CHAPTER 3 - APPENDIX A

SUPPLEMENTARY MATERIALS

Table 3A.1: Total energies for the optimized geometries of water, chloride, hydroxide and ammonia.

Ligand	Point Group	HF/6-311+G*	MP2/6-311+G*	B3LYP/6-311+G*
H_2O	C_{2v}	-76.0377596	-76.2447096	76.4438090
Cl^-	K_h	-459.5654251	-459.7035702	-460.3037272
OH^-	$C_{\infty v}$	-75.3958926	-75.6209813	-75.8181221
NH_3	C_{3v}	-56.2043573	-56.3860912	-56.5728247

Table 3A.2: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-31G*/ CEP-121G**	**MP2/6-31G*/ CEP-121G**	**B3LYP/6-31G*/ CEP-121G**
1	C_{2v}	-78.7377472	-78.9469606	-79.2054817
2	D_{2h}	-154.8225026	-155.2234019	-155.6970915
	D_{2d}	-154.8226915	-155.2237237	-155.6977034
	C_s	-154.8405075	-155.2424163	-155.7165205
	C_2	-154.8405441	-155.2424559	-155.7165518
3	D_{3h} #1	-230.9101693	-231.5037497	-232.1938288
	D_{3h} #2	-230.9105263	-231.5040845	-232.1925527
	D_3	-230.9112251	-231.5049971	-232.1945861
	C_{2v} #1	-230.9193143	-231.5127354	-232.1995976
	C_{2v} #2	-230.9172259	-231.5127354	-232.1995976
	C_{3v} #1	-230.9261653	-231.5193654	-232.2075058
	C_{3v} #2	-230.9281585	-231.5213897	-232.2093809
	C_2 #1	-230.9193145	-231.5127356	-232.1995975
	C_s #1	-230.9307040	-231.5244127	-232.2119734
	C_s #2	-230.9298960	-231.5234079	-232.2110618
	C_3	-230.9323120	-231.5263775	-232.2137844
4	D_{4h} #1	-306.9768628	-307.7597674	-308.6592724
	D_{4h} #2	-306.9768076	-307.7601108	-308.6607978
	D_4	-306.9807339	-307.7643463	-308.6648855
	D_{2h}	-306.9807115	-307.7642568	-308.6646823
	C_{4v} #1	-306.9919497	-307.7752468	-308.6757340
	C_{4v} #2	-306.9907649	-307.7749602	-308.6744382
	D_{2d} #1	-306.9871132	-307.7724685	-308.6759044
	D_{2d} #2	-306.9870797	-307.7724280	-308.6758919
	C_4	-307.0020351	-307.7879272	-308.6878995
	C_2	-307.0024184	-307.7880679	-308.6878997

5	C_{2v}	-383.0656888	-384.0418419	-385.1522804
	C_s	-383.0657029	-384.0419928	-385.1525866
6	T_h	-459.1082585	-460.2737465	-461.5981403
	C_3	-459.1175918	-460.2850989	-461.6073987
7	C_{2v}	-535.1585025	-536.5165178	-538.0495704
	C_s #1	-535.1615583	-536.5221873	-538.0453274
	C_s #2	-535.1585109	-536.5142886	-538.0499601
	C_1	-535.1616300	-536.5271729	-538.0636887
8	D_{4h} #1	-611.1693931	-612.7144696	-614.4588421
	D_{4h} #2	-611.1689227	-612.7136368	-614.4581961
	D_{4d} #1	-611.1877488	-612.7342801	-614.4774269
	D_{4d} #2	-611.1902368	-612.7377258	-614.4806632
	S_8	-611.2033245	-612.7557317	-614.5039034
	D_4	-611.2014672	-612.7556186	-614.5038127
	C_2	-611.2033246	-612.7557315	-614.4125757
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.2297735	-688.9695517	-690.9225435
	D_{3h} #2	-687.2072430	-688.9443490	-690.8980267
	D_{3h} #3	-687.2256673	-688.9634636	-690.9170316
	D_{3h} #4	-687.2028488	-688.9375707	-690.8919417
	D_3	-687.2385848	-688.9794620	-690.9349374
	C_{3h}	-687.2341129	-688.9783871	-690.9342263
	C_3	-687.2400789	-688.9877497	-690.9398215
	C_1	N/A	N/A	-690.9464575

Detached structure

Table 3A.3: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-31G*/ LANL2DZ**	**MP2/6-31G*/ LANL2DZ**	**B3LYP/6-31G*/ LANL2DZ**
1	C_{2v}	-78.7113685	-78.9221672	-79.1764042
2	D_{2h}	-154.7875492	-155.1899972	-155.6596311
	D_{2d}	-154.7877133	-155.1902731	-155.6601566
	C_s	-154.8043986	-155.2074456	-155.6775700
	C_2	-154.8044244	-155.2074674	-155.6776037
3	D_{3h} #1	-230.8642076	-231.4587129	-232.1442714
	D_{3h} #2	-230.8647449	-231.4593123	-232.1433186
	D_3	-230.8653286	-231.4600734	-232.1451477
	C_{2v} #1	-230.8742338	-231.4685673	-232.1514622
	C_{2v} #2	-230.8742338	-231.4685673	-232.1514622
	C_{3v} #1	-230.8791143	-231.4729493	-232.1570007
	C_{3v} #2	- 230.8809968	-231.4749463	-232.1589283
	C_2 #1	-230.8742338	-231.4685673	-232.1514622
	C_s #1	-230.8836045	-231.4780223	-232.1615468
	C_s #2	-230.8828273	-231.4770123	-232.1606332
	C_3	-230.8851859	-231.4799189	-232.1632470
4	D_{4h} #1	-306.9238822	-307.7071950	-308.6025532
	D_{4h} #2	-306.9242797	-307.7082151	-308.6050083
	D_4	-306.9949190	-307.7954899	-308.6901516
	D_{2h}	-306.9950176	-307.7953496	-308.6900944
	C_{4v} #1	-306.8933281	-307.8019446	-308.6967035
	C_{4v} #2	-307.0023790	-307.8016722	-308.6958341
	D_{2d} #1	-306.9995716	-307.8001543	-308.6981141
	D_{2d} #2	-306.9995278	-307.8001082	-308.6980861
	C_4	-307.0133192	-307.8151181	-308.7082150
	C_2	-307.0142840	-307.8154999	-308.7085091
5	C_{2v}	-383.0829421	-384.0807729	-385.1830736
	C_s	-383.0829420	-384.0807729	-385.1831023
6	T_h	-459.1335715	-460.3266414	-461.6418377
	C_3	-459.1390483	-460.3338796	-461.6280642
7	C_{2v}	-535.0864883	-536.4445470	-537.9780126
	C_s #1	-535.0855366	-536.4445067	-537.9821902
	C_s #2	-535.0864883	-536.4446189	-537.9781230
	C_1	-535.0865358	-536.4546541	-537.9968456
8	D_{4h} #1	-611.1994817	-612.7826570	-614.5144617
	D_{4h} #2	-611.1990729	-612.7822415	-614.5142059
	D_{4d} #1	-611.2196570	-612.8076924	-614.5364951
	D_{4d} #2	-611.2207799	-612.8088248	-614.5373136

	S_8	-611.2364877	-612.8267254	-614.5572950
	D_4	-611.2334911	-612.8253800	-614.5564501
	C_2	-611.1196803	-612.6690373	-614.3738816
	C_1	-611.1381743	-612.6748938	N/A
9	D_{3h} #1	-687.1425370	-688.8774289	-690.8252232
	D_{3h} #2	-687.1255706	-688.8577582	-690.8085378
	D_{3h} #3	-687.1397500	-688.8730431	-690.8215774
	D_{3h} #4	-687.1199400	-688.8498931	-690.7990302
	D_3	-687.1504980	-688.8865496	-690.8774423
	C_{3h}	-687.1458467	-688.8858507	-690.8368029
	C_3	-687.1623866	-688.8943984	-690.8469998
	C_1	N/A	-688.9108165	-690.8681842

Detached structure

Table 3A.4: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-31G*/ SDD**	**MP2/6-31G*/ SDD**	**B3LYP/6-31G*/ SDD**
1	C_{2v}	-78.6856476	-78.8978027	-79.1541896
2	D_{2h}	-154.7578353	-155.1623753	-155.6321885
	D_{2d}	-154.7579285	-155.1625441	-155.6324970
	C_s	-154.7699458	-155.1765462	-155.6460497
	C_2	-154.7699779	-155.1766338	-155.6461774
3	D_{3h} #1	-230.8301436	-231.4278184	-232.1119160
	D_{3h} #2	-230.8299055	-231.4270531	-232.1099207
	D_3	-230.8307133	-231.4283672	-232.1122095
	C_{2v} #1	-230.8358275	-231.4343141	-232.1153073
	C_{2v} #2	-230.8358275	-231.4343141	-232.1153073
	C_{3v} #1	-230.8397521	-231.4387160	-232.1207111
	C_{3v} #2	-230.8410182	-231.4403360	-232.1220304
	C_2 #1	-230.8358278	-231.4343141	-232.1153072
	C_s #1	-230.8429341	-231.4425899	-232.1238755
	C_s #2	-230.8423652	-230.8392139	-232.1231510
	C_3	-230.8440759	-231.4439433	-232.1250225
4	D_{4h} #1	-306.8873058	-307.6745668	-308.5676066
	D_{4h} #2	-306.8879020	-307.6759206	-308.5702245
	D_4	-307.0900079	-307.9633326	-308.7931019
	D_{2h}	-307.0901351	-307.9631097	-308.7930737
	C_{4v} #1	-307.0979196	-307.9697113	-308.7995259
	C_{4v} #2	-307.0971071	-307.9689306	-308.7980951
	D_{2d} #1	-307.0944231	-307.9674265	-308.8009087
	D_{2d} #2	-307.0944024	-307.9674150	-308.8009310
	C_4	-307.1089687	-307.9837903	-308.8113061
	C_2	-307.1098367	-307.9840638	-308.8115716
5	C_{2v}	-383.2010581	-384.2902031	-385.3105054
	C_s	-383.2010579	-384.2902031	-385.3105420
6	T_h	-459.2729277	-460.5750655	-461.7924979
	C_3	-459.2793741	-460.5840590	-461.7805372
7	C_{2v}	-535.0395369	-536.4033182	-537.9321492
	C_s #1	-535.0392630	-536.4046993	-537.9364830
	C_s #2	-535.0393490	-536.4034666	-537.9323561
	C_1	-535.0468328	-536.4137013	Dissociation
8	D_{4h} #1	-611.3799044	-613.1089061	-614.7091184
	D_{4h} #2	-611.3796169	-613.1079916	-614.7089315
	D_{4d} #1	-611.4014529	-613.1360704	-614.7325685
	D_{4d} #2	-611.4030365	-613.1380009	-614.7340585

	S_8	-611.4196341	-613.1564548	-614.7561475
	D_4	-611.4167693	-613.1546660	-614.7553386
	C_2	-611.0775596	-612.6337286	-614.5573388
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.1011810	-688.8392482	-690.7836827
	D_{3h} #2	-687.0860609	-688.8218307	-690.7689989
	D_{3h} #3	-687.0985985	-688.8348671	-690.7801315
	D_{3h} #4	-687.0818169	-688.8150077	-690.7613392
	D_3	-687.1081093	-688.8488514	-690.8342303
	C_{3h}	-687.1042748	-688.8494388	-690.7974764
	C_3	-687.1154069	-688.8570034	-690.8063236
	C_1	N/A	Dissociation	Dissociation

Detached structure

Table 3A.5: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
N	**Point Group**	**HF/6-31+G*/ CEP-121G**	**MP2/6-31+G*/ CEP-121G**	**B3LYP/6-31+G*/ CEP-121G**
1	C_{2v}	-78.7407600	-78.9529010	-79.2102498
2	D_{2h}	-154.8289705	-155.2372082	-155.7082047
	D_{2d}	-154.8291321	-155.2374860	-155.7086224
	C_s	-154.8461208	-155.2546645	-155.7260389
	C_2	-154.8462440	-155.2548004	-155.7262298
3	D_{3h} #1	-230.9196925	-231.5245433	-232.2105538
	D_{3h} #2	-230.9189736	-231.5232412	-232.2077983
	D_3	-230.9202495	-231.5251143	-232.2107921
	C_{2v} #1	-230.9282991	-231.5328684	-232.2154721
	C_{2v} #2	-230.9282991	-231.5328684	-232.2154721
	C_{3v} #1	-230.9342829	-231.5382958	-232.2222172
	C_{3v} #2	-230.9363472	-231.5405084	-232.2241916
	C_2 #1	-230.9282992	-231.5328684	-232.2154721
	C_s #1	-230.9391052	-231.5437632	-232.2270037
	C_s #2	-230.9381773	-231.5427583	-232.2259831
	C_3	-230.9405840	-231.5456288	-232.2284542
4	D_{4h} #1	-306.9902162	-307.7891959	-308.6833087
	D_{4h} #2	-306.9910888	-307.7907321	-308.6862407
	D_4	-306.9277483	-307.7119146	-308.6084108
	D_{2h}	-306.9277917	-307.7119313	-308.6083372
	C_{4v} #1	-306.9350794	-307.7185695	-308.6148173
	C_{4v} #2	-306.9345108	-307.7189917	-308.6145037
	D_{2d} #1	-306.9311344	-307.7166831	-308.6152492
	D_{2d} #2	-306.9310789	-307.7166205	-308.6152165
	C_4	-306.9447670	-307.7308392	-308.6264836
	C_2	-306.9452933	-307.7310611	-308.6264837
5	C_{2v}	-383.0001569	-383.9760426	-385.0825021
	C_s	-383.0002719	-383.9764209	-385.0830480
6	T_h	-459.0385421	-460.2030107	-461.5229214
	C_3	-459.0454660	-460.2121020	-461.5308181
7	C_{2v}	-535.1866362	-536.5780732	-538.0982229
	C_s #1	-535.1842313	-536.5769527	-538.0923315
	C_s #2	-535.1806802	-536.5724886	-538.0982861
	C_1	-535.1905746	-536.5843396	Dissociation
8	D_{4h} #1	-611.0909145	-612.6321259	-614.3716937
	D_{4h} #2	-611.0906645	-612.6316520	-614.3713854
	D_{4d} #1	-611.1061832	-612.6498232	-614.3879586
	D_{4d} #2	-611.1080541	-612.6523725	-614.3900951

	S_8	-611.1196805	-612.6690373	-614.4125510
	D_4	-611.1179788	-612.6688951	-614.4125084
	C_2	-611.2364877	-612.8267254	-614.4734671
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.2660952	-689.0532518	-690.9887174
	D_{3h} #2	-687.2415237	-689.0252398	-690.9619018
	D_{3h} #3	-687.2614313	-689.0487437	-690.9839858
	D_{3h} #4	-687.2365044	-689.0185683	-690.9564085
	D_3	-687.2760524	-689.0648175	-691.0198403
	C_{3h}	-687.2698253	-689.0606241	-690.9958570
	C_3	-687.2765304	-689.0677926	-691.0044055
	C_1	N/A	N/A	N/A

Detached structure

Table 3A.6: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
N	**Point Group**	**HF/6-31+G*/ LANL2DZ**	**MP2/6-31+G*/ LANL2DZ**	**B3LYP/6-31+G*/ LANL2DZ**
1	C_{2v}	-78.7186093	-78.9323502	-79.1857826
2	D_{2h}	-154.7986578	-155.2083607	-155.6756807
	D_{2d}	-154.7988002	-155.2086060	-155.6759998
	C_s	-154.8143762	-155.2242015	-155.6919716
	C_2	-154.8144734	-155.2243146	-155.6921734
3	D_{3h} #1	-230.8793705	-231.4850742	-232.1669163
	D_{3h} #2	-230.8792607	-231.4849672	-232.1651702
	D_3	-230.8801724	-231.5251143	-232.1674057
	C_{2v} #1	-230.8872505	-231.4929107	-232.1719991
	C_{2v} #2	-230.8872505	-231.4929107	-232.1719991
	C_{3v} #1	-230.8917342	-231.4967894	-232.1771366
	C_{3v} #2	-230.8934287	-231.4986406	-232.1787277
	C_2 #1	-230.8872505	-231.4929107	-232.1719991
	C_s #1	-230.8960274	-231.5017462	-232.1813914
	C_s #2	-230.8952127	-231.5007996	-232.1804620
	C_3	-230.8973330	-231.5033420	-232.1826281
4	D_{4h} #1	-306.9428337	-307.7422598	-308.6332319
	D_{4h} #2	-306.9441432	-307.7444801	-308.6367236
	D_4	-306.9475018	-307.7484859	-308.6400274
	D_{2h}	-306.9475680	-307.7483973	-308.6399274
	C_{4v} #1	-306.9503925	-307.7499581	-308.6412049
	C_{4v} #2	-306.9508185	-307.7511179	-308.6419439
	D_{2d} #1	-306.9499652	-307.7513743	-308.6446038
	D_{2d} #2	-306.9498866	-307.7512072	-308.6445072
	C_4	-306.9600711	-307.7623549	-308.6520103
	C_2	-306.9610183	-307.7627601	-308.6524077
5	C_{2v}	-383.0207657	-384.0186068	-385.1180450
	C_s	-383.0207657	-384.0186068	-385.1180420
6	T_h	-459.0686241	-460.2616720	-461.5729839
	C_3	-459.0708113	-460.2649182	-461.5791262
7	C_{2v}	-535.1152461	-536.5088077	-538.0316785
	C_s #1	-535.1152021	-536.5069562	-538.0339358
	C_s #2	-535.1172185	-536.5088076	-538.0316976
	C_1	-535.1221187	-536.5161575	Dissociation
8	D_{4h} #1	-611.1272091	-612.7089304	-614.4372166
	D_{4h} #2	-611.1269918	-612.7086223	-614.4370716
	D_{4d} #1	-611.1441297	-612.7300107	-614.4553964
	D_{4d} #2	-611.1447679	-612.7306242	-614.4557119

