)_8^{2+}$ C_{2h} #2	-137.2994032	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_{2v} #1	-137.2999160	n/a	n/a
$Pb(H_2O)_8^{2+}$ [7+1] C_{2v} #1	-137.3100587	-137.9046247	-137.9348977
$Pb(H_2O)_8^{2+}$ [7+1] C_2 #1	-137.3114345	-137.9054422	-137.9357178
$Pb(H_2O)_8^{2+}$ [7+1] C_s #1	-137.3158681	-137.9059176	-137.9363953
$Pb(H_2O)_8^{2+}$ [7+1] C_s #2	-137.3110318	-137.9052475	-137.9356892
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #1	**-137.3155990**	**-137.9061264**	**-137.9365583**
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #2	**-137.3168382**	**-137.9074181**	**-137.9380717**
$Pb(H_2O)_9^{2+}$ D_{3h} #1	-154.0961215	-154.7659341	-154.7991124
$Pb(H_2O)_9^{2+}$ D_{3h} #2	-154.0790794	-154.7414869	-154.7739838
$Pb(H_2O)_9^{2+}$ D_{3h} #3	-154.0807115	-154.7462143	-154.7788857
$Pb(H_2O)_9^{2+}$ D_{3h} #4	-154.0983701	-154.7699874	-154.8033683
$Pb(H_2O)_9^{2+}$ D_3 #1	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #2	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #3	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #4	-154.1045510	-154.7793030	-154.8131550
$Pb(H_2O)_9^{2+}$ C_{3h} #1	-154.1014713	-154.7751973	-154.8089169
$Pb(H_2O)_9^{2+}$ C_{3h} #2	-154.1013030	-154.7735646	-154.8070324
$Pb(H_2O)_9^{2+}$ C_{3h} #3	C_{3h} #1	C_{3h} #1	C_{3h} #1
$Pb(H_2O)_9^{2+}$ C_{3h} #4	C_{3h} #2	C_{3h} #2	C_{3h} #2
$Pb(H_2O)_9^{2+}$ C_3	-154.1049199	**-154.7794634**	**-154.8135468**
$Pb(H_2O)_9^{2+}$ D_3 [6+3]	-154.1045644	-154.7842838	-154.8184119
$Pb(H_2O)_9^{2+}$ C_3 [6+3]	**-154.1203557**	**-154.7894699**	**-154.8241273**
$Pb(H_2O)_{18}^{2+}$ T	-305.2210454	-306.6369871	-306.7076464

	HF/LANL2MB (5d)	HF/LANL2DZ (5d)	HF/SDD (6d)
Pb^{2+} K_h	**-2.6011289**	**-2.6017087**	**-2.5880503**
$Pb(H_2O)^{2+}$ C_{2v}	**-77.7080783**	**-78.7223821**	**-78.6953868**
$Pb(H_2O)_2^{2+}$ D_{2d}	-152.7577432	-154.8069190	-154.7746089
$Pb(H_2O)_2^{2+}$ C_s	-152.7969695	-154.8247453	-154.7880062
$Pb(H_2O)_2^{2+}$ C_2	(ip C_{2v}) **-152.7985824**	**-154.8248069**	**-154.7880523**
$Pb(H_2O)_2^{2+}$ [1+1] C_s	**-152.7695050**	$PbOH^+ + H_3O^+$	**-154.7688463**
$PbOH^+ + H_3O^+$ C_s		**-154.8046360**	**-154.7683184**
$Pb(H_2O)_3^{2+}$ D_{3h} #1	-227.8137833	-230.8902884	-230.8531037
$Pb(H_2O)_3^{2+}$ D_{3h} #2	-227.8218061	-230.8904919	-230.8534421
$Pb(H_2O)_3^{2+}$ D_3	D_{3h} #2	-230.8913759	-230.8540798
$Pb(H_2O)_3^{2+}$ C_{3v} #1	-227.8724969	-230.9086696	-230.8656458
$Pb(H_2O)_3^{2+}$ C_{3v} #2	-227.8654811	-230.9063196	-230.8641443
$Pb(H_2O)_3^{2+}$ C_3	**-227.8729279**	**-230.9130643**	**-230.8691309**
$Pb(H_2O)_3^{2+}$ [2+1] C_{2v}	**-227.8502945**	**-230.8994652**	**-230.8593758**
$Pb(H_2O)_4^{2+}$ D_{2d} #1	-302.8654789	-306.9625021	-306.9223534
$Pb(H_2O)_4^{2+}$ D_{2d} #2	-302.8654457	-306.9624098	-306.9222796
$Pb(H_2O)_4^{2+}$ S_4	-302.8660346	-306.9632929	-306.9230167
$Pb(H_2O)_4^{2+}$ C_{2v} #1	-302.9049930	-306.9730881	-306.9276396
$Pb(H_2O)_4^{2+}$ C_{2v} #2	-302.9103137	-306.9723886	-306.9269851
$Pb(H_2O)_4^{2+}$ C_{2v} #3	-302.9124407	-306.9778425	-306.9311669
$Pb(H_2O)_4^{2+}$ C_2	-302.9127208	**-306.9778821**	**-306.9312510**
$Pb(H_2O)_4^{2+}$ C_s	**-302.9135505**	n/a	n/a
$Pb(H_2O)_4^{2+}$ [3+1] C_s #1	-302.9110418	-306.9782231	-306.9323911
$Pb(H_2O)_4^{2+}$ [3+1] C_s #2	**-302.9132857**	**-306.9793565**	**-306.9333531**
$Pb(H_2O)_5^{2+}$ C_{2v} #1	-377.9282114	-383.0277437	-382.9818019
$Pb(H_2O)_5^{2+}$ C_{2v} #2	-377.9367945	-383.0272884	-382.9808594
$Pb(H_2O)_5^{2+}$ C_{2v} #3	**-377.9392634**	**-383.0371870**	**-382.9889392**
$Pb(H_2O)_5^{2+}$ C_{2v} #4	-377.9305121	-383.0272909	-382.9813964
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #1	**-377.9443001**	-383.0371557	-382.9895672
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #2	-377.9400506	-383.0360072	-382.9885881
$Pb(H_2O)_5^{2+}$ [4+1] C_2 #1	n/a	-383.0372974	-382.9896673
$Pb(H_2O)_5^{2+}$ [4+1] C_s #1	n/a	-383.0374095	**-382.9899537**
$Pb(H_2O)_5^{2+}$ [4+1] C_s #4	-377.9428389	**-383.0378755**	-382.9898003
$Pb(H_2O)_6^{2+}$ T_h	-452.9139336	-459.0786455	-459.0341368
$Pb(H_2O)_6^{2+}$ C_3	**-452.9442821**	**-459.0848447**	**-459.0364433**
$Pb(H_2O)_6^{2+}$ [5+1] C_s #1	**-452.9667999**	**-459.0937461**	**-459.0443675**

$Pb(H_2O)_7^{2+}$ C_{2v} #1	[5+2]	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_{2v} #2	[5+2]	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_{2v} #3	-527.9183494	[6+1]	[6+1]
$Pb(H_2O)_7^{2+}$ C_{2v} #4	[5+2]	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_{2v} #5	-527.9125549	-535.1033857	-535.0606127
$Pb(H_2O)_7^{2+}$ C_{2v} #6	-527.9165876	-535.1100200	-535.0663807
$Pb(H_2O)_7^{2+}$ C_{2v} #7	-527.9140491	-535.1034163	-535.0606125
$Pb(H_2O)_7^{2+}$ C_{2v} #8	-527.9232285	-535.1157628	-535.0707184
$Pb(H_2O)_7^{2+}$ C_{2v} #9	[5+2]	-535.1150128	[6+1]
$Pb(H_2O)_7^{2+}$ C_{2v} #10	-527.9137218	-535.1048327	-535.0618692
$Pb(H_2O)_7^{2+}$ C_{2v} #11	-527.9185545		
$Pb(H_2O)_7^{2+}$ C_{2v} #12	-527.9151844	-535.1048344	-535.0618692
$Pb(H_2O)_7^{2+}$ C_{2v} #13	-527.9213665	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_{2v} #14	-527.9202698		
$Pb(H_2O)_7^{2+}$ C_{2v} #15	[5+2]	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_{2v} #16	-527.9224049	-535.1203009	-535.0751227
$Pb(H_2O)_7^{2+}$ C_2 #1	[5+2]	[5+2]	[5+2]
$Pb(H_2O)_7^{2+}$ C_s #16	-527.9395314	[4+3]	[4+3]
$Pb(H_2O)_7^{2+}$ C_1 #1	[6+1] **-527.9604546**	[4+3] **-535.1429779**	[4+3] **-535.0989415**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #1	-527.9574108	-535.1242633	-535.0765309
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #2	**-527.9848990**	-535.1445914	-535.0946541
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #3	-527.9663983	-535.1284240	-535.0795249
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #4	-527.9646616	-535.1243392	-535.0755780
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #5	-527.9649305	-535.1266210	-535.0781947
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #6	-527.9682625	-535.1352137	-535.0845095
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #7	-527.9686340	-535.1383147	-535.0878888
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #8	-527.9796675	-535.1444124	-535.0950799
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #9	-527.9616710	-535.1298676	-535.0812184
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #10	-527.9691694	-535.1418262	-535.0925654
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #11	**-527.9724417**	-535.1411042	-535.0916338
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #12	-527.9686204	-535.1342717	-535.0841535
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #1	[5+2] C_{2v} #2	[5+2] C_2 #2	[5+2] C_2 #2
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #2	n/a	-535.1452600	-535.0953616
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #3	-527.9680455	**-535.1372506**	**-535.0867859**
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #4	[5+2] C_{2v} #2	[5+2] C_2 #2	[5+2] C_2 #2
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #5	[5+2] C_2 #3	[5+2] C_{2v} #7	[5+2] C_{2v} #7
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #6	[5+2] C_{2v} #2	[5+2] C_2 #2	[5+2] C_2 #2
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #7	**-527.9687311**	n/a	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #8	[5+2] C_{2v} #2	[5+2] C_2 #2	[5+2] C_2 #2
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #9	C_2 #7	C_{2v} #7	C_{2v} #7
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #10	[5+2] C_{2v} #11	-535.1419835	-535.0928772
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #11	n/a	[5+2] C_2 #10	[5+2] C_2 #10
$Pb(H_2O)_7^{2+}$ [5+2] C_s #5	n/a	-535.1298681	-535.0812181
$Pb(H_2O)_7^{2+}$ [5+2] C_s #7	n/a	-535.1244282	-535.0823780
$Pb(H_2O)_7^{2+}$ [5+2] C_s #9	n/a	-535.1356972	-535.0848704