	S_8	-611.1585195	-612.7464960	-614.4734305
	D_4	-611.1555154	-612.7453855	-614.4727371
	C_2	(S_8) -611.1585195	(S_8) -612.7464960	-614.4284662
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.1851672	-688.9689999	-690.9012587
	D_{3h} #2	-687.1685320	-688.9483886	-690.8844076
	D_{3h} #3	-687.1816396	-688.9650281	-690.8977989
	D_{3h} #4	-687.1605233	-688.9389423	-690.8742102
	D_3	-687.1939245	-688.9790247	-690.9487108
	C_{3h}	-687.1879599	-688.9743524	-690.9067512
	C_3	-687.2037381	-688.9807650	-690.9146162
	C_1	N/A	-689.0010051	Dissociation

Detached structure

Table 3A.7: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-31+G*/ SDD**	**MP2/6-31+G*/ SDD**	**B3LYP/6-31+G*/ SDD**
1	C_{2v}	-78.6887845	-78.9036772	-79.1589271
2	D_{2h}	-154.7646301	-155.1760743	-155.6433967
	D_{2d}	-154.7647076	-155.1761957	-155.6436029
	C_s	-154.7760427	-155.1888775	-155.6560580
	C_2	-154.7760942	-155.1890372	-155.6562323
3	D_{3h} #1	-230.8406201	-231.4491798	-232.1294956
	D_{3h} #2	-230.8402169	-231.4482128	-232.1275881
	D_3	-230.8411230	-231.4862000	-232.1297535
	C_{2v} #1	-230.8456377	-231.4549455	-232.1323058
	C_{2v} #2	-230.8456377	-230.8420144	-232.1323058
	C_{3v} #1	-230.8489972	-231.4582291	-232.1368291
	C_{3v} #2	-230.8500699	-231.4596061	-232.1378098
	C_2 #1	-230.8456378	-231.4549455	-232.1323058
	C_s #1	-230.8522202	-231.4623934	-232.1400629
	C_s #2	-230.8516670	-231.4615670	-232.1393763
	C_3	-230.8533597	-231.4636854	-232.1411263
4	D_{4h} #1	-306.9017274	-307.7046260	-308.5933333
	D_{4h} #2	-306.9029158	-307.7068214	-308.5963971
	D_4	-307.0414624	-307.9153900	-308.7419352
	D_{2h}	-307.0415069	-307.9152931	-308.7418125
	C_{4v} #1	-307.0443223	-307.9167632	-308.7430334
	C_{4v} #2	-307.0443272	-307.9175854	-308.7431909
	D_{2d} #1	-307.0434566	-307.9177574	-308.7462741
	D_{2d} #2	-307.0433618	-307.9175204	-308.7461713
	C_4	-307.0544090	-307.9300214	-308.7540167
	C_2	-307.0552486	-307.9303076	-308.7543461
5	C_{2v}	-383.1377696	-384.2272172	-385.2444960
	C_s	-383.1377695	-384.2272521	-385.2444929
6	T_h	-459.2070243	-460.5105119	-461.7229838
	C_3	-459.2099392	-460.5145047	-461.7310006
7	C_{2v}	-535.0684502	- 536.4631444	-537.9841858
	C_s #1	-535.0671922	-536.4639845	-537.9866245
	C_s #2	-535.0682253	-536.4649724	-537.9842322
	C_1	-535.0741748	-536.4724537	Dissociation
8	D_{4h} #1	-611.3067485	-613.0355939	-614.6311753
	D_{4h} #2	-611.3065600	-611.2996822	-614.6310587
	D_{4d} #1	-611.3251558	-613.0581204	-614.6510404
	D_{4d} #2	-611.3261312	-613.0596290	-614.6518280

	S_8	-611.3406024	-613.0757873	-614.6713345
	D_4	-611.3375426	-613.0742731	-614.6707319
	C_2	-611.1119883	-612.7039112	-614.7561793
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.1400534	-688.9266706	-690.8563110
	D_{3h} #2	-687.1241694	-688.9065678	-690.8403009
	D_{3h} #3	-687.1371057	-688.9230867	-690.8534028
	D_{3h} #4	-687.1185858	-688.8996317	-690.8326612
	D_3	-687.1479599	-688.9358534	-690.9024724
	C_{3h}	-687.1424797	-688.9321235	-690.8631214
	C_3	-687.1552649	-688.9378662	-690.8700002
	C_1	N/A	-688.9493645	Dissociation

Detached structure

Table 3A.8: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-311+G*/ CEP-121G**	**MP2/6-311+G*/ CEP-121G**	**B3LYP/6-311+G*/ CEP-121G**
1	C_{2v}	-78.6856476	-78.9954020	-79.2367178
2	D_{2h}	-154.8773625	-155.3217742	-155.7606335
	D_{2d}	-154.8775707	-155.3221118	-155.7611074
	C_s	-154.8948546	-155.3396358	-155.7786285
	C_2	-154.8948926	-155.3397004	-155.7787640
3	D_{3h} #1	-230.9916009	-231.6507293	-232.2884047
	D_{3h} #2	-230.9908332	-231.6494099	-232.2857735
	D_3	-230.9921749	-231.4496673	-232.2887014
	C_{2v} #1	-231.0006241	-231.6597473	-232.2935190
	C_{2v} #2	-231.0006241	-231.6597473	-232.2935190
	C_{3v} #1	-231.0063151	-231.6647555	-232.3000053
	C_{3v} #2	-231.0087042	-231.6675325	-232.3023638
	C_2 #1	-231.0006241	-231.6597473	-232.2935190
	C_s #1	-231.0114081	-231.6706105	-232.3050259
	C_s #2	-231.0105017	-231.6696126	-232.3039776
	C_3	-231.0131730	-231.6728206	-232.3066271
4	D_{4h} #1	-307.0847180	-307.9562198	-308.7857439
	D_{4h} #2	-307.0858704	-307.9577108	-308.7887178
	D_4	-306.8906723	-307.6789059	-308.5728202
	D_{2h}	-306.8907032	-307.6789068	-308.5727411
	C_{4v} #1	-306.8933281	-307.6822326	-308.5750852
	C_{4v} #2	-306.8933203	-307.6826140	-308.5752463
	D_{2d} #1	-306.8938378	-307.6829059	-308.5790823
	D_{2d} #2	-306.8937975	-307.6828546	-308.5790528
	C_4	-306.9013667	-307.6928632	-308.5850721
	C_2	-306.9017051	-307.6930599	-308.5850823
5	C_{2v}	-382.9551861	-383.9367149	-385.0392987
	C_s	-382.9551898	-383.9368387	-383.2010579
6	T_h	-458.9981433	-460.1671492	-461.4833222
	C_3	-459.0003096	-460.1726562	-461.4929109
7	C_{2v}	-535.3483958	-536.8679984	-538.2751208
	C_s #1	-535.3466550	-536.8675032	-538.2696298
	C_s #2	-535.3440772	-536.8646490	-538.2751548
	C_1	-535.3531842	-536.8716667	Dissociation
8	D_{4h} #1	-611.0524732	-612.5971842	-614.3334376
	D_{4h} #2	-611.0523190	-612.5968794	-614.3332691
	D_{4d} #1	-611.0651740	-612.6126964	-614.3474910

	D_{4d} #2	-611.0664732	-612.6144746	-614.3487372
	S_8	-611.0775596	-612.6337284	-614.3739204
	D_4	-611.0766877	-612.6336945	-614.3740495
	C_2	-611.4196341	-613.1564549	-614.6713881
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.4687360	-689.4216873	-691.2072569
	D_{3h} #2	-687.4435472	-689.3945429	-691.1796954
	D_{3h} #3	-687.4650758	-689.4182736	-691.2038694
	D_{3h} #4	-687.0818169	-689.3853106	-691.1738298
	D_3	-687.4804415	-689.4344218	-691.2442125
	C_{3h}	-687.4743817	-689.4303975	-691.2176112
	C_3	-687.4809019	-689.4360664	-691.2264051
	C_1	N/A	N/A	N/A

Detached structure

Table 3A.9: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-311+G*/ LANL2DZ**	**MP2/6-311+G*/ LANL2DZ**	**B3LYP/6-311+G*/ LANL2DZ**
1	C_{2v}	-78.7425715	-78.9954020	-79.2118563
2	D_{2h}	-154.8463339	-155.2923513	-155.7275239
	D_{2d}	-154.8465129	-155.2926955	-155.7278824
	C_s	-154.8623322	-155.3086605	-155.7439787
	C_2	-154.8623470	-155.3086670	-155.7441074
3	D_{3h} #1	-230.9502242	-231.6103011	-232.2439511
	D_{3h} #2	-230.9500351	-231.6104019	-232.2422314
	D_3	-230.9509788	-231.6513209	-232.2444331
	C_{2v} #1	-230.9585142	-231.6190367	-232.2491986
	C_{2v} #2	-231.0006241	-231.6190367	-232.2491986
	C_{3v} #1	-230.9628773	-231.6226742	-232.2542603
	C_{3v} #2	-230.9648017	-231.6249699	-232.2560728
	C_2 #1	-230.9585142	-231.6190367	-232.2491986
	C_s #1	-230.9673908	-231.6278731	-232.2586525
	C_s #2	-230.9665710	-231.6269919	-232.2577290
	C_3	-230.9688320	-231.6297403	-232.2599407
4	D_{4h} #1	-307.0364668	-307.9087446	-308.7348484
	D_{4h} #2	-307.0378286	-307.9107622	-308.7382693
	D_4	-306.9056930	-307.7100834	-308.5991397
	D_{2h}	-306.9057331	-307.7099262	-308.5990349
	C_{4v} #1	-306.9062769	-307.7105786	-308.5989276
	C_{4v} #2	-306.9068786	-307.7115742	-308.5998354
	D_{2d} #1	-306.9082554	-307.7128476	-308.6040410
	D_{2d} #2	-306.9081812	-307.7127079	-308.6039418
	C_4	-306.9144487	-307.7213411	-308.6082581
	C_2	-306.9149033	-307.7216313	-308.6084470
5	C_{2v}	-382.9734466	-383.9761585	-385.0722767
	C_s	-382.9734460	-383.9761585	-385.0722820
6	T_h	-459.0230909	-460.2194758	-461.5278488
	C_3	-459.0236445	-460.2222236	-461.5332471
7	C_{2v}	-535.2794376	-536.8001360	-538.2075121
	C_s #1	-535.2768063	-536.8007319	-538.2102140
	C_s #2	-535.2794376	-536.8001349	-538.2075290
	C_1	-535.2847386	-536.8068100	Dissociation
8	D_{4h} #1	-611.0850196	-612.6697849	-614.3954131
	D_{4h} #2	-611.0848542	-612.6695075	-614.3952767
	D_{4d} #1	-611.0990517	-612.688488	-614.4107581
	D_{4d} #2	-611.0996899	-612.6889346	-614.4108679

	S_8	-611.1119883	-612.7039112	-614.4283727
	D_4	-611.1097764	-612.7032473	-614.4281413
	C_2	-611.3406024	-613.0757873	-614.6255398
	C_1	N/A	N/A	N/A
9	D_{3h} #1	-687.3877084	-689.3382002	-691.1199795
	D_{3h} #2	-687.3699362	-689.3169861	-691.1017126
	D_{3h} #3	-687.3847152	-689.3351296	-691.2038694
	D_{3h} #4	-687.4379900	-689.3061115	-691.0915656
	D_3	-687.3975603	-689.3490003	-691.1717224
	C_{3h}	-687.3913350	-689.3434121	-691.1271165
	C_3	-687.4098784	-689.3495215	-691.1355611
	C_1	N/A	N/A	-691.1721536

Detached structure

Table 3A.10: Total energies for the stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=0 – 9.

Total Energy (Hartrees)				
n	**Point Group**	**HF/6-311+G*/ SDD**	**MP2/6-311+G*/ SDD**	**B3LYP/6-311+G*/ SDD**
0	K_h	-2.5880503	-2.6036578	-2.6448270
1	C_{2v}	-78.7125289	-78.9460579	-79.1847890
2	D_{2h}	-154.8116111	-155.2600652	-155.6944643
	D_{2d}	-154.8116918	-155.2602101	-155.6946794
	C_s	-154.8233871	-155.2735072	-155.7075267
	C_2	-154.8234126	-155.2736366	-155.7076847
3	D_{3h} #1	-230.9107314	-231.5748563	-232.2058003
	D_{3h} #2	-230.9101989	-231.5738827	-232.2037714
	D_3	-230.9111906	-231.6116218	-232.2060349
	C_{2v} #1	-230.9160398	-231.5812006	-232.2086750
	C_{2v} #2	-230.9160398	-231.5812006	-232.2086750
	C_{3v} #1	-230.9194157	-231.5845509	-232.2133776
	C_{3v} #2	-230.9205926	-231.5861931	-232.2144873
	C_2 #1	-230.9160397	-231.5812006	-232.2086750
	C_s #1	-230.9228121	-231.5888791	-232.2167117
	C_s #2	-230.9222539	-231.5880399	-232.2160465
	C_3	-230.9240418	-231.5902606	-232.2178114
4	D_{4h} #1	-306.9943100	-307.8713319	-308.6938381
	D_{4h} #2	-306.9956033	-307.8734982	-308.6969489
	D_4	-306.9985743	-307.8771321	-308.6999670
	D_{2h}	-306.9985868	-307.8769049	-308.6998172
	C_{4v} #1	-306.9993564	-307.8779883	-308.7000018
	C_{4v} #2	-306.9996660	-307.8787549	-308.7004494
	D_{2d} #1	-307.0010280	-307.880043	-308.7050082
	D_{2d} #2	-307.0009416	-307.8798824	-308.7049076
	C_4	-307.0079296	-307.8893675	-308.7095326
	C_2	-307.0083078	-307.8895713	-308.709697
5	C_{2v}	-383.089435	-384.1852774	-385.1978795
	C_s	-383.0894349	-384.1852775	-385.1978815
6	T_h	-459.1605451	-460.4685201	-461.6769699
	C_3	-459.1616546	-460.4724224	-461.6843908
7	C_{2v}	-535.2283295	-536.7570254	-538.1591309
	C_s #1	-535.2277694	-536.7570691	-538.1620020
	C_s #2	-535.2293787	-536.7570254	-538.1591885
	C_1	-535.2346418	-536.7637132	Dissociation
8	D_{4h} #1	-611.2640311	-612.9975471	-614.5887282
	D_{4h} #2	-611.2639007	-612.9968052	-614.5886017
	D_{4d} #1	-611.2793901	-613.0180626	-614.6054820

	D_{4d} #2	-611.2801195	-613.0191125	-614.6058638
	S_8	-611.2931957	-613.0339214	-614.6254594
	D_4	-611.2910371	-613.0329382	-614.6253075
	C_2	(S_8) -611.2931957	(S_8) -613.0339215	-614.6255390
	C_1	-n/a-	-n/a-	-n/a-
9	D_{3h} #1	-687.3417754	-689.2968058	-691.0739133
	D_{3h} #2	-687.3247661	-689.2757725	-691.0566572
	D_{3h} #3	-687.3392885	-689.2939517	-691.0719396
	D_{3h} #4	-687.3615867	-689.2677376	-691.0489961
	D_3	-687.3506609	-689.3066781	-691.1247042
	C_{3h}	-687.3449529	-689.3020315	-691.0825786
	C_3	-687.3603808	-689.3073688	-691.1065563
	C_1	-N/A-	-689.3175287	-691.1123918

Detached structure

Table 3A.11: Pb-O bond lengths for stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=1 – 9.

		Optimized Pb-O Bond Lengths (Å)		
n	**Point Group Symmetry**	**HF SDD/6-311+G***	**MP2 SDD/6-311+G***	**B3LYP/ SDD/6-311+G***
1	C_{2v}	2.382	2.365	2.357
2	C_2	2.423	2.403	2.399
3	C_3	2.462	2.438	2.442
4	C_2	2.591 2.484	2.554 2.461	2.563 2.467
5	C_s	2.455 2.643 2.635	2.429 2.599 2.585	2.383 2.885 2.600
6	C_3	2.557 2.800	2.495 2.785	--
7	C_1	--	--	--
8	D_4	2.783	2.735	2.762
	C_2	--	--	2.760
	S_8	2.773	2.725	2.756
	C_1	-N/A-	-N/A-	-N/A-
9	C_3	--	--	--
	C_1	-N/A-	--	--

Table 3A.12: Vibrational stretching frequencies of stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=1 – 9, calculated at HF/SDD/6-311+G*.

n	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Rep. Symmetry	Mixing
1	C_{2v}	317.7	a_1	
2	C_2	280.1 297.6	b a	
3	C_3	254.3 278.9	e a	 H_2O twisting
4	C_2	184.9 217.3 223.2 263.3	b a b a	H_2O twisting H_2O twisting
5	C_s	176.0 188.1 203.7 215.6 253.9	a” a’ a’ a’ a’	H_2O wagging H_2O wagging H_2O wagging
6	C_3	158.4 169.0 205.8 235.8	e a e a	 H_2O twisting H_2O rocking
7	C_1	--	--	
8	D_4	143.4 146.5 150.7 159.9 167.1 202.6	a_2 e b_2 b_1 e a_1	H_2O wagging H_2O wagging
	C_2	--	--	--
	S_8	134.6 136.5 144.8 155.4 201.6	e_1 b e_2 e_3 a	H_2O twisting H_2O wagging H_2O rocking H_2O wagging
	C_1	--	--	--
9	C_3	--	--	
	C_1	--	--	

Table 3A.13: Vibrational stretching frequencies of stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=1 – 9, calculated at MP2/SDD/6-311+G*.

n	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Rep. Symmetry	Mixing
1	C_{2v}	335.3	a_1	
2	C_2	298.7 316.1	b a	
3	C_3	273.3 300.0	e a	
4	C_2	208.8 232.2 247.6 283.2	b a b a	H_2O twisting H_2O twisting
5	C_s	195.4 209.9 220.9 231.9 276.4	a” a’ a’ a’ a’	H_2O wag./rock. H_2O twisting H_2O twisting H_2O wagging
6	C_3	176.5 185.6 233.9 265.5	e a e a	H_2O twisting H_2O twisting H_2O twisting
7	C_1	--	--	
8	D_4	170.1 172.0 172.8 179.5 194.6 224.7	b_2 a_2 e b_1 e a_1	H_2O twisting H_2O twisting H_2O wagging H_2O twisting H_2O wagging H_2O wagging
	C_2	--	--	--
	S_8	167.9 172.0 172.3 184.4 223.3	b e_2 e_1 e_3 a	H_2O twisting H_2O wagging H_2O wagging H_2O wagging H_2O wagging
	C_1	--	--	
9	C_3	156.1 166.3 176.1 191.1	e a e a	H_2O twisting H_2O twisting H_2O twisting H_2O twisting

		191.6 227.5	e a	H_2O wagging H_2O rocking
	C_1	--		

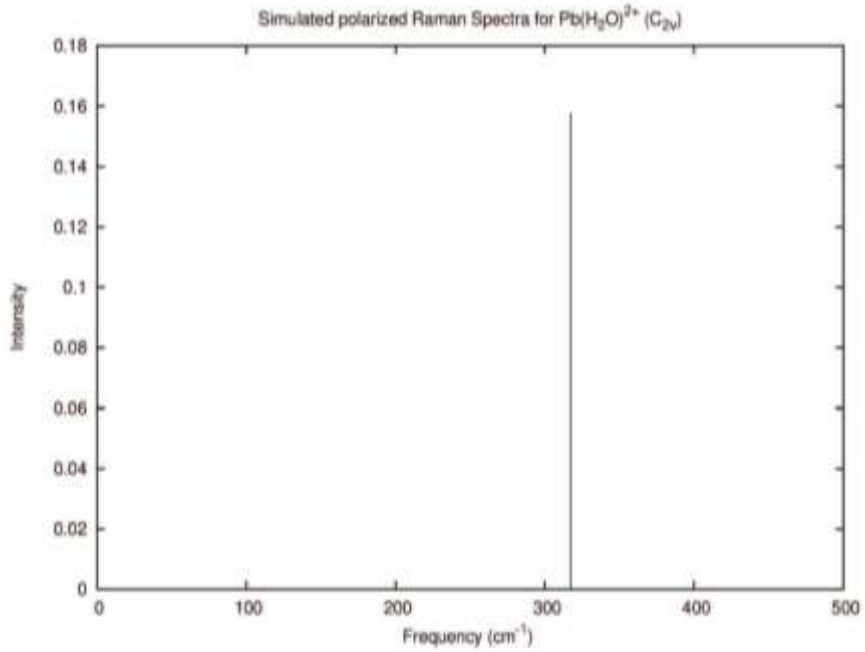
Table 3A.14: Vibrational stretching frequencies of stable geometries of $[Pb(H_2O)_n]^{2+}$, where n=1 – 9, calculated at B3LYP/SDD/6-311+G*.

n	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Rep. Symmetry	Mixing
1	C_{2v}	333.5	a_1	
2	C_2	294.1 310.1	b a	
3	C_3	265.8 292.9	e a	H_2O wagging H_2O twisting
4	C_2	197.7 225.1 237.5 274.4	b a b a	H_2O twisting H_2O twisting
5	C_s	183.3 196.5 211.3 223.3 266.8	a” a’ a’ a’ a’	H_2O wagging H_2O twisting H_2O twisting H_2O wagging
6	C_3	--	--	
7	C_1	--	--	
8	D_4	100.1 109.9 187.1 188.8 208.4 225.2	b_1 b_2 e a_2 e a_1	 H_2O wagging H_2O wagging H_2O wagging
	C_2	176.9 179.6 184.2 190.3 192.8 193.1 232.3	a a a b b b a	H_2O twisting H_2O twisting H_2O twisting H_2O twisting H_2O twisting H_2O twisting H_2O wagging
	S_8	91.7 183.9 193.9 194.0 222.8	e_2 b e_1 e_3 a	 H_2O twisting H_2O twisting H_2O twisting H_2O wagging
	C_1	--	--	--

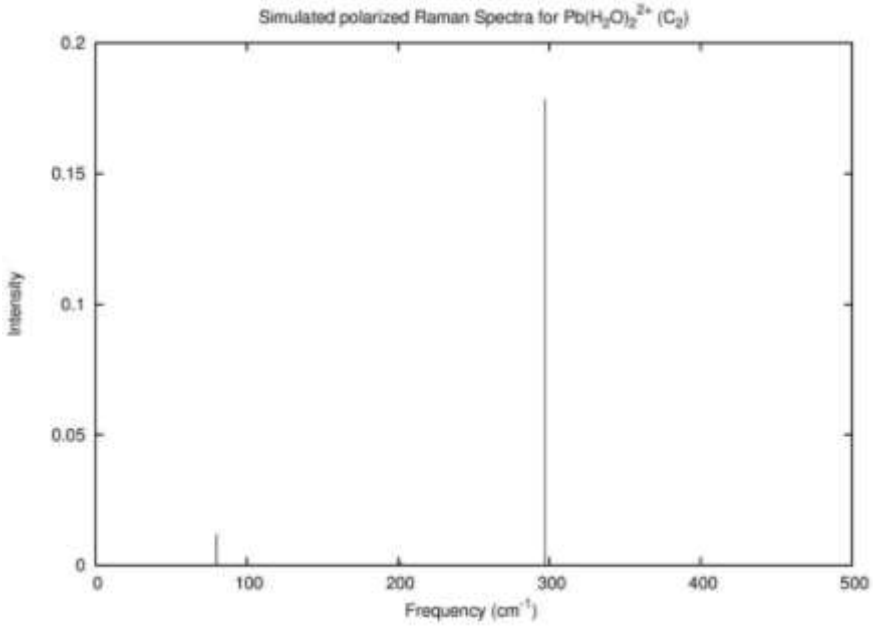
9	C_3	--	--	
	C_1	--	--	

Figure 3A-1: Simulated polarized Raman spectra for $[Pb(H_2O)_n]^{2+}$, where n=1 – 9.