$Pb(H_2O)_7^{2+}$ [5+2] C_s #11	**-527.9687152**	**-535.1385812**	**-535.0880251**
$Pb(H_2O)_7^{2+}$ [5+2] C_s #15	-527.9630328	-535.1320649	-535.0831369
$Pb(H_2O)_7^{2+}$ [5+2] C_s #17	-527.9738548	-535.1432775	-535.0936066
$Pb(H_2O)_7^{2+}$ [5+2] C_s #21	-527.9829629	**-535.1456419**	**-535.0956935**
$Pb(H_2O)_7^{2+}$ [5+2] C_1 #11	n/a	**-535.1440757**	**-535.0943086**
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #1	-527.9582486	-535.1281962	-535.0821424
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #2	-527.9639270	-535.1369755	-535.0878753
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #3	-527.9567767	-535.1294494	-535.0829659
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #4	-527.9596135	-535.1335809	-535.0848530
$Pb(H_2O)_7^{2+}$ [6+1] C_2 #2	n/a	-535.1370164	-535.0879150
$Pb(H_2O)_7^{2+}$ [6+1] C_s #3	-527.9643365	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #4	**[5+2] -527.9795828**	**[5+2] -535.1426371**	**[5+2] -535.0920921**
$Pb(H_2O)_7^{2+}$ [6+1] C_s #5	-527.9626579	[6+1] C_{2v} #4	[6+1] C_{2v} #4
$Pb(H_2O)_7^{2+}$ [6+1] C_s #7	-527.9617081	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #8	**[5+2] -527.9796062**	[6+1] C_s #4	[6+1] C_s #4

$Pb(H_2O)_8^{2+}$ D_{4h} #1	-602.9002392	-611.1239053	-611.0833627
$Pb(H_2O)_8^{2+}$ D_{4h} #2	-602.9004069	-611.1240774	-611.0834987
$Pb(H_2O)_8^{2+}$ D_{4d} #1	-602.9128516	-611.1458972	-611.1019324
$Pb(H_2O)_8^{2+}$ D_{4d} #2	-602.9124839	-611.1432395	-611.0997399
$Pb(H_2O)_8^{2+}$ D_4 #1	-602.9178848	-611.1580759	-611.1135665
$Pb(H_2O)_8^{2+}$ C_{4h} #1	-602.9125704	-611.1556082	-611.1119789
$Pb(H_2O)_8^{2+}$ S_8 #1	-602.9205293	-611.1603531	**-611.1149646**
$Pb(H_2O)_8^{2+}$ D_{2d} #1	-602.9078892	-611.1412522	-611.0985168
$Pb(H_2O)_8^{2+}$ D_{2d} #2	-602.9097257	-611.1399978	-611.0968325
$Pb(H_2O)_8^{2+}$ D_{2d} #4	-602.9120378	-611.1394044	-611.0962643
$Pb(H_2O)_8^{2+}$ D_{2d} #5	-602.9168637	-611.1569739	-611.1126982
$Pb(H_2O)_8^{2+}$ D_{2h} #2	-602.9103614	-611.1475786	-611.1040130
$Pb(H_2O)_8^{2+}$ C_{4v} #1	-602.9185401	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_{4v} #2	-602.9172392	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_4 #1	[4+4] -602.9864819	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_4 #2	[4+4] -602.9895902	-611.1582506	**-611.1141058**
$Pb(H_2O)_8^{2+}$ D_2 #3	-602.9186236	D_4 #1	D_4 #1
$Pb(H_2O)_8^{2+}$ S_4 #3	-602.9173410	D_{2d} #5	D_{2d} #5
$Pb(H_2O)_8^{2+}$ S_4 #4	-602.9168691	D_{2d} #5	D_{2d} #5
$Pb(H_2O)_8^{2+}$ C_{2h} #2	-602.9108207	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_{2v} #1	-602.9120829	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_{2v} #2	[4+4] -602.9852353	[4+4] -611.1762686	[4+4] -611.1263561
$Pb(H_2O)_8^{2+}$ C_{2v} #3	[6+2] -602.9556934	[6+2] -611.1708280	[6+2] -611.1238597
$Pb(H_2O)_8^{2+}$ C_2 [4+4]	-602.9934726	n/a	n/a
$Pb(H_2O)_8^{2+}$ C_1	[4+4] **-602.9937329**	[4+3+1] **-611.1869928**	n/a
$Pb(H_2O)_8^{2+}$ [7+1] C_{2v} #1	-602.9416834	-611.1716313	-611.1254848
$Pb(H_2O)_8^{2+}$ [7+1] C_2 #1	-602.9419759	-611.1716322	-611.1254859
$Pb(H_2O)_8^{2+}$ [7+1] C_s #1	[6+2]	[4+4] -611.1922760	[6+2] -611.1337743
$Pb(H_2O)_8^{2+}$ [7+1] C_s #2	[5+3]	[6+2] -611.1781970	[6+2] -611.1306729
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #1	[6+2] **-602.9683653**	[5+3] **-611.1903737**	[5+3] **-611.1381949**
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #2	n/a	[4+4] **-611.1923331**	[5+3] **-611.1389731**
$Pb(H_2O)_9^{2+}$ D_{3h} #1	-677.9059153	-687.1762825	-687.1330949
$Pb(H_2O)_9^{2+}$ D_{3h} #2	-677.8968551	-687.1520308	-687.1117746
$Pb(H_2O)_9^{2+}$ D_{3h} #3	-677.8959352	-687.1617251	-687.1186713
$Pb(H_2O)_9^{2+}$ D_{3h} #4	-677.9069442	-687.1786305	-687.1351823
$Pb(H_2O)_9^{2+}$ D_3 #1	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #2	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #3	D_3 #4	[6+3]	[6+3]
$Pb(H_2O)_9^{2+}$ D_3 #4	-677.9116990	-687.1887294	-687.1442824
$Pb(H_2O)_9^{2+}$ C_{3h} #1	-677.9097518	-687.1840421	-687.1409321
$Pb(H_2O)_9^{2+}$ C_{3h} #2	-677.9079084	-687.1840983	-687.1407077
$Pb(H_2O)_9^{2+}$ C_{3h} #3	C_{3h} #1	[6+3] -687.1946459	C_{3h} #1
$Pb(H_2O)_9^{2+}$ C_{3h} #4	C_{3h} #2	[6+3] -687.2255363	-687.1392200
$Pb(H_2O)_9^{2+}$ C_3	[6+3] -677.9536839	[6+3] -687.2210670	[6+3] **-687.1714432**
$Pb(H_2O)_9^{2+}$ D_3 [6+3]	-677.9417913	-687.2287523	-687.1827338

$Pb(H_2O)_9^{2+}$ *C3* [6+3]	**-677.9864407**	**-687.2338605**	**-687.1847869**
$Pb(H_2O)_{18}^{2+}$ *T*	-1352.8875269	**-306.7076464**	**-1371.5267755**