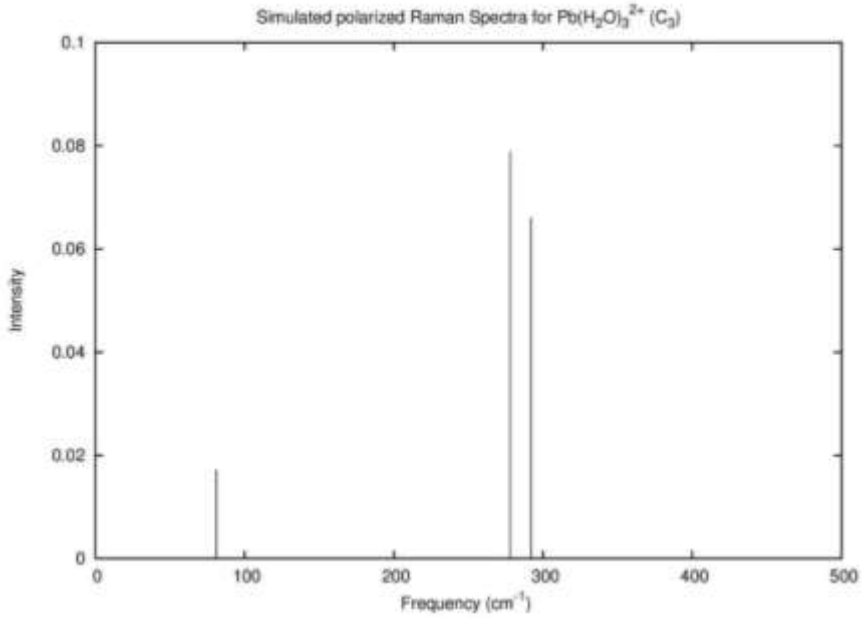
$[Pb(H_2O)]^{2+}$



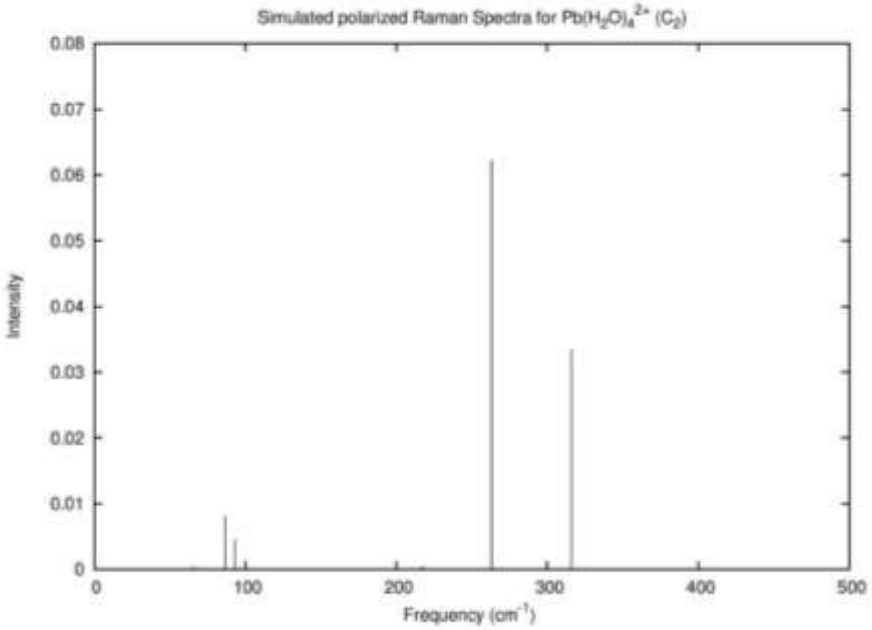
$[Pb(H_2O)_2]^{2+}$



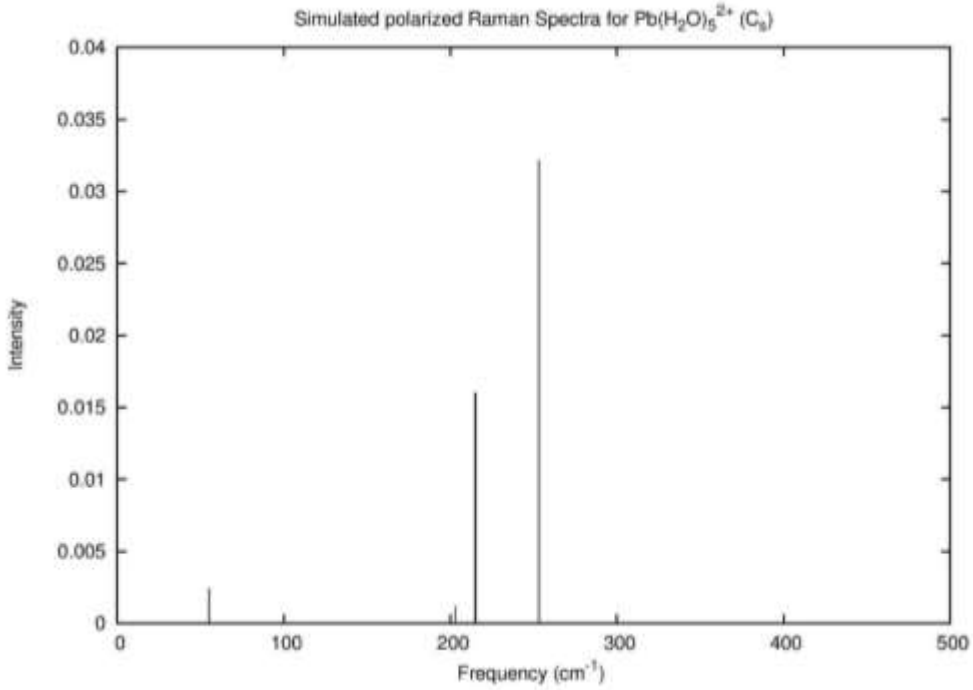
$[Pb(H_2O)_3]^{2+}$



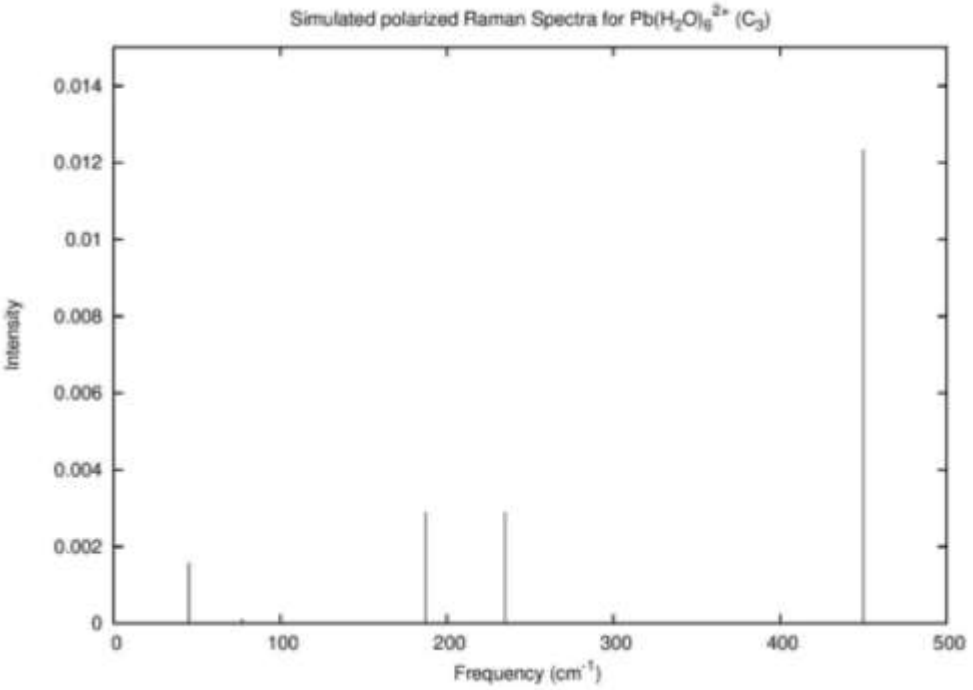
$[Pb(H_2O)_4]^{2+}$



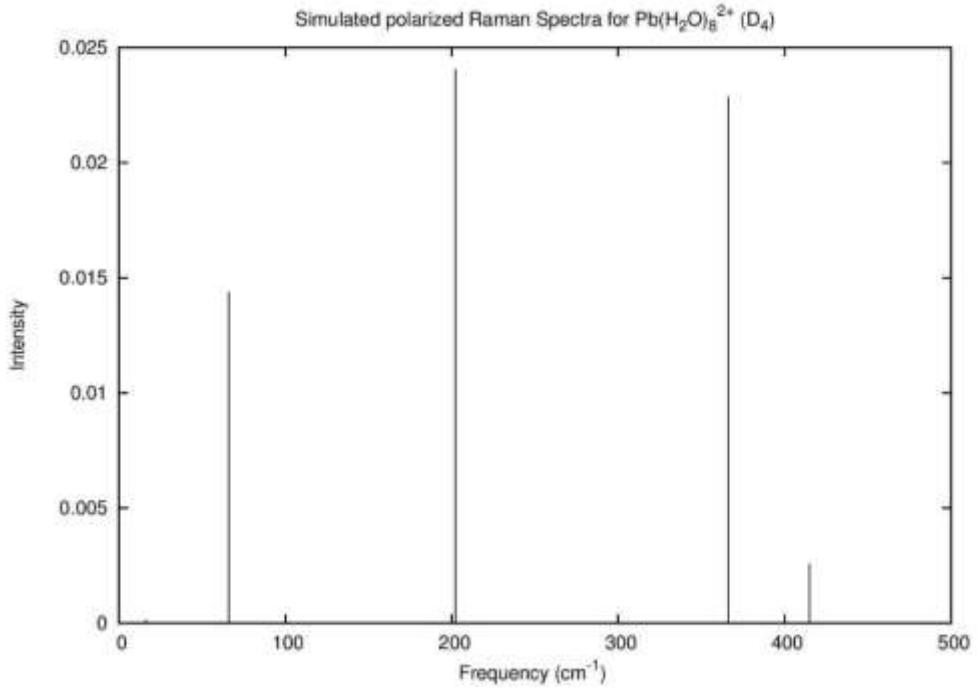
$[Pb(H_2O)_5]^{2+}$



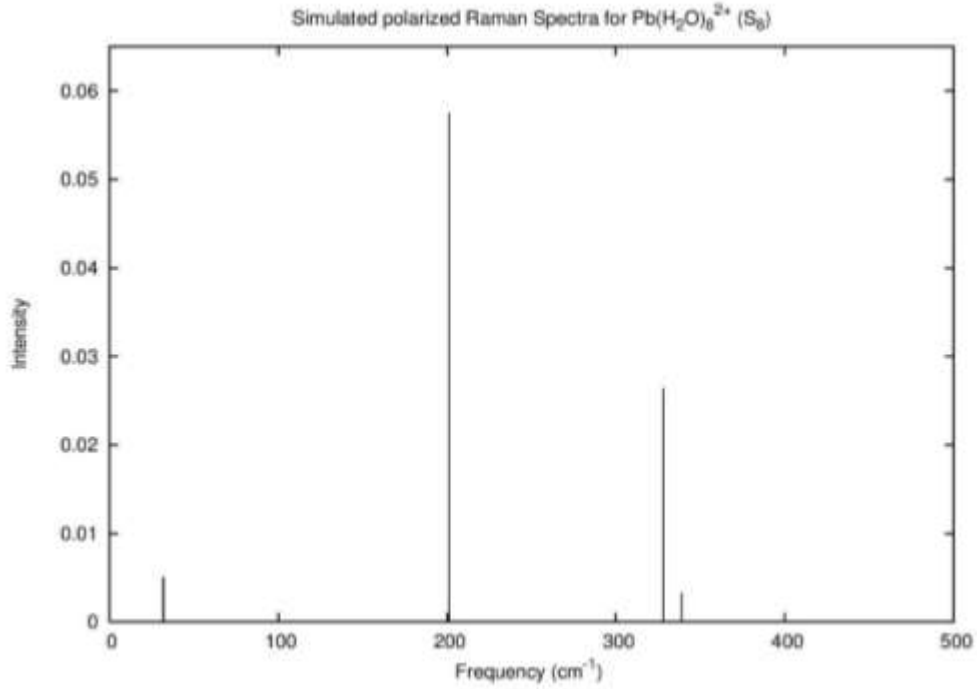
$[Pb(H_2O)_6]^{2+}$



$[Pb(H_2O)_8]^{2+}$



$[Pb(H_2O)_8]^{2+}$



CHAPTER 4 - APPENDIX A

SUPPLEMENTARY MATERIALS

Table 4A.1: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ CEP-121G**	**MP2/6-31G*/ CEP-121G**	**B3LYP/6-31G*/ CEP-121G**
1	0	$C_{\infty v}$	-462.6489162	-462.8072232	-463.4697184
1	1	C_{2v}	-538.6905728	-539.0394160	-539.9151785
		C_s	-538.7251366	-539.0727010	-539.9480345
1	2	C_{2v} #1	-614.7736113	-615.3105508	-616.3981406
		C_{2v} #2	-614.7840389	-615.3212764	-616.4078363
		C_s	-614.7933166	-615.3308577	-616.4175918
1	3	C_{3v} #1	-614.7933168	-691.5563514	-692.8570451
		C_{3v} #2	-690.8291156	-691.5744165	-692.8725845
		C_3	-690.8459725	-691.5744164	N/A
		C_s	N/A	N/A	N/A
1	4	C_{4v} #1	-766.8723438	-767.7892528	-769.2994363
		C_{4v} #2	-766.8940855	-767.8123895	-769.3197865
		C_4	N/A	-767.8127855	-769.3212694
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.9198322	-844.0286791	-845.7480803
		C_{2v} #2	-842.8996729	-844.0077980	-845.7306521
		C_{2v} #3	-842.9151971	-844.0251984	-845.7463598
		C_{2v} #4	-842.9138271	-844.0237642	-845.7448338
		C_{2v} #5	-842.9198699	-844.0287440	-845.7481281
		C_2 #1	-842.9198815	-844.0298449	N/A
		C_2 #2	N/A	N/A	-845.7509487
		C_s #1	-842.9265040	-844.0411130	-845.7614680
		C_s #2	N/A	N/A	-845.7502360
		C_1	-842.9290076	-844.0441243	-845.7620474
2	0	$D_{\infty h}$	-922.4006680	-922.6949239	-923.9695210
		C_{2v}	-922.4517487	-922.7422932	-924.0151697
2	1	C_{2v} #1	-998.4715514	-998.9517336	-1000.4369080
		C_{2v} #2	-998.4710949	-998.9513092	-1000.4365180
		C_2	-998.4715515	-998.9517336	-1000.4369080
		C_s #1	-998.4805975	-998.9609777	-1000.4445655
		C_s #2	-998.5068496	-998.9892149	-1000.4726135
		C_s #3	-998.5007433	-998.9799794	-1000.4627802
		C_s #4	-998.4775307	-998.9578086	-1000.4424300
		C_1	-998.5068498	-998.9892148	-1000.4726596

2	2	D_{2h} #1	-1074.4980206	-1075.1680827	-1076.8627601
		D_{2h} #2	-1074.4840185	-1075.1539362	-1076.8497236
		C_{2v} #1	-1074.5524941	-1075.2269678	-1076.9208179
		C_{2v} #2	-1074.5028271	-1075.1737911	-1076.8681788
2	3	D_{3h} #1	-1150.5205579	-1151.3790010	-1153.2854951
		D_{3h} #2	-1150.5427828	-1151.4026431	-1153.3079690
		C_{3v} #1	-1150.5462866	-1151.4110455	-1153.3165141
		C_{3v} #2	-1150.5278634	-1151.3925049	-1153.3026736
		C_3	-1150.5462888	-1151.4120305	-1153.3198888
		C_s	-1150.5762755	-1151.4420402	-1153.3477481
		C_1	Dissociation	-1151.4479673	-1153.3531185
2	4	D_{4h} #1	-1226.5760328	-1227.6247131	-1229.7395827
		D_{4h} #2	-1226.5478508	-1227.5950496	-1229.7109859
		C_{4h}	-1226.5779918	-1227.6297931	-1229.7481746
		D_{2d}	-1226.5854548	-1227.6411611	-1229.7558943
		C_{4v}	-1226.5821883	-1227.6373437	-1229.7517676
		C_{2v}	-1226.5924250	-1227.6476763	-1229.7636235
		C_s	-1226.5987136	-1227.6566048	-1229.7715643
		C_1	-1226.6105977	-1227.6711764	-1229.7862771
3	0	D_{3h}	-1382.0480339	-1382.4710930	-1384.3491067
		C_{3v}	-1382.0795201	-1382.5000609	-1384.3758886
3	1	C_{2v} #1	-1458.0739478	-1458.6853974	-1460.7716770
		C_{2v} #2	-1458.0610873	-1458.6708328	-1460.7584618
		C_s #1	-1458.1093569	-1458.7231267	-1460.8101127
		C_s #2	-1458.0972614	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.1182873	-1534.9237761	-1537.2211954
		C_{2v} #2	-1534.1300711	-1534.9352669	-1537.2321350
		C_2	-1534.1371644	-1534.9464339	-1537.2441472
		C_s #1	-1534.1378495	-1534.9474461	-1537.2452144
		C_s #2	-1534.1322602	-1534.9372707	-1537.2343541
3	3	C_{3v} #1	-1610.1341764	-1611.1261020	-1613.6330523
		C_{3v} #2	-1610.1725388	-1611.1745977	-1613.6836568
		C_{3v} #3	-1610.1369465	-1611.1342496	-1613.6434433
		C_{3v} #4	-1610.1434385	-1611.1270019	-1613.6368223
		C_{2v} #1	-1610.1420476	-1611.1375110	-1613.6418955
		C_{2v} #2	-1610.1496585	-1611.1448233	-1613.6538719
		C_{2v} #3	-1610.1260580	-1611.1183524	-1613.6254170
		C_{2v} #4	-1610.1418933	-1611.1363834	-1613.6450923
		C_2	-1610.1607381	-1611.1604281	-1613.6687108
		C_s	-1610.1665942	-1611.1655886	-1613.6733779
4	0	D_{4h}	-1841.5171539	-1842.0648079	-1844.5402487
		T_d	-1841.5492869	-1842.0983742	-1844.5754918
		C_{4v}	-1841.5232741	-1842.0724743	-1844.5482897

4	1	C_{2v}	-1917.5665573	-1918.3064028	-1920.9923115
		C_s #1	-1917.5812182	-1918.3251134	-1921.0128140
		C_s #2	-1917.5876521	-1918.3285836	-1921.0153264
4	2	D_{2h}	-1993.5607540	-1994.4854936	-1997.3800426
		C_{2v} #1 (cis)	-1993.6110317	-1994.5463203	-1997.4416727
		C_{2v} #2	-1993.5705391	-1994.4978270	-1997.3932230
		C_{2h} (trans)	-1993.5943885	-1994.5285479	-1997.4262034
		C_2 #1	-1993.6082896	-1994.5539520	-1997.4506851
		C_2 #2	-1993.5854650	-1994.5154356	-1997.4102592
		C_s #1	-1993.6126276	-1994.5457340	-1997.4447801
		C_s #2	-1993.6181312	Dissociation	Dissociation

Detached structure

Table 4A.2: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ LANL2DZ**	**MP2/6-31G*/ LANL2DZ**	**B3LYP/6-31G*/ LANLDZ**
1	0	$C_{\infty v}$	-462.6238064	-462.7825147	-463.4413000
1	1	C_{2v}	-538.6981915	-539.0526257	-539.9257604
		C_s	-538.7303017	-539.0834241	-539.9554246
1	2	C_{2v} #1	-614.7814370	-615.3290713	-616.4116424
		C_{2v} #2	-614.7934783	-615.3420292	-616.4232470
		C_s	-614.8020588	-615.3508366	-616.4313693
1	3	C_{3v} #1	-690.8400762	-691.5826643	-692.8761797
		C_{3v} #2	-690.8585831	-691.6033028	-692.8939526
		C_3	-690.7874179	-691.5155026	N/A
		C_s	N/A	N/A	N/A
1	4	C_{4v} #1	-766.8085036	-767.7241245	-769.2297990
		C_{4v} #2	-766.8270644	-767.7444448	-769.2474844
		C_4	N/A	-767.7447448	-769.2485855
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.8510779	-843.9573615	-845.6721514
		C_{2v} #2	-842.8328413	-843.9379039	-845.6556403
		C_{2v} #3	-842.8462681	-843.9532473	-845.6694546
		C_{2v} #4	-842.8451662	-843.9520552	-845.6682080
		C_{2v} #5	-842.8511004	-843.9573996	-845.6720788
		C_2 #1	-842.8511004	-843.9581392	N/A
		C_2 #2	N/A	N/A	-845.6741180
		C_s #1	-842.8537700	-843.9654063	N/A
		C_s #2	N/A	N/A	-845.6728028
		C_1	-842.8599761	-843.9709428	-845.6852351
2	0	$D_{\infty h}$	-922.3682473	-922.6619896	-923.9338734
		C_{2v}	-922.4132715	-922.7036660	-923.9724216
2	1	C_{2v} #1	-998.4315822	-998.9099855	-1000.3905539
		C_{2v} #2	-998.4312758	-998.9097322	-1000.3903719
		C_2	-998.4315822	-998.9099855	-1000.3905539
		C_s #1	-998.4372249	-998.9166563	-1000.3962438
		C_s #2	-998.4562761	-998.9380675	-1000.4165065
		C_s #3	-998.4504354	-998.9295339	-1000.4076674
		C_s #4	-998.4348466	-998.9140779	-1000.3945124
		C_1	-998.4562761	-998.9380675	-1000.4165018
2	2	D_{2h} #1	-1074.4461275	-1075.1153516	-1076.8063036

		D_{2h} #2	-1074.4331256	-1075.1020027	-1076.7940796
		C_{2v} #1	-1074.4920342	-1075.1654069	-1076.8540390
		C_{2v} #2	-1074.4518259	-1075.1217122	-1076.8120129
2	3	D_{3h} #1	-1150.4602268	-1151.3168735	-1153.2184915
		D_{3h} #2	-1150.5427828	-1151.3386917	-1153.2390924
		C_{3v} #1	-1150.4843144	-1151.3482891	-1153.2485686
		C_{3v} #2	-1150.4666646	-1151.3293443	-1153.2337254
		C_3	-1150.4843143	-1151.3490905	-1153.2511372
		C_s	-1150.5119239	-1151.3750889	-1153.2755289
		C_1	-1150.5801836	-1151.3791923	-1153.2790947
2	4	D_{4h} #1	-1226.5072681	-1227.5539464	-1229.6635302
		D_{4h} #2	-1226.4823808	-1227.5274573	-1229.6384628
		C_{4h}	-1226.5085123	-1227.5578345	-1229.6697266
		D_{2d}	-1226.5157620	-1227.5689343	-1229.6787020
		C_{4v}	-1226.5138233	-1227.5680218	-1229.6767333
		C_{2v}	-1226.5214992	-1227.5768431	-1229.6876988
		C_s	-1226.5270703	-1227.5824817	-1229.6915862
		C_1	-1226.5374047	-1226.6033105	-1229.7048678
3	0	D_{3h}	-1382.0044608	-1382.4269536	-1384.3000376
		C_{3v}	-1382.0285017	-1382.4487720	-1384.3196816
3	1	C_{2v} #1	-1458.0234168	-1458.6338764	-1460.7159252
		C_{2v} #2	-1458.0132487	-1458.6213658	-1460.7047565
		C_s #1	-1458.0548651	-1458.6663470	-1460.7483728
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.0598895	-1534.8647004	-1537.1570071
		C_{2v} #2	-1534.0640554	-1534.8665207	-1537.1585216
		C_2	-1534.0729770	-1534.8796010	-1537.1723594
		C_s #1	-1534.0740173	-1534.8815795	-1537.1738786
		C_s #2	-1534.0694618	-1534.8710598	-1537.1629990
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-1610.1074983	-1611.1035845	-1613.6074184
		C_{3v} #3	Dissociation	-1611.1342496	Dissociation
		C_{3v} #4	-1610.0937818	-1611.0767616	-1613.5818474
		C_{2v} #1	-1610.0751483	-1611.0717886	-1613.5735557
		C_{2v} #2	-1610.0807262	-1611.0734979	-1613.5763362
		C_{2v} #3	-1610.0606709	-1611.0505580	-1613.5522892
		C_{2v} #4	-1610.0738492	-1611.0644919	-1613.5676863
		C_2	-1610.0916110	-1611.0880778	-1613.5905410
		C_s	-1610.0979257	-1611.0936127	-1613.5919868
4	0	D_{4h}	-1841.4693275	-1842.0156990	-1844.4870987
		T_d	-1841.4985222	-1842.0469856	-1844.5177752
		C_{4v}	-1841.4707274	-1842.0178042	-1844.4894803
4	1	C_{2v}	-1917.5098917	-1918.2488529	-1920.9289599

		C_s #1	-1917.5326846	-1918.2721359	-1920.9538975
		C_s #2	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-1993.4983457	-1994.4213917	-1997.3099438
		C_{2v} #1 (cis)	-1993.5492691	-1994.4825060	-1997.3722012
		C_{2v} #2	-1993.5090706	-1994.4349272	-1997.2879240
		C_{2h} (trans)	-1993.5305788	-1994.4621371	-1997.3538367
		C_2 #1	-1993.5531031	-1994.4909884	-1997.3822998
		C_2 #2	-1993.5231555	-1994.4519636	-1997.3413602
		C_s #1	-1993.5622084	-1994.4896628	-1997.3830406
		C_s #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 4A.3: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ SDD**	**MP2/6-31G*/ SDD**	**B3LYP/6-31G*/ SDD**
1	0	$C_{\infty v}$	-462.5973792	-462.7657747	-463.4146803
1	1	C_{2v}	-538.7464374	-539.1270281	-539.9788676
		C_s	-538.7803310	-539.1596186	-540.0102489
1	2	C_{2v} #1	-614.8533884	-615.4449809	-616.4905049
		C_{2v} #2	-614.8670245	-615.4601260	-616.5036500
		C_s	-614.8761032	-615.4697452	-616.5121530
1	3	C_{3v} #1	-690.9346911	-691.7392861	-692.9794689
		C_{3v} #2	-690.9558456	-691.7639502	-693.0000672
		C_3	-690.7471327	-691.4861444	N/A
		C_s	N/A	N/A	N/A
1	4	C_{4v} #1	-766.7692081	-767.6965018	-769.1914237
		C_{4v} #2	-766.7849448	-767.7134834	-769.2060488
		C_4	N/A	-767.7139378	-769.2071988
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.8093113	-843.9256242	-845.6306443
		C_{2v} #2	-842.7936329	-843.9092521	-845.6166609
		C_{2v} #3	-842.8049647	-843.9219909	-845.6280708
		C_{2v} #4	-842.8039708	-843.9208873	-845.6269893
		C_{2v} #5	-842.8093286	-843.9256684	-845.6307530
		C_2 #1	-842.8093286	-843.9266011	N/A
		C_2 #2	N/A	N/A	-845.6326890
		C_s #1	-842.8113056	-843.9328635	N/A
		C_s #2	N/A	N/A	-845.6313902
		C_1	-842.8163569	-843.9347438	-845.6438213
2	0	$D_{\infty h}$	-922.3375847	-922.6441503	-923.9013176
		C_{2v}	-922.3800021	-922.6871475	-923.9393847
2	1	C_{2v} #1	-998.3983179	-998.8926952	-1000.3574911
		C_{2v} #2	-998.3979617	-998.8923453	-1000.3570939
		C_2	-998.3983179	-998.8926952	-1000.3574911
		C_s #1	-998.4034095	-998.8990290	-1000.3625428
		C_s #2	-998.4179629	-998.9164152	-1000.3793307
		C_s #3	-998.4126755	-998.9086016	-1000.3708528
		C_s #4	-998.4011595	-998.8967635	-1000.3609388
		C_1	-998.4179630	-998.9164152	-1000.3793377
2	2	D_{2h} #1	-1074.4088021	-1075.0907069	-1076.7686302

		D_{2h} #2	-1074.3971989	-1075.0787181	-1076.7572655
		C_{2v} #1	-1074.4513038	-1075.1408234	-1076.8145740
		C_{2v} #2	-1074.4137288	-1075.0963840	-1076.7740576
2	3	D_{3h} #1	-1150.4226413	-1151.2912600	-1153.1805207
		D_{3h} #2	-1150.4803961	-1151.3100803	-1153.1985531
		C_{3v} #1	-1150.4455109	-1151.3201897	-1153.2104161
		C_{3v} #2	-1150.4295140	-1151.3042663	-1153.1969171
		C_3	-1150.4455410	-1151.3218440	-1153.2136929
		C_s	-1150.4713757	-1151.3500456	-1153.2360887
		C_1	-1150.5144046	-1151.3616125	-1153.2490549
2	4	D_{4h} #1	-1226.4664387	-1227.5243141	-1229.6224761
		D_{4h} #2	-1226.4441041	-1227.5004471	-1229.5997568
		C_{4h}	-1226.4676028	-1227.5291710	-1229.6289461
		D_{2d}	-1226.4757045	-1227.5385679	-1229.6390509
		C_{4v}	-1226.4742969	-1227.5384123	-1229.6381048
		C_{2v}	-1226.4808505	-1227.5489008	-1229.6473189
		C_s	-1226.4840436	-1227.6566048	-1229.6597335
		C_1	Dissociation	Dissociation	Dissociation
3	0	D_{3h}	-1381.9695920	-1382.4055875	-1384.2648421
		C_{3v}	-1381.9910999	-1382.4309241	-1384.2835391
3	1	C_{2v} #1	-1457.9871685	-1458.6108589	-1460.6792876
		C_{2v} #2	-1457.9783172	-1458.6014678	-1460.6694694
		C_s #1	-1458.0177497	-1458.6487757	-1460.7127389
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.0237949	-1534.8413849	-1537.1205337
		C_{2v} #2	-1534.0245176	-1534.8433338	-1537.1197307
		C_2	-1534.0346151	-1534.8566636	-1537.1349942
		C_s #1	-1534.0355889	-1534.8583027	-1537.1362373
		C_s #2	-1534.0290657	-1534.8480260	-1537.1244490
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-1610.0710214	-1611.0851746	-1613.5720303
		C_{3v} #3	Dissociation	-1611.0778067	-1613.5467747
		C_{3v} #4	-1610.0562227	-1611.0582977	-1613.5459229
		C_{2v} #1	-1610.0362050	-1611.0410842	-1613.5331852
		C_{2v} #2	-1610.0417688	-1611.0467372	-1613.5380134
		C_{2v} #3	-1610.0232207	-1611.0248439	-1613.5154772
		C_{2v} #4	-1610.0347755	-1611.0403885	-1613.5289076
		C_2	-1610.0522747	-1611.0611010	-1613.5515230
		C_s	-1610.0550299	-1611.0648456	-1613.5551575
4	0	D_{4h}	-1841.4347768	-1841.9964148	-1844.4523945
		T_d	-1841.4633326	-1842.0250939	-1844.4830471
		C_{4v}	-1841.4351545	-1841.9989237	-1844.4538705
4	1	C_{2v}	-1917.4735705	-1918.2237151	-1920.8925331

		C_s #1	-1917.4973796	Dissociation	-1920.9191257
		C_s #2	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-1993.4610258	-1994.3966324	-1997.2727398
		C_{2v} #1 (cis)	-1993.5096465	-1994.4548418	-1997.3336600
		C_{2v} #2	-1993.4717569	-1994.4086793	-1997.4448865
		C_{2h} (trans)	-1993.4954973	-1994.4408167	-1997.3192326
		C_2 #1	-1993.5155435	-1994.4653683	-1997.3453414
		C_2 #2	-1993.4851103	-1994.4236440	-1997.3031713
		C_s #1	Dissociation	-1994.4683675	-1997.3483942
		Cs #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 4A.4: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ CEP-121G**	**MP2/6-31+G*/ CEP-121G**	**B3LYP/6-31+G*/ CEP-121G**
1	0	$C_{\infty v}$	-462.6504538	-462.8093870	-463.4709860
1	1	C_{2v}	-538.6606493	-539.0090718	-539.8810267
		C_s	-538.6881766	-539.0359810	-539.9073856
1	2	C_{2v} #1	-614.7281482	-615.2650023	-616.3485704
		C_{2v} #2	-614.7374032	-615.2746624	-616.3573231
		C_s	-614.7444350	-615.2820114	-616.3643378
1	3	C_{3v} #1	-690.7722967	-691.4987314	-692.7944254
		C_{3v} #2	-690.7874179	-691.5155026	-692.8090352
		C_3	-690.8585831	-691.6033028	N/A
		C_s	-690.8585830	-691.6049015	N/A
1	4	C_{4v} #1	-766.8885721	-767.8273539	-769.3279733
		C_{4v} #2	-766.9124529	-767.8547677	-769.3514324
		C_4	N/A	N/A	N/A
		C_s	N/A	N/A	-769.2061280
		C_1	N/A	N/A	-769.3171289
1	5	C_{2v} #1	-842.9443740	-844.0826564	-845.7904660
		C_{2v} #2	-842 .9213146	-844.0567620	-845.7679605
		C_{2v} #3	-842.9384855	-844.0768536	-845.7855361
		C_{2v} #4	-842.9368891	-844.0750691	-845.7837124
		C_{2v} #5	-842.9443904	-844.0826693	-845.7902796
		C_2 #1	-842.9443904	-844.0826694	N/A
		C_2 #2	N/A	N/A	-845.7905081
		C_s #1	-842.9487833	-844.0892877	N/A
		C_s #2	N/A	N/A	-845.7917861
		C_1	-842.9502465	-844.0934920	-845.7983028
2	0	$D_{\infty h}$	-922.4039478	-922.7017602	-923.9745972
		C_{2v}	-922.4544124	-922.7480020	-924.0188882
2	1	C_{2v} #1	-998.4810762	-998.9707183	-1000.4521737
		C_{2v} #2	-998.4803600	-998.9698649	-1000.4512505
		C_2	-998.4810763	-998.9707183	-1000.4521737
		C_s #1	-998.4896467	-998.9795627	-1000.4591700
		C_s #2	-998.5127851	-999.0033836	-1000.4812025
		C_s #3	-998.5077488	-998.9967959	-1000.4743354
		C_s #4	-998.4855287	-998.9747100	-1000.4548876
		C_1	-998.5127851	-999.0033835	-1000.4812261
2	2	D_{2h} #1	-1074.5120613	-1075.1990559	-1076.8867557

		D_{2h} #2	-1074.4961513	-1075.1812252	-1076.8712644
		C_{2v} #1	-1074.5620595	-1075.2504240	-1076.9355301
		C_{2v} #2	-1074.5167611	-1075.2039631	-1076.8919474
2	3	D_{3h} #1	-1150.5376378	-1151.4165549	-1153.3159325
		D_{3h} #2	-1150.4403021	-1151.4441874	-1153.3402547
		C_{3v} #1	-1150.5647243	-1151.4508719	-1153.3476253
		C_{3v} #2	-1150.5423820	-1151.4259799	-1153.3249810
		C_3	-1150.5647243	-1151.4508719	-1153.2136929
		C_s	-1150.5907805	-1151.4758259	-1153.3704748
		C_1	-1150.5955107	-1151.4829262	-1153.3751633
2	4	D_{4h} #1	-1226.6033251	-1227.6830037	-1229.7852505
		D_{4h} #2	-1226.5718806	-1227.6464383	-1229.7530526
		C_{4h}	-1226.6037094	-1227.6835852	-1229.7875359
		D_{2d}	-1226.6104225	-1227.6938028	-1229.7974450
		C_{4v}	-1226.6074686	-1227.6910312	-1229.7939590
		C_{2v}	-1226.6134691	-1227.6966380	-1229.7982233
		C_s	-1226.6194244	-1227.5824817	-1229.8056893
		C_1	-1226.6296812	-1227.5945543	-1229.6777511
3	0	D_{3h}	-1382.0562895	-1382.4873647	-1384.3623728
		C_{3v}	-1382.0866317	-1382.5144980	-1384.3875091
3	1	C_{2v} #1	-1458.0887019	-1458.7163690	-1460.7969083
		C_{2v} #2	-1458.0751717	-1458.7001315	-1460.7829401
		C_s #1	-1458.1212701	-1458.6487757	-1460.8297135
		C_s #2	-1458.1102723	-1458.7350365	Dissociation
3	2	C_{2v} #1	-1534.1384146	-1534.9653018	-1537.2550385
		C_{2v} #2	-1534.1454990	-1534.9705876	-1537.2574567
		C_2	-1534.1520582	-1534.9806244	-1537.2691261
		C_s #1	-1534.1526292	-1534.9812116	-1537.2697487
		C_s #2	-1534.1477764	-1534.9732938	-1537.2603996
3	3	C_{3v} #1	-1610.1341763	-1611.1769131	-1613.6737189
		C_{3v} #2	-1610.1923994	-1611.2197888	-1613.7167011
		C_{3v} #3	-1610.1629244	-1611.0595039	-1613.5467747
		C_{3v} #4	-1610.1722977	-1611.1816854	-1613.6884602
		C_{2v} #1	-1610.1673720	-1611.1885363	-1613.6854674
		C_{2v} #2	-1610.1727360	-1611.1963676	-1613.6917798
		C_{2v} #3	-1610.1508548	-1611.1724855	-1613.6682038
		C_{2v} #4	-1610.1633906	-1611.1837433	-1613.6812319
		C_2	-1610.1823327	-1611.2096515	-1613.7051275
		C_s	Dissociation	-1611.2119593	-1613.7060543
4	0	D_{4h}	-1841.5342592	-1842.0965707	-1844.5703458
		T_d	-1841.5670778	-1842.1311982	-1844.6047883
		C_{4v}	-1841.5386052	-1842.1026963	-1844.5760030
4	1	C_{2v}	-1917.5902233	-1918.3542282	-1921.0327068

		C_s #1	-1917.6026373	-1918.3678195	-1921.0535231
		C_s #2	-1917.6126395	-1918.3743816	-1921.0562162
4	2	D_{2h}	-1993.5921993	-1994.5496670	-1997.4347219
		C_{2v} #1 (cis)	-1993.6369378	-1994.5993730	-1997.4846143
		C_{2v} #2	-1993.5998657	-1994.5594098	-1997.3810705
		C_{2h} (trans)	-1993.6194623	-1994.5808524	-1997.4690912
		C_2 #1	-1993.6392470	-1994.6062721	-1997.4932568
		C_2 #2	-1993.6151076	-1994.5776669	-1997.4618983
		C_s #1	-1993.6437961	-1994.6007173	Dissociation
		Cs #2	-1993.6429186	Dissociation	Dissociation

Detached structure

Table 4A.5: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ LANL2DZ**	**MP2/6-31+G*/ LANL2DZ**	**B3LYP/6-31+G*/ LANL2DZ**
1	0	$C_{\infty v}$	-462.6279655	-462.7877278	-463.4457535
1	1	C_{2v}	-538.6698650	-539.0245679	-539.8943731
		C_s	-538.6955685	-539.0497576	-539.9178681
1	2	C_{2v} #1	-614.7390639	-615.2873876	-616.3665498
		C_{2v} #2	-614.7493901	-615.2988669	-616.3764195
		C_s	-614.7553937	-615.3049924	-616.3817375
1	3	C_{3v} #1	-614.7553937	-691.5297757	-692.8193324
		C_{3v} #2	-690.7870558	-691.5483423	-692.8349371
		C_3	-690.8030934	-691.5483423	N/A
		C_s	-690.8030949	-691.5491881	N/A
1	4	C_{4v} #1	-766.8284130	-767.7664066	-769.2646047
		C_{4v} #2	-766.8478168	-767.7894671	-769.2833295
		C_4	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.8778675	-844.0144968	-845.7190307
		C_{2v} #2	-842.8583340	-843.9926439	-845.7001792
		C_{2v} #3	-842.8726257	-844.0093838	-845.7147750
		C_{2v} #4	-842.8713446	-844.0078030	-845.7132006
		C_{2v} #5	-842.8778837	-844.0145170	-845.7188896
		C_2 #1	-842.8778837	-844.0145170	N/A
		C_2 #2	N/A	N/A	-845.7190965
		C_s #1	-842.8798155	-844.0183857	N/A
		C_s #2	N/A	N/A	-845.7192568
		C_1	-842.8849649	-844.0234577	-845.7283251
2	0	$D_{\infty h}$	-922.3735883	-922.6714346	-923.9411055
		C_{2v}	-922.4171720	-922.7112580	-923.9781305
2	1	C_{2v} #1	-998.4419114	-998.9309204	-1000.4083252
		C_{2v} #2	-998.4413830	-998.9302834	-1000.4076500
		C_2	-998.4419114	-998.9309204	-1000.4083252
		C_s #1	-998.4472149	-998.9371293	-1000.4131279
		C_s #2	-998.4633398	-998.9543435	-1000.4280030
		C_s #3	-998.4583713	-998.9480977	-1000.4216415
		C_s #4	-998.4438174	-998.9328640	-1000.4094800
		C_1	-998.4633398	-998.9543435	-1000.4279633
2	2	D_{2h} #1	-1074.4630761	-1075.1497792	-1076.8344144

		D_{2h} #2	-1074.4479741	-1075.1326271	-1076.8197226
		C_{2v} #1	-1074.5032681	-1075.1916290	-1076.8728038
		C_{2v} #2	-1074.4676267	-1075.1548765	-1076.8390780
2	3	D_{3h} #1	-1150.4803355	-1151.3589487	-1153.2542484
		D_{3h} #2	-1150.5616637	-1151.3848993	-1153.2767896
		C_{3v} #1	-1150.5061613	-1151.3938188	-1153.2851766
		C_{3v} #2	-1150.4854419	-1151.3696196	-1153.2634980
		C_3	-1150.5061613	-1151.3938189	-1153.3477005
		C_s	-1150.5282091	-1151.4122941	-1153.3704749
		C_1	-1150.5383796	-1151.4247903	-1153.3066297
2	4	D_{4h} #1	-1226.5370399	-1227.6159775	-1229.7144278
		D_{4h} #2	-1226.5089685	-1227.5834008	-1229.6858954
		C_{4h}	-1226.5372612	-1227.6167376	-1229.7163647
		D_{2d}	-1226.5435006	-1227.6275975	-1229.7253675
		C_{4v}	-1226.5417315	-1227.6264329	-1229.7240240
		C_{2v}	-1226.5454530	-1227.6294881	-1229.7279176
		C_s	-1226.5508230	-1227.5510442	-1229.7326716
		C_1	Dissociation	-1227.7161528	-1229.8168297
3	0	D_{3h}	-1382.0136190	-1382.4447780	-1384.3154679
		C_{3v}	-1382.0359167	-1382.4644551	-1384.3335495
3	1	C_{2v} #1	-1458.0398235	-1458.6674759	-1460.7442560
		C_{2v} #2	-1458.0286602	-1458.6526005	-1460.7322786
		C_s #1	-1458.0691413	-1458.7484549	-1460.7732622
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.0821781	-1534.9099928	-1537.1955710
		C_{2v} #2	-1534.0826797	-1534.9065375	-1537.1904569
		C_2	-1534.0907353	-1534.9186528	-1537.2031371
		C_s #1	-1534.0920443	-1534.9214827	-1537.2049060
		C_s #2	-1534.0290657	-1534.9113955	-1537.1969582
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-1610.1324175	-1611.1533914	-1613.6472968
		C_{3v} #3	Dissociation	-1611.1901282	-1613.6878051
		C_{3v} #4	-1610.1219279	-1611.1318874	-1613.6349141
		C_{2v} #1	-1610.1029376	-1611.1289178	-1613.6215322
		C_{2v} #2	-1610.1067554	-1611.1293094	-1613.6207068
		C_{2v} #3	-1610.0875929	-1611.1077311	-1613.6062696
		C_{2v} #4	-1610.0986778	-1611.1179017	-1613.6112654
		C_2	-1610.1164646	-1611.1423307	-1613.6335134
		C_s	Dissociation	Dissociation	-1613.6345498
4	0	D_{4h}	-1841.4883591	-1842.0501832	-1844.5205187
		T_d	-1841.5167535	-1842.0798646	-1844.5495662
		C_{4v}	-1841.4886629	-1842.0509526	-1844.5214867
4	1	C_{2v}	-1917.5354529	-1918.2979907	-1920.9730209