	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*
Pb^{2+} K_h	**-2.6357016**	**-2.6357016**	**-2.6357016**	**-2.6357016**
$Pb(H_2O)^{2+}$ C_{2v}	**-19.7746554**	**-19.7901036**	**-78.9439801**	**-78.9498238**
$Pb(H_2O)_2^{2+}$ D_{2d}	-36.8835170	-36.9145559	-155.2175285	-155.2313917
$Pb(H_2O)_2^{2+}$ C_s	-36.8993726	-36.9307610	-155.2364418	-155.2486993
$Pb(H_2O)_2^{2+}$ C_2	**-36.8995127**	**-36.9308409**	**-155.2364845**	**-155.2488226**
$Pb(H_2O)_2^{2+}$ [1+1] C_s	$PbOH^+ + H_3O^+$ C_s	$PbOH^+ + H_3O^+$ C_s	$PbOH^+ + H_3O^+$ C_s	$PbOH^+ + H_3O^+$ C_s
$PbOH^+ + H_3O^+$ C_s	**-36.8720265**	**-36.9027440**	**-155.2072202**	**-155.2230073**
$Pb(H_2O)_3^{2+}$ D_{3h} #1	-53.9936533	-54.0405220	-231.4948650	-231.5143630
$Pb(H_2O)_3^{2+}$ D_{3h} #2	-53.9942859	-54.0408185	-231.4946360	-231.5155822
$Pb(H_2O)_3^{2+}$ D_3	-53.9950305	-54.0418015	-231.4958340	-231.5161888
$Pb(H_2O)_3^{2+}$ C_{3v} #1	-54.0084582	-54.0557310	-231.5123776	-231.5316590
$Pb(H_2O)_3^{2+}$ C_{3v} #2	-54.0066609	-54.0539202	-231.5103370	-231.5295037
$Pb(H_2O)_3^{2+}$ C_3	**-54.0135204**	**-54.0613648**	**-231.5173824**	**-231.5369070**
$Pb(H_2O)_3^{2+}$ [2+1] C_{2v}	**-53.9922464**	**-54.0387157**	**-231.4959122**	**-231.5162788**
$Pb(H_2O)_4^{2+}$ D_{2d} #1	-71.0937945	-71.1562832	-307.7603272	-307.7885414
$Pb(H_2O)_4^{2+}$ D_{2d} #2	-71.0937054	-71.1561911	-307.7602835	-307.7885050
$Pb(H_2O)_4^{2+}$ D_2	D_{2d} #1	D_{2d} #1	D_{2d} #1	-307.7885492
$Pb(H_2O)_4^{2+}$ S_4	-71.0945700	-71.1572448	-307.7611085	-307.7895583
$Pb(H_2O)_4^{2+}$ C_{2v} #1	-71.1010129	-71.1643585	-307.7694299	-307.7977216
$Pb(H_2O)_4^{2+}$ C_{2v} #2	-71.0996580	-71.1629193	-307.7675321	-307.7965073
$Pb(H_2O)_4^{2+}$ C_{2v} #3	-71.1068047	-71.1703457	-307.7753732	-307.8036249
$Pb(H_2O)_4^{2+}$ C_2	**-71.1070558**	**-71.1708894**	**-307.7759495**	**-307.8040751**
$Pb(H_2O)_4^{2+}$ [3+1] C_s #1	-71.0970284	-71.1601427	-307.7670117	-307.7950524
$Pb(H_2O)_4^{2+}$ [3+1] C_s #2	-71.0979562	**-71.1608462**	-307.7677536	-307.7958656
$Pb(H_2O)_4^{2+}$ [3+1] C_1 #1	**-71.0979591**	n/a	**-307.7678043**	n/a
$Pb(H_2O)_5^{2+}$ C_{2v} #1	-88.1835961	-88.2626676	-384.0152100	-384.0547243
$Pb(H_2O)_5^{2+}$ C_{2v} #2	-88.1837438	-88.2625319	-384.0162039	-384.0551322
$Pb(H_2O)_5^{2+}$ C_{2v} #3	**-88.1948069**	**-88.2747307**	**-384.0265374**	**-384.0665172**
$Pb(H_2O)_5^{2+}$ C_{2v} #4	-88.1830736	-88.2619274	-384.0143384	-384.0545685
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #1	-88.1833856	-88.2621655	-384.0167851	-384.0553125
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #2	-88.1826769	-88.2618310	-384.0165751	-384.0547539
$Pb(H_2O)_5^{2+}$ [4+1] C_2 #1	-88.1844505	-88.2637904	-384.0188507	-384.0566331
$Pb(H_2O)_5^{2+}$ [4+1] C_s #1	-88.1852073	-88.2637176	-384.0190972	-384.0563369
$Pb(H_2O)_5^{2+}$ [4+1] C_s #2	[4+1] C_s #1	[4+1] C_s #1	[4+1] C_s #1	-384.0562042
$Pb(H_2O)_5^{2+}$ [4+1] C_s #3	-88.1826930	-88.2619603	-384.0168461	-384.0547834
$Pb(H_2O)_5^{2+}$ [4+1] C_s #4	-88.1850022	-88.2643974	-384.0189439	-384.0571982
$Pb(H_2O)_5^{2+}$ [4+1] C_1 #1	**-88.1850440**	**-88.2645728**	**-384.0195554**	**-384.0572649**
$Pb(H_2O)_5^{2+}$ [4+1] C_1 #2	**-88.1895125**	**-88.2686259**	**-384.0237320**	**-384.0611528**
$Pb(H_2O)_6^{2+}$ T_h	-105.2632299	-105.3584592	-460.2552926	-460.3095380
$Pb(H_2O)_6^{2+}$ S_6	n/a	n/a	-460.2558101	n/a
$Pb(H_2O)_6^{2+}$ C_3	**-105.2707331**	**-105.3666233**	**-460.2666074**	**-460.3168474**
$Pb(H_2O)_6^{2+}$ [5+1] C_s #1	**-105.2711219**	**-105.3662393**	**-460.2690752**	**-460.3175527**

$Pb(H_2O)_7^{2+}$ C_{2v} #1	-122.3369252	-122.4486271	-536.4948215	-536.5582666
$Pb(H_2O)_7^{2+}$ C_{2v} #2	-122.3317315	-122.4426600	-536.4896434	-536.5530413
$Pb(H_2O)_7^{2+}$ C_{2v} #3	-122.3292210	-122.4399652	-536.4869634	-536.5499368
$Pb(H_2O)_7^{2+}$ C_{2v} #4	-122.3300163	-122.4408642	-536.4898292	-536.5512417
$Pb(H_2O)_7^{2+}$ C_{2v} #5	-122.3147944	-122.4252326	-536.4735317	-536.5356266
$Pb(H_2O)_7^{2+}$ C_{2v} #6	-122.3235340	-122.4344131	-536.4820849	-536.5440012
$Pb(H_2O)_7^{2+}$ C_{2v} #7	-122.3170981	-122.4283689	-536.4778555	-536.5382711
$Pb(H_2O)_7^{2+}$ C_{2v} #8	-122.3307000	-122.4422513	-536.4890999	-536.5518215
$Pb(H_2O)_7^{2+}$ C_{2v} #9	-122.3318520	-122.4430240	-536.4895497	-536.5525756
$Pb(H_2O)_7^{2+}$ C_{2v} #10	-122.3197943	-122.4290631	-536.4765606	-536.5395470
$Pb(H_2O)_7^{2+}$ C_{2v} #11	-122.3263941	-122.4365975	-536.4848552	-536.5473836
$Pb(H_2O)_7^{2+}$ C_{2v} #12	-122.3197952	-122.4290816	-536.4767570	-536.5395600
$Pb(H_2O)_7^{2+}$ C_{2v} #13	-122.3280475	-122.4389993	-536.4864142	-536.5489965
$Pb(H_2O)_7^{2+}$ C_{2v} #14	-122.3290248	-122.4398661	-536.4869422	-536.5497121
$Pb(H_2O)_7^{2+}$ C_{2v} #15	-122.3315704	-122.4427758	-536.4896834	-536.5527477
$Pb(H_2O)_7^{2+}$ C_{2v} #16	-122.3353644	-122.4466961	-536.4924970	-536.5565061
$Pb(H_2O)_7^{2+}$ C_2 #1	-122.3378039	-122.4494103	-536.4969775	-536.5590533
$Pb(H_2O)_7^{2+}$ C_s #1	-122.3394797	-122.4518104	-536.5004941	-536.5608471
$Pb(H_2O)_7^{2+}$ C_s #16	-122.3366109	-122.4481805	-536.4948594	-536.5576737
$Pb(H_2O)_7^{2+}$ C_1	**-122.3396163**	**-122.4519688**	**-536.5007520**	**-536.5615593**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #1	-122.3167413	-122.4268421	-536.4773659	-536.5376488
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #2	-122.3404625	-122.4506150	-536.5027642	-536.5617341
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #3	[7+0] C_{2v} #4	[7+0] C_{2v} #4	[7+2] C_{2v} #4	[7+2] C_{2v} #4
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #4	-122.3184164	-122.4284810	-536.4788880	-536.5395675
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #5	-122.3190874	-122.4289615	-536.4791892	-536.5394901
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #6	-122.3303363	-122.4415731	-536.4899273	-536.5519293
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #7	-122.3319857	-122.4429955	-536.4909060	-536.5525246
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #8	-122.3399099	-122.4500019	-536.5012267	-536.5611084
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #9	[7+0] C_{2v} #2	[7+0] C_{2v} #2	[7+0] C_{2v} #2	[7+0] C_{2v} #2
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #10	-122.3378844	-122.4486193	-536.4999154	-536.5593117
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #11	-122.3391033	-122.4504293	-536.5020302	-536.5609486
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #12	-122.3274659	-122.4384140	-536.4866781	-536.5492934
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #2	-122.3414331	-122.4521745	-536.5039501	-536.5630704
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #7	n/a	n/a	-536.4918780	-536.5525334
$Pb(H_2O)_7^{2+}$ [5+2] C_s #7	-122.3188087	-122.4294113	-536.4808380	-536.5408102
$Pb(H_2O)_7^{2+}$ [5+2] C_s #9	-122.3304647	-122.4416793	-536.4910404	-536.5521005
$Pb(H_2O)_7^{2+}$ [5+2] C_s #10	-122.3305707	-122.4420472	-536.4914404	-536.5522157
$Pb(H_2O)_7^{2+}$ [5+2] C_s #11	**-122.3319875**	n/a	-536.4915212	-536.5525261
$Pb(H_2O)_7^{2+}$ [5+2] C_s #12	n/a	**-122.4430045**	[6+1]	-536.5525328
$Pb(H_2O)_7^{2+}$ [5+2] C_s #17	-122.3399438	-122.4502008	-536.5031171	-536.5605334
$Pb(H_2O)_7^{2+}$ [5+2] C_s #18	**-122.3409076**	**-122.4526029**	**-536.5058614**	**-536.5628506**
$Pb(H_2O)_7^{2+}$ [5+2] C_s #20	-122.3274663	n/a	-536.4871788	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_s #21	**-122.3431256**	122.4539715	**-536.5064643**	**-536.5648659**
$Pb(H_2O)_7^{2+}$ [5+2] C_1 #7	n/a	n/a	C_1 #1 [7+0]	**-536.5525500**
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #1	-122.3329402	-122.4427794	-536.4928929	-536.5534059