		C_s #1	-1917.5569346	-1918.3181635	-1920.9978611
		C_s #2	Dissociation	-1918.3204520	Dissociation
4	2	D_{2h}	-1993.5325437	-1994.4878079	-1997.3702219
		C_{2v} #1 (cis)	-1993.5783269	-1994.5402931	-1997.4215118
		C_{2v} #2	-1993.5409448	-1994.4979350	-1997.3448167
		C_{2h} (trans)	-1993.5589019	-1994.5180007	-1997.4690913
		C_2 #1	-1993.5818630	-1994.5483128	-1997.4314635
		C_2 #2	-1993.5555389	-1994.5159825	-1997.3974325
		C_s #1	Dissociation	-1994.5485386	Dissociation
		Cs #2	-1993.5815670	Dissociation	Dissociation

Detached structure

Table 4A.6: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ SDD**	**MP2/6-31+G*/ SDD**	**B3LYP/6-31+G*/ SDD**
1	0	$C_{\infty v}$	-462.5985448	-462.7680210	-463.4162148
1	1	C_{2v}	-538.7176662	-539.0987739	-539.9474406
		C_s	-538.7452304	-539.1257957	-539.9724941
1	2	C_{2v} #1	-614.8107394	-615.4031600	-616.4451979
		C_{2v} #2	-614.8220271	-615.4162469	-616.4559680
		C_s	-614.8285819	-615.4232672	-616.4617586
1	3	C_{3v} #1	-690.8810504	-691.6860337	-692.9221817
		C_{3v} #2	-690.8986694	-691.7076603	-692.9394469
		C_3	-690.7602063	-691.5151129	N/A
		C_s	N/A	-691.5154182	N/A
1	4	C_{4v} #1	-766.7869067	-767.7348489	-769.2239276
		C_{4v} #2	-766.8029208	-767.7537507	-769.2391423
		C_4	N/A	N/A	-769.2391627
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.8335572	-843.9783881	-845.6750094
		C_{2v} #2	-842.8169452	-843.9593518	-845.6589512
		C_{2v} #3	-842.8289739	-843.9735361	-845.6713804
		C_{2v} #4	-842.8278352	-843.9720952	-845.6699678
		C_{2v} #5	-842.8335707	-843.9784082	-845.6749619
		C_2 #1	-842.8335707	-843.9784083	N/A
		C_2 #2	N/A	N/A	-845.6751781
		C_s #1	-842.8349561	-843.9819506	N/A
		C_s #2	N/A	N/A	-845.6751202
		C_1	-842.8401192	-843.9877917	-845.6836507
2	0	$D_{\infty h}$	-922.4525452	-922.6514870	-923.9073574
		C_{2v}	-922.3827713	-922.6937688	-923.9442677
2	1	C_{2v} #1	-998.4071779	-998.9112790	-1000.3738289
		C_{2v} #2	-998.4067245	-998.9107179	-1000.3732551
		C_2	-998.4071780	-998.9112790	-1000.3738289
		C_s #1	-998.4120233	-998.9175319	-1000.3783262
		C_s #2	-998.4242159	-998.9312288	-1000.3903881
		C_s #3	-998.4197512	-998.9255974	-1000.3843247
		C_s #4	-998.4089022	-998.9139082	-1000.3748870
		C_1	-998.4242160	-998.9312288	-1000.3903677
2	2	D_{2h} #1	-1074.4231927	-1075.1208329	-1076.7945896

		D_{2h} #2	-1074.4105233	-1075.1068333	-1076.7820191
		C_{2v} #1	-1074.4617336	-1075.1647474	-1076.8327882
		C_{2v} #2	-1074.4278503	-1075.1272950	-1076.7997718
2	3	D_{3h} #1	-1150.4412973	-1151.3308655	-1153.2154840
		D_{3h} #2	-1150.5025671	-1151.3521817	-1153.2349931
		C_{3v} #1	-1150.4646262	-1151.3605048	-1153.2443256
		C_{3v} #2	-1150.4457849	-1151.3392804	-1153.2244178
		C_3	-1150.4646261	-1151.3605931	-1153.2854474
		C_s	-1150.4867628	-1151.3842002	-1153.3032250
		C_1	-1150.4895919	-1151.3970961	-1153.5087244
2	4	D_{4h} #1	-1226.4927784	-1227.5797495	-1229.6704576
		D_{4h} #2	-1226.4686195	-1227.5524407	-1229.6457338
		C_{4h}	-1226.4930524	-1227.5813332	-1229.6728846
		D_{2d}	-1226.5002095	-1227.5910592	-1229.6828538
		C_{4v}	-1226.4988448	-1227.5907777	-1229.6821269
		C_{2v}	-1226.5027119	-1227.5981793	-1229.6870683
		C_s	-1226.5066929	-1227.7046686	-1229.6899073
		C_1	Dissociation	Dissociation	-1229.7414937
3	0	D_{3h}	-1381.9787848	-1382.4234034	-1384.2809890
		C_{3v}	-1381.9987220	-1382.4474283	-1384.2978611
3	1	C_{2v} #1	-1458.0030124	-1458.6435592	-1460.7076456
		C_{2v} #2	-1457.9935645	-1458.6318114	-1460.6974302
		C_s #1	-1458.0318297	-1458.6943126	-1460.7375831
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.0444477	-1534.8833173	-1537.1579198
		C_{2v} #2	-1534.0426545	-1534.8808151	-1537.1517721
		C_2	-1534.0516886	-1534.8927416	-1537.1653549
		C_s #1	-1534.0527053	-1534.8945921	-1537.1666210
		C_s #2	-1534.0481389	-1534.8868807	-1537.1582556
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-1610.0949268	-1611.1321228	-1613.6117346
		C_{3v} #3	Dissociation	-1611.1349689	-1613.6007079
		C_{3v} #4	-1610.0838812	-1611.1132629	-1613.5985813
		C_{2v} #1	-1610.0627490	-1611.0970040	-1613.5808302
		C_{2v} #2	-1610.0661998	-1611.0983041	-1613.5811164
		C_{2v} #3	-1610.0493311	-1611.0793927	-1613.5664661
		C_{2v} #4	-1610.0591342	-1611.0907693	-1613.5726170
		C_2	-1610.0760874	-1611.1116296	-1613.5939603
		C_s	-1610.0791272	Dissociation	-1613.5964950
4	0	D_{4h}	-1841.4544393	-1842.0313744	-1844.4869925
		T_d	-1841.4820614	-1842.0590167	-1844.5159275
		C_{4v}	-1841.4544521	-1842.0331826	-1844.4876205
4	1	C_{2v}	-1917.4993429	-1918.2733721	-1920.9376602

		C_s #1	-1917.5219292	Dissociation	-1920.9640119
		C_s #2	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-1993.4947140	-1994.4609543	-1997.3330942
		C_{2v} #1 (cis)	-1993.5383076	-1994.5102460	-1997.3830824
		C_{2v} #2	-1993.5036247	-1994.4718547	-1997.6120563
		C_{2h} (trans)	-1993.5229592	-1994.4943150	-1997.4032989
		C_2 #1	-1993.5437272	-1994.5202900	-1997.3942539
		C_2 #2	-1993.5174728	-1994.4882600	-1997.3600655
		C_s #1	-1993.5576661	-1994.5276716	Dissociation
		Cs #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 4A.7: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ CEP-121G**	**MP2/6-311+G*/ CEP-121G**	**B3LYP/6-311+G*/ CEP-121G**
1	0	$C_{\infty v}$	-462.6759889	-462.8426014	-463.4992514
1	1	C_{2v}	-538.6333770	-538.9910103	-539.8525950
		C_s	-538.6548463	-539.0138220	-539.8747291
1	2	C_{2v} #1	-614.6931485	-615.2415336	-616.3141586
		C_{2v} #2	-614.7010830	-615.2497745	-616.3216998
		C_s	-614.7057474	-615.2551499	-616.3269953
1	3	C_{3v} #1	-690.7345519	-691.4726345	-692.7575489
		C_{3v} #2	-690.7471327	-691.7639502	-692.7692311
		C_3	-690.9558456	-691.7639502	N/A
		C_s	N/A	-691.7651912	N/A
1	4	C_{4v} #1	-767.0052788	-768.0240592	-769.4551619
		C_{4v} #2	-767.0318907	-768.0561237	-769.4812922
		C_4	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-843.0850270	-844.3237247	-845.9435917
		C_{2v} #2	-843.0592362	-844.2933318	-845.9182650
		C_{2v} #3	-843.0779721	-844.3155173	-845.9375211
		C_{2v} #4	-843.0762747	-844.3134273	-845.9355128
		C_{2v} #5	-843.0850318	-844.3237388	-845.9433790
		C_2 #1	-843.0850318	-844.3237389	N/A
		C_2 #2	N/A	N/A	-845.9435934
		C_s #1	-843.0895076	-844.3305630	N/A
		C_s #2	N/A	N/A	-845.9449926
		C_1	-843.0905031	-844.3339605	-845.9510702
2	0	$D_{\infty h}$	-922.4239719	-922.7665886	-924.0307236
		C_{2v}	-922.5049289	-922.8142367	-924.0761700
2	1	C_{2v} #1	-998.5528900	-999.0768440	-1000.5330491
		C_{2v} #2	-998.5520436	-999.0759379	-1000.5319415
		C_2	-998.5528901	-999.0768440	-1000.5330491
		C_s #1	-998.5626606	-999.0870282	-1000.5409156
		C_s #2	-998.5858416	-999.1103058	-1000.5628279
		C_s #3	-998.5824969	-999.1058947	-1000.5577913
		C_s #4	-998.5575195	-999.0807409	-1000.5356273
		C_1	-998.5858416	-999.1103058	-1000.5628381
2	2	D_{2h} #1	-1074.6093349	-1075.3492674	-1076.9951116

		D_{2h} #2	-1074.5920097	-1075.3297854	-1076.9783095
		C_{2v} #1	-1074.6569998	-1075.3974432	-1077.0408655
		C_{2v} #2	-1074.6137574	-1075.3539780	-1077.0000283
2	3	D_{3h} #1	-1150.6567991	-1151.6064982	-1153.4479132
		D_{3h} #2	-1150.6826807	-1151.6365453	-1153.4741214
		C_{3v} #1	-1150.6859390	-1151.6432121	-1153.4814481
		C_{3v} #2	-1150.6592182	-1151.6125331	-1153.4543116
		C_3	-1150.6859390	-1151.6432121	-1153.2449433
		C_s	-1150.7067528	-1151.6621577	-1153.2630032
		C_1	-1150.7128803	-1151.6712388	-1153.5087244
2	4	D_{4h} #1	-1226.7464553	-1227.9158270	-1229.9427174
		D_{4h} #2	-1226.7133464	-1227.8766321	-1229.9088669
		C_{4h}	-1226.7464553	-1227.9158270	-1229.9429752
		D_{2d}	-1226.5435006	-1227.9255415	-1229.9547907
		C_{4v}	-1226.7505995	-1227.9239316	-1229.9512903
		C_{2v}	-1226.7547573	-1227.9267439	-1229.9534543
		C_s	-1226.7609511	-1227.6337994	-1229.9610239
		C_1	-1226.7696216	-1227.9456550	-1229.9701182
3	0	D_{3h}	-1382.1309755	-1382.5857714	-1384.4488230
		C_{3v}	-1382.1626095	-1382.6139735	-1384.4747735
3	1	C_{2v} #1	-1458.1874824	-1458.8574819	-1460.9089553
		C_{2v} #2	-1458.1723469	-1458.8395940	-1460.8933571
		C_s #1	-1458.2167695	-1458.6770580	-1460.9372103
		C_s #2	-1458.2080781	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.2600340	-1535.1466305	-1537.3915075
		C_{2v} #2	-1534.2651082	-1535.1502573	-1537.3924695
		C_2	-1534.2707506	-1535.1583355	-1537.4024513
		C_s #1	-1534.2714202	-1535.1591760	-1537.4033112
		C_s #2	-1534.2655435	-1535.1484789	-1537.3922554
3	3	C_{3v} #1	-1610.1568658	-1611.4001726	-1613.8315236
		C_{3v} #2	-1610.3219973	-1611.4363627	-1613.8721182
		C_{3v} #3	-1610.3030972	-1611.1163460	-1613.8447915
		C_{3v} #4	-1610.3108551	-1611.4002397	-1613.8434382
		C_{2v} #1	-1610.3129859	-1611.4163814	-1613.8482134
		C_{2v} #2	-1610.3156573	-1611.4177223	-1613.8515611
		C_{2v} #3	-1610.2951862	-1611.3952765	-1613.8300338
		C_{2v} #4	-1610.3047999	-1611.4034780	-1613.8397116
		C_2	-1610.3245401	-1611.4297234	-1613.8636950
		C_s	Dissociation	-1611.4313507	-1613.8639710
4	0	D_{4h}	-1841.6355030	-1842.2285983	-1844.6872383
		T_d	-1841.6689471	-1842.2637647	-1844.7221554
		C_{4v}	-1841.6402935	-1842.2358055	-1844.6934541
4	1	C_{2v}	-1917.7158061	-1918.5292855	-1921.1752858

		C_s #1	-1917.7250933	-1918.5391337	-1921.1886781
		C_s #2	-1917.6829946	-1918.5482442	-1921.1976822
4	2	D_{2h}	-1993.7406844	-1994.7657048	-1997.6015032
		C_{2v} #1 (cis)	-1993.7844008	-1994.8144383	-1997.6505811
		C_{2v} #2	-1993.7486924	-1994.7760623	-1997.5479833
		C_{2h} (trans)	-1993.7642780	-1994.7931208	-1997.3682278
		C_2 #1	-1993.7851823	-1994.8182433	-1997.6571618
		C_2 #2	-1993.7647559	-1994.7954853	-1997.6299860
		C_s #1	Dissociation	-1994.8130404	Dissociation
		Cs #2	-1993.7905640	Dissociation	Dissociation

Detached structure

Table 4A.8: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ LANL2DZ**	**MP2/6-311+G*/ LANL2DZ**	**B3LYP/6-311+G*/ LANL2DZ**
1	0	$C_{\infty v}$	-462.6536465	-462.8211889	-463.4744627
1	1	C_{2v}	-538.6396328	-539.0032788	-539.8632103
		C_s	-538.6592798	-539.0238100	-539.8823536
1	2	C_{2v} #1	-614.7017833	-615.2604587	-616.3298144
		C_{2v} #2	-614.7100577	-615.2697592	-616.3377284
		C_s	-614.7138887	-615.2736852	-616.3416384
1	3	C_{3v} #1	-690.7472628	-691.5005647	-692.7804924
		C_{3v} #2	-690.7602063	-691.5151129	-692.7929388
		C_3	-690.8986694	-691.7076603	N/A
		C_s	-690.8986724	-691.7084596	N/A
1	4	C_{4v} #1	-766.9442660	-767.9626846	-769.3910171
		C_{4v} #2	-766.9657439	-767.9895367	-769.4118478
		C_4	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-843.0167555	-844.2544223	-845.8706590
		C_{2v} #2	-842.9949219	-844.2284673	-845.8490903
		C_{2v} #3	-843.0105377	-844.2471762	-845.8653089
		C_{2v} #4	-843.0092102	-844.2453264	-845.8636174
		C_{2v} #5	-843.0167663	-844.2544443	-845.8704864
		C_2 #1	-843.0167664	-844.2544444	N/A
		C_2 #2	N/A	N/A	-845.8706797
		C_s #1	-843.0190066	-844.2584797	N/A
		C_s #2	N/A	N/A	-845.8709292
		C_1	-843.0245783	-844.2627512	-845.8795682
2	0	$D_{\infty h}$	-922.3928905	-922.7378838	-923.9993584
		C_{2v}	-922.4681794	-922.7779887	-924.0361776
2	1	C_{2v} #1	-998.5135797	-999.0368891	-1000.4890945
		C_{2v} #2	-998.5130526	-999.0364065	-1000.4883995
		C_2	-998.5135797	-999.0368890	-1000.4890945
		C_s #1	-998.5199486	-999.0445086	-1000.4948584
		C_s #2	-998.5365593	-999.0616065	-1000.5100401
		C_s #3	-998.5327834	-999.0570762	-1000.5049228
		C_s #4	-998.5159216	-999.0391358	-1000.4905972
		C_1	-998.5365593	-999.0616065	-1000.5099961
2	2	D_{2h} #1	-1074.5601080	-1075.3001062	-1076.9427525