$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #2	-122.3403694	-122.4513822	-536.5005124	-536.5614824
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #3	-122.3337731	-122.4437107	-536.4929623	-536.5545206
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #4	-122.3361753	-122.4468519	-536.4960535	-536.5570278
$Pb(H_2O)_7^{2+}$ [6+1] C_2 #2	-122.3416840	-122.4531699	**-536.5034472**	-536.5630397
$Pb(H_2O)_7^{2+}$ [6+1] C_s #3	-122.3406318	-122.4517276	-536.5013502	-536.5617181
$Pb(H_2O)_7^{2+}$ [6+1] C_s #4	-122.3414011	-122.4526053	-536.5020949	-536.5624520
$Pb(H_2O)_7^{2+}$ [6+1] C_s #5	-122.3389175	-122.4509975	-536.5034591	-536.5603902
$Pb(H_2O)_7^{2+}$ [6+1] C_s #6	n/a	n/a	-536.4932987	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #7	-122.3388905	-122.4501722	-536.5018148	-536.5597758
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #2	**-122.3420165**	**-122.4534691**	n/a	**-536.5632547**
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #4	**-122.3425913**	**-122.4539353**	C_2 -536.5034442	**-536.5639040**

$Pb(H_2O)_8^{2+}$ D_{4h} #1	-139.3646547	-139.4900095	-612.6884918	-612.7596475
$Pb(H_2O)_8^{2+}$ D_{4h} #2	-139.3650753	-139.4907087	-612.6893092	-612.7599749
$Pb(H_2O)_8^{2+}$ D_{4d} #1	-139.3898198	-139.5172679	-612.7124447	-612.7858440
$Pb(H_2O)_8^{2+}$ D_{4d} #2	-139.3890072	-139.5150885	-612.7091447	-612.7847179
$Pb(H_2O)_8^{2+}$ D_4 #1	**-139.4060471**	**-139.5342340**	**-612.7309690**	**-612.8031013**
$Pb(H_2O)_8^{2+}$ D_4 #3	D_{4d} #1	D_{4d} #1	-612.7126361	D_{4d} #1
$Pb(H_2O)_8^{2+}$ C_{4h} #1	-139.4020152	-139.5304704	-612.7276393	-612.7990826
$Pb(H_2O)_8^{2+}$ S_8 #1	**-139.4067861**	-139.5349414	-612.7296590	**-612.8044468**
$Pb(H_2O)_8^{2+}$ D_{2d} #1	-139.3869840	-139.5140109	-612.7101670	-612.7823026
$Pb(H_2O)_8^{2+}$ D_{2d} #2	-139.3855621	-139.5112581	-612.7075442	-612.7816385
$Pb(H_2O)_8^{2+}$ D_{2d} #4	-139.3842642	-139.5113703	-612.7092638	-612.7805833
$Pb(H_2O)_8^{2+}$ D_{2d} #5	-139.4037225	-139.5312937	-612.7265157	-612.8010983
$Pb(H_2O)_8^{2+}$ D_{2h} #2	-139.3935781	-139.5208900	-612.7156461	-612.7895640
$Pb(H_2O)_8^{2+}$ S_4 #3	-139.4037885	-139.5316586	**-612.7282840**	D_{2d} #5
$Pb(H_2O)_8^{2+}$ S_4 #4	-139.4033301	**-139.5313710**	**-612.7282762**	-612.7998542
$Pb(H_2O)_8^{2+}$ C_4 #1	n/a	**-139.5349452**	**-612.7303314**	n/a
$Pb(H_2O)_8^{2+}$ C_4 #3	**-139.4071882**	**-139.5354507**	-612.7310807	**-612.8042820**
$Pb(H_2O)_8^{2+}$ C_{2h} #2	n/a	n/a	-612.7156529	n/a
$Pb(H_2O)_8^{2+}$ C_1	n/a	n/a	(3i) -612.7310886	n/a
$Pb(H_2O)_8^{2+}$ [7+1] C_{2v} #1	-139.4066729	-139.5336005	-612.7278105	-612.8027133
$Pb(H_2O)_8^{2+}$ [7+1] C_2 #1	-139.4079949	-139.5351192	-612.7313824	-612.8033786
$Pb(H_2O)_8^{2+}$ [7+1] C_s #1	-139.4084852	-139.5357037	-612.7319583	-612.8044178
$Pb(H_2O)_8^{2+}$ [7+1] C_s #2	-139.4078011	-139.5349779	-612.7302130	-612.8039987
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #1	**-139.4093473**	**-139.5369641**	**-612.7356095**	**-612.8078797**
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #2	**-139.4113012**	**-139.5391673**	**-612.7374489**	**-612.8078795**
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #3	C_1 #2	**-139.5391115**	C_1 #2	C_1 #2
$Pb(H_2O)_9^{2+}$ D_{3h} #1	-156.4496115	-156.5929086	-688.9350265	-689.0227403
$Pb(H_2O)_9^{2+}$ D_{3h} #2	-156.4209847	-156.5634632	-688.9089519	-688.9926199
$Pb(H_2O)_9^{2+}$ D_{3h} #3	-156.4281693	-156.5702061	-688.9158733	-688.9993275
$Pb(H_2O)_9^{2+}$ D_{3h} #4	-156.4556250	-156.5988257	-688.9411756	-689.0275167
$Pb(H_2O)_9^{2+}$ D_3 #1	D_3 #4	D_3 #4	-688.9513279	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #2	D_3 #4	D_3 #4	D_3 #1	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #3	D_3 #4	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #4	-156.4657632	-156.6100704	-688.9512555	-689.0391982
$Pb(H_2O)_9^{2+}$ C_{3h} #1	-156.4634460	-156.6074838	-688.9510054	-689.0359325
$Pb(H_2O)_9^{2+}$ C_{3h} #2	-156.4613907	-156.6056387	-688.9502155	-689.0350507
$Pb(H_2O)_9^{2+}$ C_{3h} #3	C_{3h} #1	C_{3h} #1	C_{3h} #1	C_{3h} #1
$Pb(H_2O)_9^{2+}$ C_{3h} #4	-156.4594237	-156.6035527	-688.9451028	C_{3h} #2
$Pb(H_2O)_9^{2+}$ C_3	**-156.4695024**	**-156.6143135**	**-688.9593247**	**-689.0427384**
$Pb(H_2O)_9^{2+}$ D_3 [6+3]	-156.4761115	-156.6177031	-688.9641888	-689.0461939
$Pb(H_2O)_9^{2+}$ C_3 [6+3]	**-156.4828732**	**-156.6251134**	**-688.9730161**	**-689.0537552**

	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*
Pb^{2+} K_h	**-2.6207713**	**-2.6017087**	**-2.5765821**
$Pb(H_2O)^{2+}$ C_{2v}	**-78.7361303**	**-78.7095748**	**-78.6762471**
$Pb(H_2O)_2^{2+}$ D_{2d}	-154.8193450	-154.7841004	-154.7475524
$Pb(H_2O)_2^{2+}$ C_s	-154.8373339	-154.8008860	-154.7611163
$Pb(H_2O)_2^{2+}$ C_2	**-154.8373685**	**-154.8009124**	**-154.7611548**
$Pb(H_2O)_2^{2+}$ [1+1] C_s	**-154.7988232**	**-154.7736982**	**-154.7374936**
$PbOH^+ + H_3O^+$ C_s	**-154.7996053**	**-154.7775706**	**-154.7367676**
$Pb(H_2O)_3^{2+}$ D_{3h} #1	-230.9056271	-230.8594072	-230.8191080
$Pb(H_2O)_3^{2+}$ D_{3h} #2	-230.9053343	-230.8589654	-230.8195109
$Pb(H_2O)_3^{2+}$ D_3	-230.9063631	-230.8600406	-230.8200406
$Pb(H_2O)_3^{2+}$ C_{3v} #1	-230.9234237	-230.8758374	-230.8316373
$Pb(H_2O)_3^{2+}$ C_{3v} #2	-230.9214164	-230.8739307	-230.8302899
$Pb(H_2O)_3^{2+}$ C_3	**-230.9276403**	**-230.8800576**	**-230.8350348**
$Pb(H_2O)_3^{2+}$ [2+1] C_{2v}	**-230.9022077**	**-230.8661108**	**-230.8241308**
$Pb(H_2O)_4^{2+}$ D_{2d} #1	-306.9807774	-306.9243134	-306.8820972
$Pb(H_2O)_4^{2+}$ D_{2d} #2	-306.9807377	-306.9242532	-306.8820520
$Pb(H_2O)_4^{2+}$ D_2	D_{2d} #1	D_{2d} #1	D_{2d} #1
$Pb(H_2O)_4^{2+}$ S_4	-306.9814648	-306.9249656	-306.8826645
$Pb(H_2O)_4^{2+}$ C_{2v} #1	-306.9909162	-306.9343605	-306.8879254
$Pb(H_2O)_4^{2+}$ C_{2v} #2	-306.9898769	-306.9329236	-306.8868275
$Pb(H_2O)_4^{2+}$ C_{2v} #3	-306.9960856	-306.9384309	-306.8913174
$Pb(H_2O)_4^{2+}$ C_2	**-306.9962250**	**-306.9385671**	**-306.8915035**
$Pb(H_2O)_4^{2+}$ [3+1] C_s #1	-306.9844785	-306.9367379	-306.8904158
$Pb(H_2O)_4^{2+}$ [3+1] C_s #2	**-306.9852363**	**-306.9375103**	**-306.8911593**
$Pb(H_2O)_5^{2+}$ C_{2v} #1	-383.0479538	-382.9837664	-382.9370099
$Pb(H_2O)_5^{2+}$ C_{2v} #2	-383.0490237	-382.9830901	-382.9360154
$Pb(H_2O)_5^{2+}$ C_{2v} #3	-383.0579440	-382.9918752	-382.9433677
$Pb(H_2O)_5^{2+}$ C_{2v} #4	-383.0476473	-382.9826334	-382.9360014
$Pb(H_2O)_5^{2+}$ C_s	**-383.0579594**	**-382.9919645**	**-382.9433873**
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #1	-383.0465013	-382.9894486	-382.9417619
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #2	-383.0459695	-382.9888545	-382.9410523
$Pb(H_2O)_5^{2+}$ [4+1] C_2 #1	-383.0473023	-382.9899910	-382.9421173
$Pb(H_2O)_5^{2+}$ [4+1] C_s #1	-383.0473004	-382.9897695	**-382.9422193**
$Pb(H_2O)_5^{2+}$ [4+1] C_s #4	-383.0478685	**-382.9905553**	-382.9422095
$Pb(H_2O)_5^{2+}$ [4+1] C_1 #1	**-383.0478788**	[4+1] C_s #4	[4+1] C_s #1
$Pb(H_2O)_5^{2+}$ [4+1] C_1 #2	**-383.0517770**	[4+1] C_s #4	n/a
$Pb(H_2O)_6^{2+}$ T_h	-459.0988460	-459.0286943	-458.9831087
$Pb(H_2O)_6^{2+}$ C_3	**-459.1082902**	**-459.0356537**	**-458.9868459**
$Pb(H_2O)_6^{2+}$ [5+1] C_s #1	**-459.1082000**	**-459.0415523**	**-458.9920067**

$Pb(H_2O)_7^{2+}$ C_{2v} #1	-535.1476360	[5+2]	-535.0242172
$Pb(H_2O)_7^{2+}$ C_{2v} #2	-535.1424486	[5+2]	-535.0203194
$Pb(H_2O)_7^{2+}$ C_{2v} #3	-535.1408804	[6+1]	-535.0181134
$Pb(H_2O)_7^{2+}$ C_{2v} #4	-535.1420544	[5+2]	-535.0195130
$Pb(H_2O)_7^{2+}$ C_{2v} #5	-535.1298802	-535.0546633	-535.0097602
$Pb(H_2O)_7^{2+}$ C_{2v} #6	-535.1363083	-535.0604218	-535.0149685
$Pb(H_2O)_7^{2+}$ C_{2v} #7	-535.1316082	-535.0558106	-535.0099717
$Pb(H_2O)_7^{2+}$ C_{2v} #8	-535.1423315	-535.0655949	-535.0188808
$Pb(H_2O)_7^{2+}$ C_{2v} #9	-535.1423567	-535.0651671	-535.0186799
$Pb(H_2O)_7^{2+}$ C_{2v} #10	-535.1317737	-535.0560888	-535.0114042
$Pb(H_2O)_7^{2+}$ C_{2v} #11	-535.1386352	[6+1]	[6+1]
$Pb(H_2O)_7^{2+}$ C_{2v} #12	-535.1318892	-535.0561008	-535.0114042
$Pb(H_2O)_7^{2+}$ C_{2v} #13	-535.1401341	-535.0644088	-535.0181776
$Pb(H_2O)_7^{2+}$ C_{2v} #14	-535.1410200	-535.0648221	-535.0186309
$Pb(H_2O)_7^{2+}$ C_{2v} #15	-535.1426330	-535.0664150	-535.0200588
$Pb(H_2O)_7^{2+}$ C_{2v} #16	-535.1459109	-535.0684355	-535.0219738
$Pb(H_2O)_7^{2+}$ C_2 #1	-535.1487879	n/a	-535.0242586
$Pb(H_2O)_7^{2+}$ C_s #1	-535.1508078	n/a	-535.0251582
$Pb(H_2O)_7^{2+}$ C_s #16	-535.1477202	-535.0700674	-535.0226628
$Pb(H_2O)_7^{2+}$ C_1 #1	**-535.1508750**	[5+2] **-535.0767045**	**-535.0253312**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #1	-535.1306100	-535.0666664	-535.0185013
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #2	-535.1524412	-535.0855115	-535.0357584
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #3	[7+2] C_{2v} #4	-535.0677711	[7+2] C_{2v} #4
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #4	-535.1325396	-535.0657697	-535.0168673
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #5	-535.1328920	-535.0659314	-535.0171465
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #6	-535.1419907	-535.0749033	-535.0244042
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #7	-535.1431268	-535.0758217	-535.0254871
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #8	-535.1510419	-535.0850539	-535.0358725
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #9	[7+2] C_{2v} #2	-535.0681793	-535.0193070
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #10	-535.1491847	-535.0831036	-535.0334762
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #11	-535.1503693	-535.0834038	-535.0334505
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #12	-535.1402953	-535.0743999	-535.0242861
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #2	-535.1528954	-535.0860828	-535.0362664
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #3	n/a	-535.0835014	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #10	-535.1503693	-535.0835014	-535.0340597
$Pb(H_2O)_7^{2+}$ [5+2] C_s #7	-535.1330401	-535.0661644	-535.0170637
$Pb(H_2O)_7^{2+}$ [5+2] C_s #9	-535.1423652	-535.0756721	-535.025087
$Pb(H_2O)_7^{2+}$ [5+2] C_s #10	-535.1424747	-535.0752138	-535.0247523
$Pb(H_2O)_7^{2+}$ [5+2] C_s #11	-535.1432929	**-535.076309**	**-535.0258432**
$Pb(H_2O)_7^{2+}$ [5+2] C_s #13	C_{2v} #2 [5+2]	C_{2v} #2 [5+2]	-535.0358736
$Pb(H_2O)_7^{2+}$ [5+2] C_s #14	-535.1510713	-535.0851002	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_s #15	n/a	-535.0839938	-535.0342405
$Pb(H_2O)_7^{2+}$ [5+2] C_s #16	n/a	-535.0681797	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_s #17	-535.1507851	-535.0845029	-535.03473
$Pb(H_2O)_7^{2+}$ [5+2] C_s #18	**-535.1514249**	**-535.0839673**	-535.0337332