		D_{2h} #2	-1074.5440990	-1075.2815747	-1076.9271516
		C_{2v} #1	-1074.5982104	-1075.3389070	-1076.9785098
		C_{2v} #2	-1074.5641773	-1075.3045783	-1076.9468822
2	3	D_{3h} #1	-1150.5987812	-1151.5487282	-1153.3857053
		D_{3h} #2	-1150.6220143	-1151.5762774	-1153.4094156
		C_{3v} #1	-1150.6254663	-1151.5840370	-1153.4174239
		C_{3v} #2	-1150.6011048	-1151.5554624	-1153.3918489
		C_3	-1150.6254664	-1151.5840371	-1153.4814483
		C_s	-1150.6438817	-1151.5988303	-1153.4988555
		C_1	-1150.6558072	-1151.6131005	-1153.4466208
2	4	D_{4h} #1	-1226.6784074	-1227.8476405	-1229.8704363
		D_{4h} #2	-1226.6491591	-1227.8134896	-1229.8406010
		C_{4h}	-1226.6784074	-1227.8476408	-1229.8709048
		D_{2d}	-1226.5002095	-1227.8580989	-1229.8812687
		C_{4v}	-1226.6828567	-1227.8568850	-1229.8796621
		C_{2v}	-1226.6857728	-1227.8568943	-1229.8791950
		C_s	-1226.6916601	-1227.5985430	-1229.8876811
		C_1	Dissociation	Dissociation	-1229.8938552
3	0	D_{3h}	-1382.0894778	-1382.5442856	-1384.4033457
		C_{3v}	-1382.1120935	-1382.5640068	-1384.4211606
3	1	C_{2v} #1	-1458.1391406	-1458.8093063	-1460.8570893
		C_{2v} #2	-1458.1263191	-1458.7927062	-1460.8434178
		C_s #1	-1458.1663160	-1458.8835565	-1460.8835840
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.2026504	-1535.0907540	-1537.3313528
		C_{2v} #2	-1534.2019517	-1535.0856705	-1537.3251903
		C_2	-1534.2094141	-1535.0966473	-1537.3368323
		C_s #1	-1534.2108287	-1535.1000581	-1537.3389363
		C_s #2	-1535.1484789	-1535.0680923	-1537.3316865
3	3	C_{3v} #1	Dissociation	-1611.3339990	Dissociation
		C_{3v} #2	-1610.2716660	-1611.3703338	-1613.8027277
		C_{3v} #3	Dissociation	-1611.4098106	-1613.7916430
		C_{3v} #4	-1610.2607121	-1611.3506235	-1613.7904103
		C_{2v} #1	-1610.2474318	-1611.3527084	-1613.7838198
		C_{2v} #2	-1610.2488915	-1611.3504855	-1613.7798778
		C_{2v} #3	-1610.2304581	-1611.3297040	-1613.7674782
		C_{2v} #4	-1610.2390836	-1611.3369914	-1613.7689039
		C_2	-1610.2583299	-1611.3627766	-1613.7517986
		C_s	Dissociation	Dissociation	-1613.7941471
4	0	D_{4h}	-1841.5912266	-1842.1837969	-1844.6392410
		T_d	-1841.6186655	-1842.2124602	-1844.6672110
		C_{4v}	-1841.5914479	-1842.1846427	-1844.6400849
4	1	C_{2v}	-1917.6609462	-1918.4733071	-1921.1158611

		C_s #1	-1917.6797951	-1918.4902190	-1921.1381753
		C_s #2	Dissociation	-1918.4938092	Dissociation
4	2	D_{2h}	-1993.6804791	-1994.7038134	-1997.5365513
		C_{2v} #1 (cis)	-1993.7262072	-1994.7559457	-1997.5879678
		C_{2v} #2	-1993.6892763	-1994.7146445	-1997.5105630
		C_{2h} (trans)	-1993.7040251	-1994.7305165	-1997.6330460
		C_2 #1	-1993.7279448	-1994.7610640	-1997.5959570
		C_2 #2	-1993.7053167	-1994.7344677	-1997.5660298
		C_s #1	Dissociation	-1994.7607647	Dissociation
		Cs #2	-1993.7288971	Dissociation	Dissociation

Detached structure

Table 4A.9: Total energies for all stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ SDD**	**MP2/6-311+G*/ SDD**	**B3LYP/6-311+G*/ SDD**
1	0	$C_{\infty v}$	-462.6243694	-462.8211889	-463.4449675
1	1	C_{2v}	-538.6874820	-539.0774358	-539.9160724
		C_s	-538.7087457	-539.0998109	-539.9366796
1	2	C_{2v} #1	-614.7733465	-615.3768753	-616.4080569
		C_{2v} #2	-614.7824150	-615.3873085	-616.4167949
		C_s	-614.7866192	-615.3917438	-616.4211213
1	3	C_{3v} #1	-690.8412339	-691.6580321	-692.8829824
		C_{3v} #2	-690.8554790	-691.6744811	-692.8968723
		C_3	-690.8554790	-691.6744811	N/A
		C_s	N/A	-691.6747389	N/A
1	4	C_{4v} #1	-766.9026452	-767.9325827	-769.3498558
		C_{4v} #2	-766.9204582	-767.9540956	-769.3670655
		C_4	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
1	5	C_{2v} #1	-842.9720544	-844.2185311	-845.8259391
		C_{2v} #2	-842.9535034	-844.1963371	-845.8075353
		C_{2v} #3	-842.9667100	-844.2124017	-845.8214140
		C_{2v} #4	-842.9655520	-844.2108554	-845.8199426
		C_{2v} #5	-842.9720631	-844.2185482	-845.8258703
		C_2 #1	-842.9720631	-842.9670725	N/A
		C_2 #2	N/A	N/A	-845.8259579
		C_s #1	-842.9737875	-844.2223273	N/A
		C_s #2	N/A	N/A	-845.8260953
		C_1	-842.9798978	-844.2274684	-845.8356452
2	0	$D_{\infty h}$	-922.3928905	-922.7189760	-923.9993584
		C_{2v}	-922.4346052	-922.7611024	-924.0024460
2	1	C_{2v} #1	-998.4798767	-999.0181815	-1000.4548306
		C_{2v} #2	-998.4794081	-999.0175974	-1000.4883995
		C_2	-998.4798767	-999.0181815	-1000.4548306
		C_s #1	-998.4853638	-999.0251551	-1000.4598181
		C_s #2	-998.4981650	-999.0391887	-1000.4724366
		C_s #3	-998.4945644	-999.0348105	-1000.4673135
		C_s #4	-998.4818183	-999.0391358	-1000.4905972
		C_1	-998.4981650	-999.0391887	-1000.4723862

2	2	D_{2h} #1	-1074.5203964	-1075.2716379	-1076.9025616
		D_{2h} #2	-1074.5068969	-1075.2563331	-1076.8890350
		C_{2v} #1	-1074.5572900	-1075.3127651	-1076.9383395
		C_{2v} #2	-1074.5246465	-1075.2774078	-1076.9071517
2	3	D_{3h} #1	-1150.5596680	-1151.5212531	-1153.3463260
		D_{3h} #2	-1150.5798424	-1151.5441239	-1153.3672597
		C_{3v} #1	-1150.5834827	-1151.5506075	-1153.3757132
		C_{3v} #2	-1150.5618879	-1151.5263610	-1153.3527374
		C_3	-1150.5834827	-1151.5506074	-1153.3757132
		C_s	-1150.6029932	-1151.5714866	-1153.4317089
		C_1	Dissociation	-1151.5861266	-1153.4466208
2	4	D_{4h} #1	-1226.6340485	-1227.8122360	-1229.8261546
		D_{4h} #2	-1226.6084603	-1227.7827343	-1229.7996525
		C_{4h}	-1226.6340486	-1227.8123161	-1229.8269636
		D_{2d}	-1226.6410158	-1227.8222804	-1229.8380476
		C_{4v}	-1226.6394401	-1227.8214172	-1229.8368975
		C_{2v}	-1226.6413903	-1227.8258834	-1229.8387225
		C_s	-1226.6470460	-1227.8299618	-1229.8441527
		C_1	-1226.6556218	Dissociation	Dissociation
3	0	D_{3h}	-1382.0555721	-1382.5240781	-1384.3688964
		C_{3v}	-1382.0760803	-1382.5479929	-1384.3855102
3	1	C_{2v} #1	-1458.1025596	-1458.7858233	-1460.8199952
		C_{2v} #2	-1458.0917777	-1458.7722986	-1460.8081519
		C_s #1	-1458.1300366	-1458.8170262	-1460.8477738
		C_s #2	Dissociation	Dissociation	Dissociation
3	2	C_{2v} #1	-1534.1649588	-1535.0642194	-1537.2934864
		C_{2v} #2	-1534.1623206	-1535.0609433	-1537.2860309
		C_2	-1534.1705959	-1535.0714031	-1537.2987430
		C_s #1	-1534.1718568	-1535.0736513	-1537.3003424
		C_s #2	-1534.1684229	-1535.0680923	-1537.2924744
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-1610.2349055	-1611.3493617	-1613.7665690
		C_{3v} #3	Dissociation	-1611.3344868	-1613.7916430
		C_{3v} #4	-1610.2235538	-1611.3327011	-1613.7539802
		C_{2v} #1	-1610.2064272	-1611.3213329	-1613.7424485
		C_{2v} #2	-1610.2080458	-1611.3199212	-1613.7396604
		C_{2v} #3	-1610.1915076	-1611.3011715	-1613.7269185

		C_{2v} #4	-1610.1996843	-1611.3106004	-1613.7296673
		C_2	-1610.2175137	-1611.3321538	-1613.7517986
		C_s	Dissociation	Dissociation	-1613.7529784
4	0	D_{4h}	-1841.5573788	-1842.1652724	-1844.6048491
		T_d	-1841.5843607	-1842.1925705	-1844.6332856
		C_{4v}	-1841.5573802	-1842.1670136	-1844.6053912
4	1	C_{2v}	-1917.6246474	-1918.4489724	-1921.0798579
		C_s #1	-1917.6451031	Dissociation	-1921.1039483
		C_s #2	Dissociation	-1918.472443	Dissociation
4	2	D_{2h}	-1993.6419929	-1994.676797	-1997.4983978
		C_{2v} #1 (cis)	-1993.6856792	-1994.7260926	-1997.5879678
		C_{2v} #2	-1993.6511497	-1994.6883794	-1997.5105630
		trans C_{2h}	-1993.6675187	-1994.7067118	-1997.5315252
		C_2 #1	-1993.6893590	-1994.7333762	-1997.5581507
		C_2 #2	-1993.6662517	-1994.7064016	-1997.5274505
		C_s #1	Dissociation	-1994.7406605	Dissociation
		Cs #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 4A.10: Pb-Cl and Pb-O bond lengths for stable geometries of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

		Optimized Bond Lengths (Å)						
n	**m**	**Point Group Symmetry**	**HF SDD/6-311+G***		**MP2 SDD/6-311+G***		**B3LYP/ SDD/6-311+G***	
			Pb-Cl	**Pb-O**	**Pb-Cl**	**Pb-O**	**Pb-Cl**	**Pb-O**
1	0	$C_{\infty v}$	2.379	N/A	2.379	N/A	2.390	N/A
1	1	C_s	2.421	2.489	2.420	2.467	2.433	2.465
1	2	C_s	2.464	2.526	2.465	2.494	2.478	2.503
1	3	C_{3v} #2	2.499	2.628	N/A	N/A	2.467	2.455
		C_3	2.499	2.627	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	2.500	2.513 2.604	N/A	N/A
1	4	C_{4v} #2	2.501	2.487	2.501	2.487	2.501	2.487
		C_4	N/A	N/A	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	N/A	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A	N/A	N/A
1	5	C_1	--	--	--	--	--	--
2	0	C_{2v}	2.505	N/A	2.498	N/A	2.518	N/A
2	1	C_1	2.553 2.553	2.579	2.546 2.546	2.539	2.572 2.571	2.555
2	2	C_{2v} #1	2.598	2.669	2.590	2.621	2.623	2.635
2	3	C_1	N/A	N/A	--	--	--	--
2	4	C_1	--	--	N/A	N/A	N/A	N/A
3	0	C_{3v}	2.645	N/A	2.621	N/A	2.659	N/A
4	0	T_d	2.937	N/A	2.877	N/A	2.911	N/A
4	1	C_s #1	--	--	N/A	N/A	--	--
4	1	C_s #2	N/A	N/A	--	--	N/A	N/A

Table 4A.11: Pb-Cl and Pb-O vibrational stretching frequencies of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n) calculated at HF/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	Cl/H_2O	Mixing
1	0	$C_{\infty v}$	361.0	σ_g	Cl	
1	1	C_s	244.9 339.0	a' a'	Cl/H_2O Cl/H_2O	
1	2	C_s	221.5 231.5 318.9	a" a' a'	H_2O Cl/H_2O Cl/H_2O	
1	3	C_{3v} #2	192.3 210.4 300.2	e a_1 a_1	H_2O Cl/H_2O Cl/H_2O	
		C_3	192.3 210.4 300.2	e a_1 a_1	H_2O Cl/H_2O Cl/H_2O	H_2O wagging
		C_s	N/A	N/A	N/A	N/A
1	4	C_{4v} #2	189.3 249.2 270.9 274.1 314.3 357.1	e e b_2 a_1 a_1 e	H_2O H_2O H_2O Cl/H_2O Cl/H_2O Cl/H_2O	H_2O twisting H_2O twisting H_2O twisting
		C_4	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A
1	5	C_1	-	-	-	-
2	0	C_{2v}	282.6 304.6	b_2 a_1	Cl Cl	
2	1	C_1	202.2 261.7 286.7	a a a	Cl/H_2O Cl Cl/ H_2O	H_2O rocking
2	2	C_{2v} #1	172.2 186.7 216.4 242.5 269.9	b_1 a_1 b_2 b_2 a_1	H_2O Cl/ H_2O Cl Cl Cl/H_2O	 H_2O rocking H_2O rocking
2	3	C_1	N/A	N/A	N/A	N/A
2	4	C_1	-	-	-	-
3	0	C_{3v}	216.4	e	Cl	

			250.9	a_1	Cl	
4	0	T_d	132.6 132.6 180.4	b_2 e a_1	Cl Cl Cl	
4	1	C_s #1	-	-	-	-
4	1	C_s #2	N/A	N/A	N/A	N/A

Table 4A.12: Pb-Cl and Pb-O vibrational stretching frequencies of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n) calculated at MP2/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	Cl/H_2O	Mixing
1	0	$C_{\infty v}$	363.4	σ_g	Cl	
1	1	C_s	260.3 342.2	a' a'	Cl/H_2O Cl/H_2O	
1	2	C_s	239.7 248.0 322.5	a" a' a'	H_2O Cl/H_2O Cl/H_2O	
1	3	C_{3v} #2	N/A	N/A	N/A	N/A
		C_3	N/A	N/A	N/A	N/A
		C_s	195.3 220.7 234.9 305.3	a" a' a' a'	H_2O Cl/H_2O Cl/H_2O Cl/H_2O	H_2O twisting H_2O twisting
1	4	C_{4v} #2	189.3 249.2 270.9 274.1 314.3 357.1	e e b_2 a_1 a_1 e	H_2O H_2O H_2O Cl/H_2O Cl/H_2O Cl/H_2O	H_2O twisting H_2O twisting H_2O twisting
		C_4	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A
1	5	C_1	-	-	-	-
2	0	C_{2v}	289.7 308.9	b_2 a_1	Cl Cl	
2	1	C_1	223.0 271.2 293.8	a a a	Cl/H_2O Cl Cl/ H_2O	 H_2O rocking
2	2	C_{2v} #1	194.4 203.1 204.2 253.1 278.7	b_1 b_2 a_1 b_2 a_1	H_2O Cl Cl/H_2O Cl Cl/H_2O	 H_2O rocking H_2O rocking
2	3	C_1	-	-	-	-
2	4	C_1	N/A	N/A	N/A	N/A
3	0	C_{3v}	231.4	e	Cl	

			260.4	a_1	Cl	
4	0	T_d	148.3 148.3 189.9	b_2 e a_1	Cl Cl Cl	
4	1	C_s #1	N/A	N/A	N/A	N/A
4	1	C_s #2	-	-	-	-