$Pb(H_2O)_7^{2+}$ [5+2] C_s #20	-535.1403795	-535.0745721	-535.0243289
$Pb(H_2O)_7^{2+}$ [5+2] C_s #21	**-535.1542391**	**-535.0872741**	**-535.0372162**
$Pb(H_2O)_7^{2+}$ [5+2] C_1 #7	**-535.1433209**	n/a	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_1 #11	n/a	n/a	**-535.0356941**
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #1	-535.1452430	-535.0731998	-535.0259025
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #2	-535.1517137	-535.0805353	-535.0315744
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #3	-535.1454274	-535.0739667	-535.0265558
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #4	-535.1482557	-535.0779554	-535.0290800
$Pb(H_2O)_7^{2+}$ [6+1] C_2 #2	-535.1526160	**-535.0811106**	**-535.0321159**
$Pb(H_2O)_7^{2+}$ [6+1] C_s #3	-535.1523066	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #4	-535.1523880	**-535.0821907**	**-535.0317925**
$Pb(H_2O)_7^{2+}$ [6+1] C_s #5	-535.1506640	C_{2v} #4	-535.0281346
$Pb(H_2O)_7^{2+}$ [6+1] C_s #6	-535.1455941	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #7	-535.1503283	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #2	**-535.1530530**	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #4	**-535.1534874**	n/a	n/a

$Pb(H_2O)_8^{2+}$ *D4h* #1	-611.1562448	-611.0776909	-611.0342426
$Pb(H_2O)_8^{2+}$ *D4h* #2	-611.1566988	-611.0779355	-611.0343983
$Pb(H_2O)_8^{2+}$ *D4d* #1	-611.1774422	-611.0950281	-611.0489425
$Pb(H_2O)_8^{2+}$ *D4d* #2	-611.1750245	-611.0932403	-611.0475536
$Pb(H_2O)_8^{2+}$ *D4* #1	**-611.1893145**	-611.1053732	**-611.0593095**
$Pb(H_2O)_8^{2+}$ *C4h* #1	-611.1856817	-611.1031016	-611.0576384
$Pb(H_2O)_8^{2+}$ *S8* #1	-611.1908965	-611.1068819	-611.0601408
$Pb(H_2O)_8^{2+}$ *D2d* #1	-611.1736085	-611.0923256	-611.0471298
$Pb(H_2O)_8^{2+}$ *D2d* #2	-611.1725330	-611.0901631	-611.0448178
$Pb(H_2O)_8^{2+}$ *D2d* #4	-611.1734825	-611.0913184	-611.0455293
$Pb(H_2O)_8^{2+}$ *D2d* #5	-611.1876950	-611.1042612	-611.0579922
$Pb(H_2O)_8^{2+}$ *D2h* #2	-611.1791553	-611.0973632	-611.0515907
$Pb(H_2O)_8^{2+}$ *S4* #3	-611.1877625	*D2d* #5	*D2d* #5
$Pb(H_2O)_8^{2+}$ *S4* #4	-611.1874389	*D2d* #5	*D2d* #5
$Pb(H_2O)_8^{2+}$ *C2h* #2	-611.1791768	n/a	n/a
$Pb(H_2O)_8^{2+}$ *C2v* #2	n/a	[4+4] -611.1033062	[4+4] -611.0534051
$Pb(H_2O)_8^{2+}$ *C1*	(2i) **-611.1909153**	**-611.1219018**	[5+3] **-611.0748284**
$Pb(H_2O)_8^{2+}$ [7+1] *C2v* #1	-611.1904505	-611.1131103	-611.0658460
$Pb(H_2O)_8^{2+}$ [7+1] *C2* #1	-611.1922531	-611.1139401	-611.0663321
$Pb(H_2O)_8^{2+}$ [7+1] *Cs* #1	-611.1929907	[6+2] -611.1194725	[6+2] -611.0696950
$Pb(H_2O)_8^{2+}$ [7+1] *Cs* #2	-611.1917973	[6+2] -611.1156799	-611.0663854
$Pb(H_2O)_8^{2+}$ [7+1] *C1* #1	**-611.1937574**	[5+3] **-611.1220544**	[5+3] **-611.0708510**
$Pb(H_2O)_8^{2+}$ [7+1] *C1* #2	**-611.1961872**	[5+3] **-611.1277330**	[5+3] **-611.0767597**
$Pb(H_2O)_8^{2+}$ [7+1] *C1* #3	*C1* #2	*C1* #1	**-611.0688687**
$Pb(H_2O)_9^{2+}$ *D3h* #1	-687.2114509	-687.1253288	-687.0795903
$Pb(H_2O)_9^{2+}$ *D3h* #2	-687.1883968	-687.1053865	-687.0622245
$Pb(H_2O)_9^{2+}$ *D3h* #3	-687.1929450	-687.1112368	-687.0665905
$Pb(H_2O)_9^{2+}$ *D3h* #4	-687.2156167	-687.1282062	-687.0821526
$Pb(H_2O)_9^{2+}$ *D3* #1	*D3* #4	*D3* #4	*D3* #4
$Pb(H_2O)_9^{2+}$ *D3* #2	*D3* #4	*D3* #4	*D3* #4
$Pb(H_2O)_9^{2+}$ *D3* #3	*D3* #4	*D3* #4	*D3* #4
$Pb(H_2O)_9^{2+}$ *D3* #4	-687.2245270	-687.1361531	-687.0892843
$Pb(H_2O)_9^{2+}$ *C3h* #1	-687.2215871	-687.1335401	-687.0871622
$Pb(H_2O)_9^{2+}$ *C3h* #2	-687.2202186	-687.1315925	-687.0855861
$Pb(H_2O)_9^{2+}$ *C3h* #3	*C3h* #1	*C3h* #1	*C3h* #1
$Pb(H_2O)_9^{2+}$ *C3h* #4	*C3h* #2	*C3h* #2	*C3h* #2
$Pb(H_2O)_9^{2+}$ *C3*	**-687.2263959**	-687.1373204	-687.0906677
$Pb(H_2O)_9^{2+}$ *D3* [6+3]	-687.2336902	-687.1613941	-687.1135865
$Pb(H_2O)_9^{2+}$ *C3* [6+3]	**-687.2409961**	**-687.1665624**	**-687.1165806**
$Pb(H_2O)_{18}^{2+}$ *T*	-1371.5355262	-1371.4619634	**-1371.4125792**

	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*
Pb^{2+} K_h	**-2.6207713**	**-2.6017087**	**-2.5765821**
$Pb(H_2O)^{2+}$ C_{2v}	**-78.7392156**	**-78.7171288**	**-78.6820545**
$Pb(H_2O)_2^{2+}$ D_{2d}	-154.8262202	-154.7962085	-154.7572719
$Pb(H_2O)_2^{2+}$ C_s	-154.8433189	-154.8116869	-154.7703175
$Pb(H_2O)_2^{2+}$ C_2	**-154.8434294**	**-154.8117830**	**-154.7703791**
$Pb(H_2O)_2^{2+}$ [1+1] C_s	**-154.8069311**	**-154.7850931**	**-154.7472427**
$PbOH^+ + H_3O^+$ C_s	**-154.8089789**	**-154.7882379**	**-154.7452334**
$Pb(H_2O)_3^{2+}$ D_{3h} #1	-230.9149361	-230.8753499	-230.8330659
$Pb(H_2O)_3^{2+}$ D_{3h} #2	-230.9155750	-230.8755071	-230.8335748
$Pb(H_2O)_3^{2+}$ D_3	-230.9161717	-230.8762913	-230.8340529
$Pb(H_2O)_3^{2+}$ C_{3v} #1	-230.9323682	-230.8894378	-230.8440259
$Pb(H_2O)_3^{2+}$ C_{3v} #2	-230.9303733	-230.8877749	-230.8429171
$Pb(H_2O)_3^{2+}$ C_3	**-230.9367672**	**-230.8935620**	**-230.8475442**
$Pb(H_2O)_3^{2+}$ [2+1] C_{2v}	**-230.9124504**	**-230.8802858**	**-230.8367676**
$Pb(H_2O)_4^{2+}$ D_{2d} #1	-306.9945425	-306.9448599	-306.9006481
$Pb(H_2O)_4^{2+}$ D_{2d} #2	-306.9945009	-306.9447797	-306.9005754
$Pb(H_2O)_4^{2+}$ D_2	D_{2d} #1	D_{2d} #1	D_{2d} #1
$Pb(H_2O)_4^{2+}$ S_4	-306.9953158	-306.9455869	-306.9012526
$Pb(H_2O)_4^{2+}$ C_{2v} #1	-307.0045212	-306.9524392	-306.9051613
$Pb(H_2O)_4^{2+}$ C_{2v} #2	-307.0034441	-306.9511556	-306.9041063
$Pb(H_2O)_4^{2+}$ C_{2v} #3	-307.0094981	-306.9562210	-306.9081264
$Pb(H_2O)_4^{2+}$ C_2	**-307.0095145**	**-306.9562379**	**-306.9082139**
$Pb(H_2O)_4^{2+}$ [3+1] C_s #1	-306.9976008	-306.9537816	-306.9065670
$Pb(H_2O)_4^{2+}$ [3+1] C_s #2	**-306.9985806**	**-306.9547751**	**-306.9074202**
$Pb(H_2O)_5^{2+}$ C_{2v} #1	-383.0672659	-383.0073185	-382.9595796
$Pb(H_2O)_5^{2+}$ C_{2v} #2	-383.0681649	-383.0065442	-382.9584119
$Pb(H_2O)_5^{2+}$ C_{2v} #3	**-383.0772409**	**-383.0149641**	**-382.9656021**
$Pb(H_2O)_5^{2+}$ C_{2v} #4	-383.0674248	-383.0068609	-382.9590796
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #1	-383.0648298	-383.0117731	-382.9631815
$Pb(H_2O)_5^{2+}$ [4+1] C_{2v} #2	-383.0639175	-383.0106092	-382.9622492
$Pb(H_2O)_5^{2+}$ [4+1] C_2 #1	-383.0653049	-383.0120091	-382.9633806
$Pb(H_2O)_5^{2+}$ [4+1] C_s #1	-383.0654191	**-383.0121434**	**-382.9636168**
$Pb(H_2O)_5^{2+}$ [4+1] C_s #4	**-383.0658258**	**-383.0122542**	-382.9633381
$Pb(H_2O)_6^{2+}$ T_h	-459.1267791	-459.0618384	-459.0135688
$Pb(H_2O)_6^{2+}$ C_3	**-459.1324316**	**-459.0641146**	**-459.0146649**
$Pb(H_2O)_6^{2+}$ [5+1] C_s #1	**-458.9920067**	**-459.0685244**	**-459.0183671**

$Pb(H_2O)_7^{2+}$ C_{2v} #1	-535.1791065	-535.1076727	-535.0583915
$Pb(H_2O)_7^{2+}$ C_{2v} #2	-535.1746009	-535.1037170	-535.0552995
$Pb(H_2O)_7^{2+}$ C_{2v} #3	-535.1722575	[6+1]	-535.0529554
$Pb(H_2O)_7^{2+}$ C_{2v} #4	-535.1730113	-535.1020250	-535.0536133
$Pb(H_2O)_7^{2+}$ C_{2v} #5	-535.1602442	-535.0909123	-535.0440575
$Pb(H_2O)_7^{2+}$ C_{2v} #6	-535.1670545	-535.0969286	-535.0495173
$Pb(H_2O)_7^{2+}$ C_{2v} #7	-535.1611930	-535.0909169	-535.0440588
$Pb(H_2O)_7^{2+}$ C_{2v} #8	-535.1730921	-535.1015326	-535.0533846
$Pb(H_2O)_7^{2+}$ C_{2v} #9	-535.1740383	-535.1020203	-535.0540743
$Pb(H_2O)_7^{2+}$ C_{2v} #10	-535.1644439	-535.0941410	-535.0469218
$Pb(H_2O)_7^{2+}$ C_{2v} #11	-535.1703833	[6+1]	
$Pb(H_2O)_7^{2+}$ C_{2v} #12	-535.1644447	-535.0941411	-535.0469219
$Pb(H_2O)_7^{2+}$ C_{2v} #13	-535.1712362	-535.1007533	-535.0528372
$Pb(H_2O)_7^{2+}$ C_{2v} #14	-535.1724230	-535.1015632	-535.0536118
$Pb(H_2O)_7^{2+}$ C_{2v} #15	-535.1740810	-535.1030295	-535.0548537
$Pb(H_2O)_7^{2+}$ C_{2v} #16	-535.1780745	-535.1061717	-535.0576390
$Pb(H_2O)_7^{2+}$ C_2 #1	-535.1799507	n/a	-535.0584844
$Pb(H_2O)_7^{2+}$ C_s #1	-535.1804779	-535.1078826	-535.0585715
$Pb(H_2O)_7^{2+}$ C_s #16	-535.1786422	n/a	n/a
$Pb(H_2O)_7^{2+}$ C_1 #1	**-535.1812511**	**-535.1080763**	**-535.0588124**
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #1	-535.1601655	-535.1001139	-535.0510203
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #2	-535.1808094	-535.1175903	-535.0670658
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #3	[7+2] C_{2v} #4	-535.1015147	[7+2] *C_{2v} #4*
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #4	-535.1620491	-535.0989768	-535.0492617
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #5	-535.1623860	-535.0996846	-535.0502734
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #6	-535.1717666	-535.1079928	-535.0568889
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #7	**-535.1729123**	-535.1094106	-535.0586110
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #8	-535.1799336	-535.1177696	-535.0676649
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #9	[7+2] C_{2v} #2	-535.1026722	-535.0531389
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #10	-535.1774672	-535.1150034	-535.0650546
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #11	-535.1779839	-535.1146011	-535.0643428
$Pb(H_2O)_7^{2+}$ [5+2] C_{2v} #12	-535.1703762	-535.1077787	-535.0570549
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #2	-535.1812820	-535.1182205	-535.0677801
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #3	n/a	**-535.1088212**	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_2 #10	-535.1779979	-535.1154329	-535.0655764
$Pb(H_2O)_7^{2+}$ [5+2] C_s #7	-535.1622881	-535.0991893	-535.0559194
$Pb(H_2O)_7^{2+}$ [5+2] C_s #9	-535.1717747	-535.1081423	-535.0570344
$Pb(H_2O)_7^{2+}$ [5+2] C_s #10	535.1718756	-535.1080008	n/a
$Pb(H_2O)_7^{2+}$ [5+2] C_s #11	n/a	**-535.1094278**	**-535.0586334**
$Pb(H_2O)_7^{2+}$ [5+2] C_s #15	n/a	-535.115547	-535.0653967
$Pb(H_2O)_7^{2+}$ [5+2] C_s #17	-535.1785236	-535.1160044	535.065836
$Pb(H_2O)_7^{2+}$ [5+2] C_s #18	**-535.1787521**	-535.1148448	-535.0643712
$Pb(H_2O)_7^{2+}$ [5+2] C_s #21	**-535.1820585**	**-535.1188468**	**-535.0682528**
$Pb(H_2O)_7^{2+}$ [5+2] C_1 #11	n/a	**-535.1167409**	**-535.0664846**
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #1	-535.1753299	-535.1083482	-535.0599584

$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #2	-535.1813884	-535.1140220	-535.0641141
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #3	-535.1759468	-535.1092590	-535.0606161
$Pb(H_2O)_7^{2+}$ [6+1] C_{2v} #4	-535.1777448	-535.1112773	-535.0616491
$Pb(H_2O)_7^{2+}$ [6+1] C_2 #2	-535.1817924	**-535.1142507**	**-535.0643189**
$Pb(H_2O)_7^{2+}$ [6+1] C_s #3	-535.1814556	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #4	-535.1818529	**-535.1142345**	**-535.0642123**
$Pb(H_2O)_7^{2+}$ [6+1] C_s #6	-535.1759472	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_s #7	-535.1787961	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #2	**-535.1819162**	n/a	n/a
$Pb(H_2O)_7^{2+}$ [6+1] C_1 #4	**-535.1825469**	n/a	n/a

$Pb(H_2O)_8^{2+}$ D_{4h} #1	-611.1908697	-611.1183872	-611.0733058
$Pb(H_2O)_8^{2+}$ D_{4h} #2	-611.1912084	-611.1185554	-611.0734390
$Pb(H_2O)_8^{2+}$ D_{4d} #1	-611.2122239	-611.1360162	-611.0881669
$Pb(H_2O)_8^{2+}$ D_{4d} #2	-611.2109963	-611.1354795	-611.0876262
$Pb(H_2O)_8^{2+}$ D_4 #1	**-611.2254105**	**-611.1473995**	**-611.0991446**
$Pb(H_2O)_8^{2+}$ C_{4h} #1	-611.2210160	-611.1447811	-611.0973065
$Pb(H_2O)_8^{2+}$ S_8 #1	**-611.2280807**	**-611.1499632**	**-611.1009230**
$Pb(H_2O)_8^{2+}$ D_{2d} #1	-611.2092262	-611.1337826	-611.0870098
$Pb(H_2O)_8^{2+}$ D_{2d} #2	-611.2092033	-611.1326987	-611.0854614
$Pb(H_2O)_8^{2+}$ D_{2d} #4	-611.2080606	-611.1318812	-611.0845574
$Pb(H_2O)_8^{2+}$ D_{2d} #5	-611.2243609	-611.1466445	-611.0985238
$Pb(H_2O)_8^{2+}$ D_{2h} #2	-611.2155449	-611.1394024	-611.0918934
$Pb(H_2O)_8^{2+}$ S_4 #3	-611.2231382	-611.1457036	D_{2d} #5
$Pb(H_2O)_8^{2+}$ C_{2h} #2	-611.2156327	-611.1394106	n/a
$Pb(H_2O)_8^{2+}$ [7+1] C_{2v} #1	-611.2278972	-611.1557997	-611.1066018
$Pb(H_2O)_8^{2+}$ [7+1] C_s #1	-611.2288330	[6+2] -611.1582727	-611.1067600
$Pb(H_2O)_8^{2+}$ [7+1] C_s #2	-611.2285500	-611.1558735	-611.1066235
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #2	**-611.2306552**	[5+3] **-611.1645473**	**-611.1071558**
$Pb(H_2O)_8^{2+}$ [7+1] C_1 #3	C_1 #2	**-611.1570209**	C_1 #2
$Pb(H_2O)_9^{2+}$ D_{3h} #1	-687.2517472	-687.1717581	-687.1243541
$Pb(H_2O)_9^{2+}$ D_{3h} #2	-687.2268638	-687.1506389	-687.1055753
$Pb(H_2O)_9^{2+}$ D_{3h} #3	-687.2320526	-687.1588491	-687.1117544
$Pb(H_2O)_9^{2+}$ D_{3h} #4	-687.2567824	-687.1757682	-687.1278958
$Pb(H_2O)_9^{2+}$ D_3 #1	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #2	D_3 #4	D_3 #4	D_3 #4
$Pb(H_2O)_9^{2+}$ D_3 #3	D_3 #4	[6+3]	[6+3]
$Pb(H_2O)_9^{2+}$ D_3 #4	-687.2668806	-687.1845942	-687.1359234
$Pb(H_2O)_9^{2+}$ C_{3h} #1	-687.2627616	-687.1805877	-687.1326107
$Pb(H_2O)_9^{2+}$ C_{3h} #2	-687.2606481	-687.1785583	-687.1304698
$Pb(H_2O)_9^{2+}$ C_{3h} #3	C_{3h} #1	C_{3h} #1	C_{3h} #1
$Pb(H_2O)_9^{2+}$ C_{3h} #4	C_{3h} #2	C_{3h} #2	C_{3h} #2
$Pb(H_2O)_9^{2+}$ C_3	**-687.2674500**	[6+3] **-687.1940695**	-687.1363552
$Pb(H_2O)_9^{2+}$ D_3 [6+3]	-687.2745908	-687.2076200	-687.1585476
$Pb(H_2O)_9^{2+}$ C_3 [6+3]	**-687.2798654**	**-687.2098793**	**-687.1596007**
$Pb(H_2O)_{18}^{2+}$ T	**-1371.6239189**	**-1371.5558187**	**-1371.5053134**

Table S2: Selected optimized structures (MP2/B, B = CEP-121G on Pb, 6-31+G* on O, H)

Z	x	y	z
$Pb(H_2O)^{2+}$ C_{2v}			
82	0.000000	0.000000	0.260646
8	0.000000	0.000000	-2.017583
1	0.000000	0.790417	-2.616136
1	0.000000	-0.790417	-2.616136
$Pb(H_2O)_2^{2+}$ C_2			
82	0.000000	0.000000	0.000000
8	1.524360	0.000000	-1.735079
1	2.438464	-0.372476	-1.697534
1	1.483344	0.531836	-2.565438
8	-1.524360	0.000000	-1.735079
1	-2.438464	0.372476	-1.697534
1	-1.483344	-0.531836	-2.565438
$Pb(H_2O)_3^{2+}$ C_3			
82	0.000000	0.000000	0.433541
8	-0.248806	1.728289	-1.124124
1	0.000000	2.673846	-1.004312
1	-0.910208	1.708887	-1.852805
8	1.621146	-0.648672	-1.124124
1	2.315618	-1.336923	-1.004312
1	1.935044	-0.066180	-1.852805
8	-1.372340	-1.079617	-1.124124
1	-2.315618	-1.336923	-1.004312
1	-1.024835	-1.642707	-1.852805
$Pb(H_2O)_4^{2+}$ C_2			
82	0.000000	0.000000	0.435170
8	0.000000	2.211690	-0.581244
8	0.000000	-2.211690	-0.581244
8	-1.778258	-0.033786	-1.119927
8	1.778258	0.033786	-1.119927
1	0.265705	3.043329	-0.130040
1	-0.485371	2.490584	-1.387242
1	-0.265705	-3.043329	-0.130040
1	0.485371	-2.490584	-1.387242
1	-1.994985	-0.868493	-1.589471
1	-2.596938	0.508811	-1.125861
1	1.994985	0.868493	-1.589471
1	2.596938	-0.508811	-1.125861

$Pb(H_2O)_5^{2+}$ C_{2v} #3

82	0.000000	0.000000	0.403541
8	0.000000	0.000000	-1.942069
8	2.339338	-0.000000	-0.412672
8	-2.339338	0.000000	-0.412672
8	0.000000	2.383409	-0.197655
8	-0.000000	-2.383409	-0.197655
1	0.797431	-0.000000	-2.510716
1	-0.797431	0.000000	-2.510716
1	2.932752	0.778922	-0.355922
1	2.932752	-0.778922	-0.355922
1	-2.932752	-0.778922	-0.355922
1	-2.932752	0.778922	-0.355922
1	0.000000	2.774343	-1.095567
1	0.000000	3.142386	0.423837
1	-0.000000	-2.774343	-1.095567
1	-0.000000	-3.142386	0.423837

$Pb(H_2O)_6^{2+}$ C_3

82	0.000000	0.000000	0.000000
8	2.568297	0.000000	0.318459
8	-1.284148	-2.224210	0.318459
8	-1.284148	2.224210	0.318459
8	0.616269	1.604186	-1.693409
8	-1.697400	-0.268389	-1.693409
8	1.081132	-1.335797	-1.693409
1	3.028175	-0.394686	1.088590
1	3.179487	0.693618	-0.003900
1	-1.855896	-2.425134	1.088590
1	-0.989052	-3.100326	-0.003900
1	-1.172280	2.819820	1.088590
1	-2.190435	2.406707	-0.003900
1	1.192767	1.536551	-2.480487
1	0.366147	2.544968	-1.587101
1	-1.927076	0.264691	-2.480487
1	-2.387080	-0.955391	-1.587101
1	0.734309	-1.801242	-2.480487
1	2.020933	-1.589576	-1.587101

$Pb(H_2O)_7^{2+}$ C_1

82	-0.009223	0.013312	-0.225142
8	-0.956355	-2.161434	0.546061
8	1.429210	-0.425177	1.703484
8	-2.476314	-0.373602	-1.049770
8	1.923734	-1.669639	-0.744338
8	-1.398385	0.544689	1.713071
8	2.155730	1.456072	-0.321784
8	-0.608441	2.523245	-0.038166
1	-0.687647	-2.957734	1.044944
1	-1.806545	-2.374331	0.109883
1	2.086035	-1.136133	1.554598
1	1.289528	-0.346832	2.667832
1	-3.254981	-0.046890	-0.556064
1	-2.791227	-0.492185	-1.969381
1	1.814235	-2.603009	-1.016944
1	2.730007	-1.365821	-1.208357
1	-1.801376	-0.018435	2.402529
1	-1.546860	1.479407	1.960718
1	2.604874	1.975752	-1.018700
1	2.761228	1.461805	0.446233
1	-1.344454	3.039870	-0.424045
1	0.150071	3.139703	-0.000102

$Pb(H_2O)_8^{2+}$ S_8

82	0.000000	0.000000	0.000000
8	1.640866	1.640866	1.128098
8	1.640866	-1.640866	1.128098
8	-1.640866	-1.640866	1.128098
8	-1.640866	1.640866	1.128098
8	0.000000	2.320535	-1.128098
8	2.320535	-0.000000	-1.128098
8	-0.000000	-2.320535	-1.128098
8	-2.320535	0.000000	-1.128098
1	2.117217	1.702990	1.979946
1	1.485196	2.560759	0.833669
1	1.702990	-2.117217	1.979946
1	2.560759	-1.485196	0.833669
1	-2.117217	-1.702990	1.979946
1	-1.485196	-2.560759	0.833669
1	-1.702990	2.117217	1.979946
1	-2.560759	1.485196	0.833669
1	0.292903	2.701294	-1.979946
1	-0.760537	2.860922	-0.833669
1	2.701294	-0.292903	-1.979946
1	2.860922	0.760537	-0.833669
1	-0.292903	-2.701294	-1.979946

1	0.760537	-2.860922	-0.833669
1	-2.701294	0.292903	-1.979946
1	-2.860922	-0.760537	-0.833669

$Pb(H_2O)_9^{2+}$ C_3

82	0.000000	0.000000	-0.020059
8	0.000000	2.617955	-0.225489
8	-2.267216	-1.308977	-0.225489
8	2.267216	-1.308977	-0.225489
8	-0.032652	-1.620494	2.018362
8	1.419715	0.781969	2.018362
8	-1.387063	0.838525	2.018362
8	-0.004270	-1.954992	-1.740822
8	1.695207	0.973798	-1.740822
8	-1.690937	0.981194	-1.740822
1	-0.252756	-2.553117	2.210113
1	0.727108	-1.390924	2.590580
1	2.337443	1.057665	2.210113
1	0.841022	1.325156	2.590580
1	-2.084686	1.495452	2.210113
1	-1.568129	0.065768	2.590580
1	0.882231	-2.347793	-1.599544
1	-0.235853	-2.139757	-2.672332
1	1.592133	1.937931	-1.599544
1	1.971011	0.865623	-2.672332
1	-2.474364	0.409862	-1.599544
1	-1.735157	1.274134	-2.672332
1	0.218509	3.405207	0.310290
1	-0.824093	2.834942	-0.707249
1	-3.058251	-1.513369	0.310290
1	-2.043086	-2.131157	-0.707249
1	2.839742	-1.891838	0.310290
1	2.867179	-0.703786	-0.707249