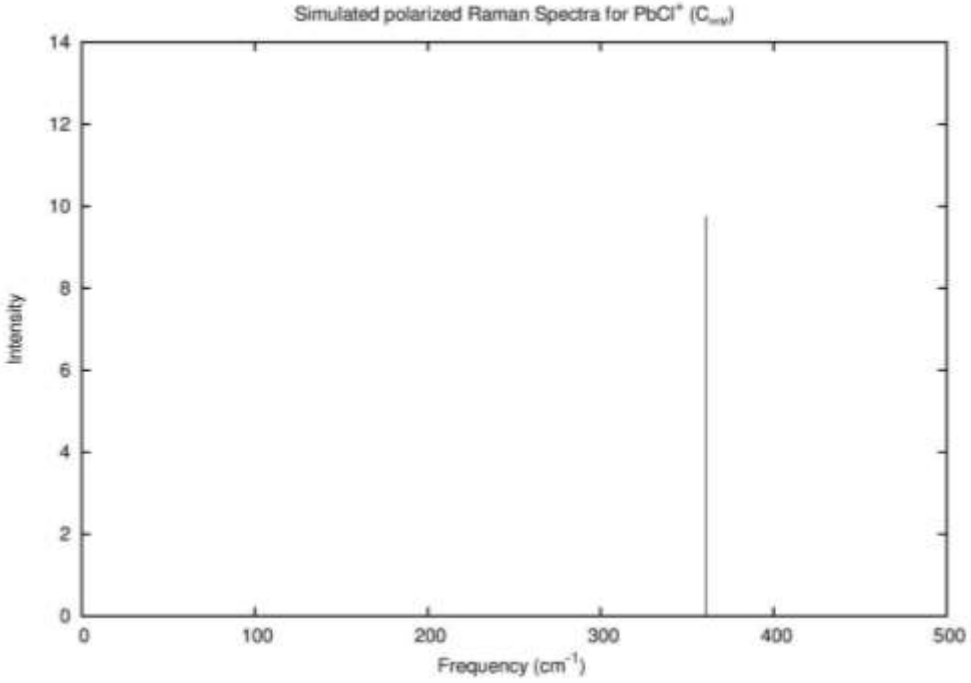
Table 4A.13: Pb-Cl and Pb-O vibrational stretching frequencies of $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n) calculated at B3LYP/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	Cl/H_2O	Mixing
1	0	$C_{\infty v}$	347.6	σ_g	Cl	
1	1	C_s	255.3 326.6	a' a'	Cl/H_2O Cl/H_2O	
1	2	C_s	226.6 239.2 307.3	a" a' a'	H_2O Cl/H_2O Cl/H_2O	H_2O twisting
1	3	C_{3v} #2	264.8 285.3 292.4	e e a_1	H_2O Cl/ H_2O Cl/ H_2O	 H_2O twisting H_2O twisting
		C_3	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	N/A	N/A
1	4	C_{4v} #2	189.3 249.2 270.9 274.1 314.3 357.1	e e b_2 a_1 a_1 e	H_2O H_2O H_2O Cl/ H_2O Cl/ H_2O Cl/ H_2O	H_2O twisting H_2O twisting H_2O twisting
		C_4	N/A	N/A	N/A	N/A
		C_s	N/A	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A
1	5	C_1	-	-	-	-
2	0	C_{2v}	272.5 292.9	b_2 a_1	Cl Cl	
2	1	C_1	209.9 253.5 277.2	a a a	Cl/H_2O Cl Cl/H_2O	 H_2O rocking
2	2	C_{2v} #1	183.8 193.7 226.3 242.2 261.8	b_1 a_1 b_2 b_2 a_1	H_2O Cl/H_2O Cl Cl Cl/H_2O	H_2O rocking H_2O rocking H_2O rocking
2	3	C_1	-	-	-	-
2	4	C_1	N/A	N/A	N/A	N/A
3	0	C_{3v}	211.6 241.7	e a_1	Cl Cl	
4	0	T_d	139.5	e	Cl	

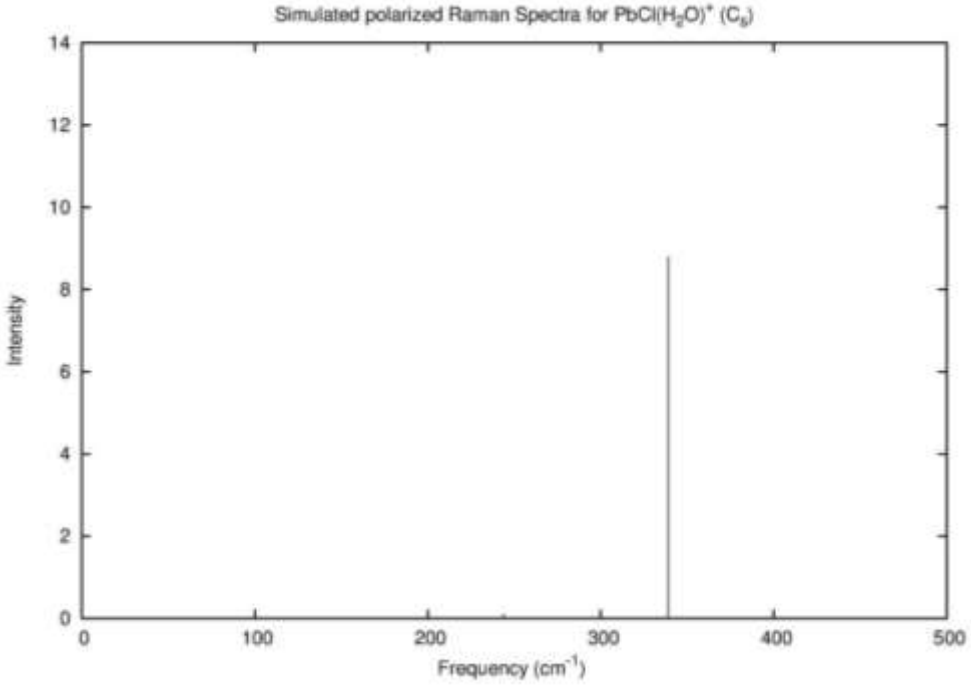
			139.5 139.5 177.7	e b_2 a_1	Cl Cl Cl	
4	1	C_s #1	-	-	-	-
4	1	C_s #2	N/A	N/A	N/A	N/A

Figure 4A-1: Simulated polarized Raman spectra for $[PbCl_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

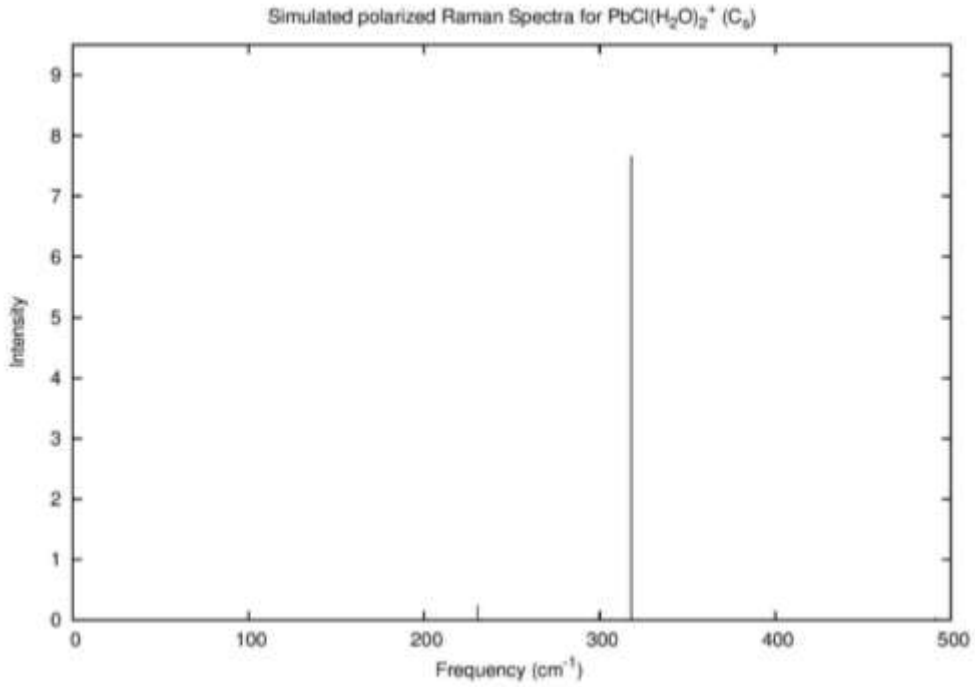
$[PbCl]^+$



$[PbCl(H_2O)]^+$



$[PbCl(H_2O)_2]^+$



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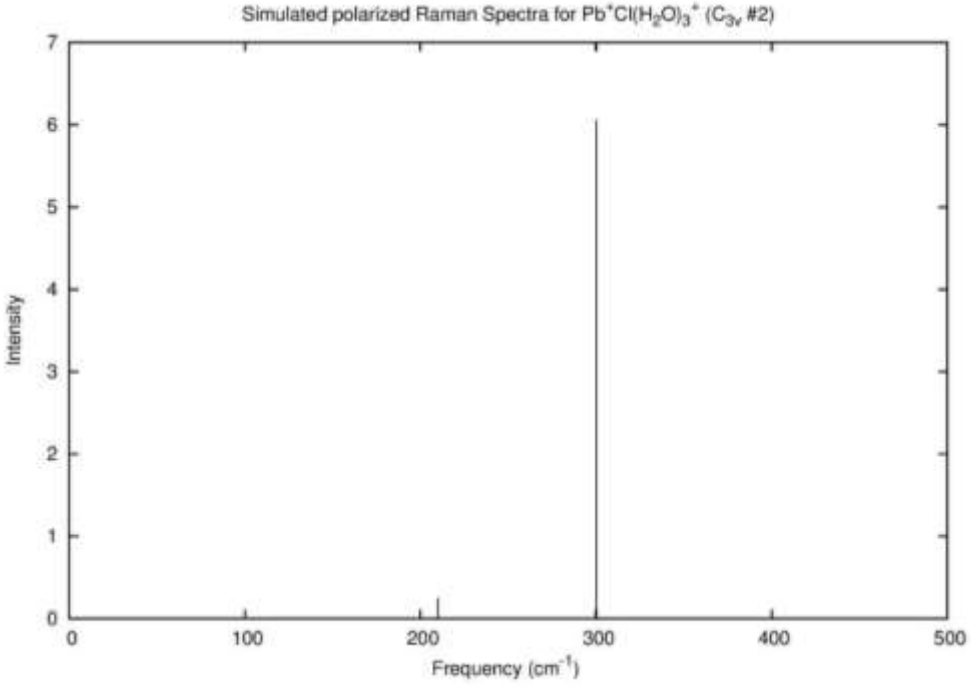

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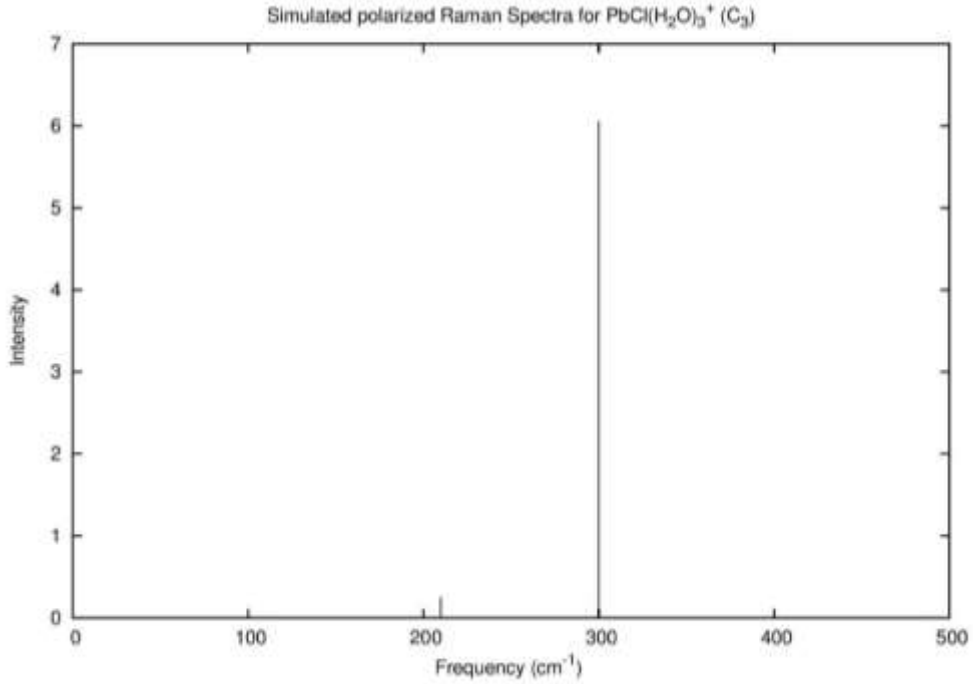

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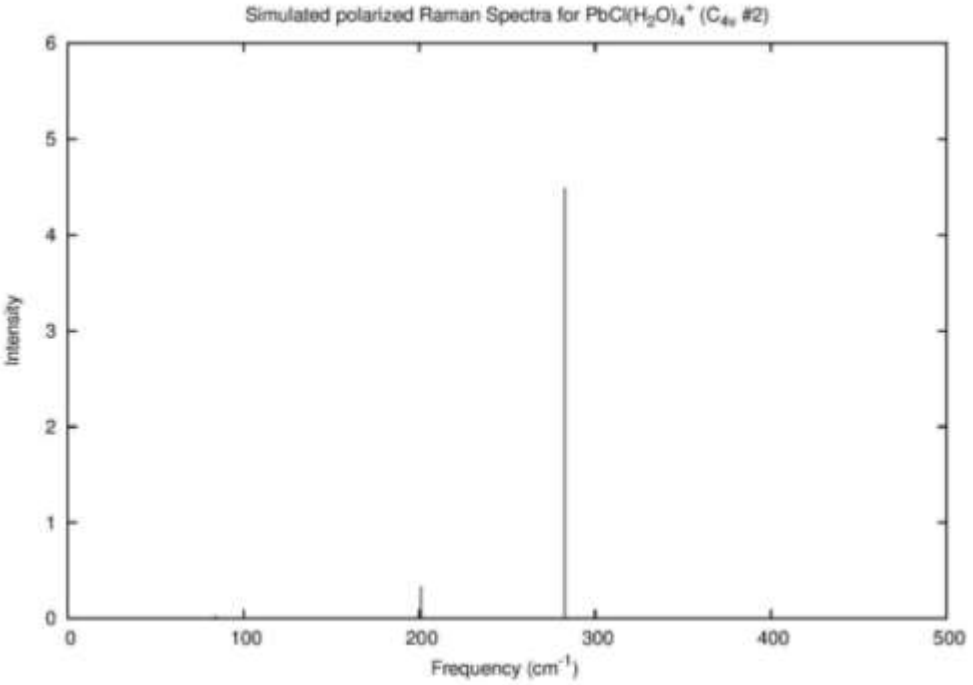
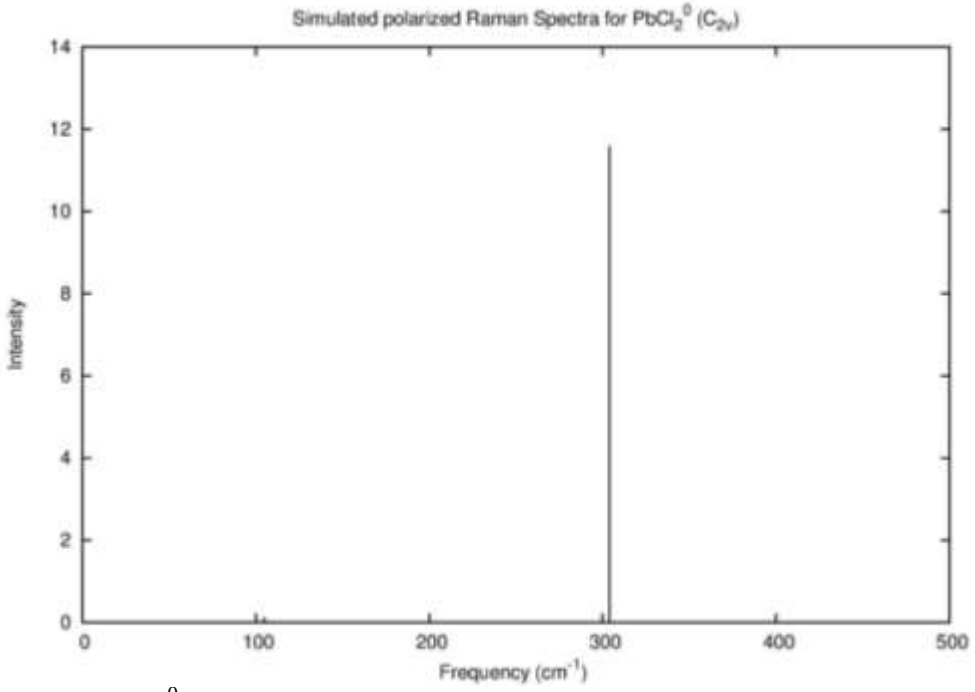
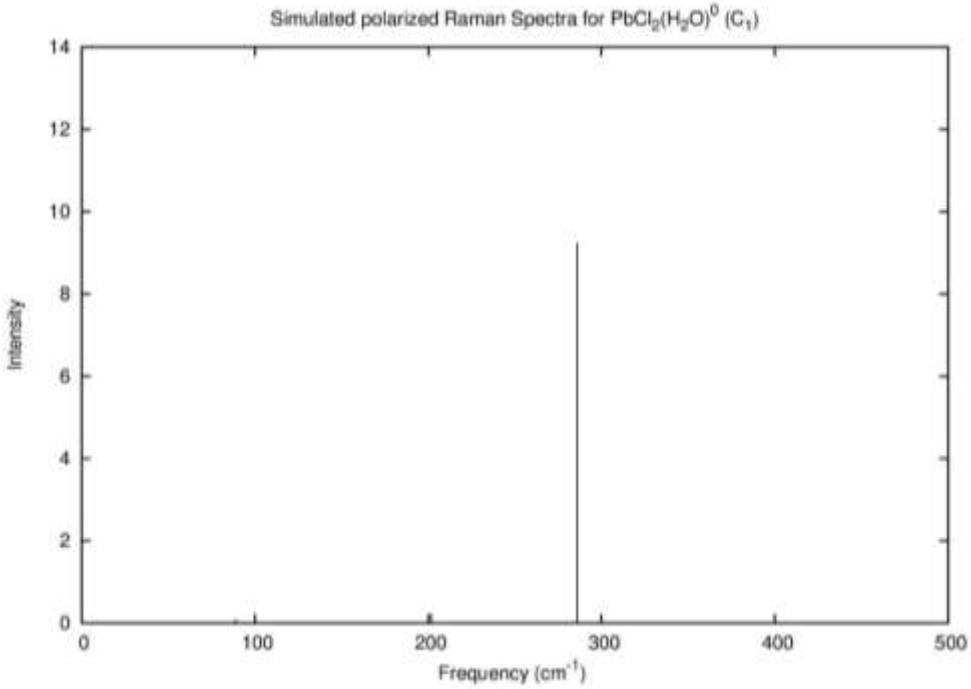


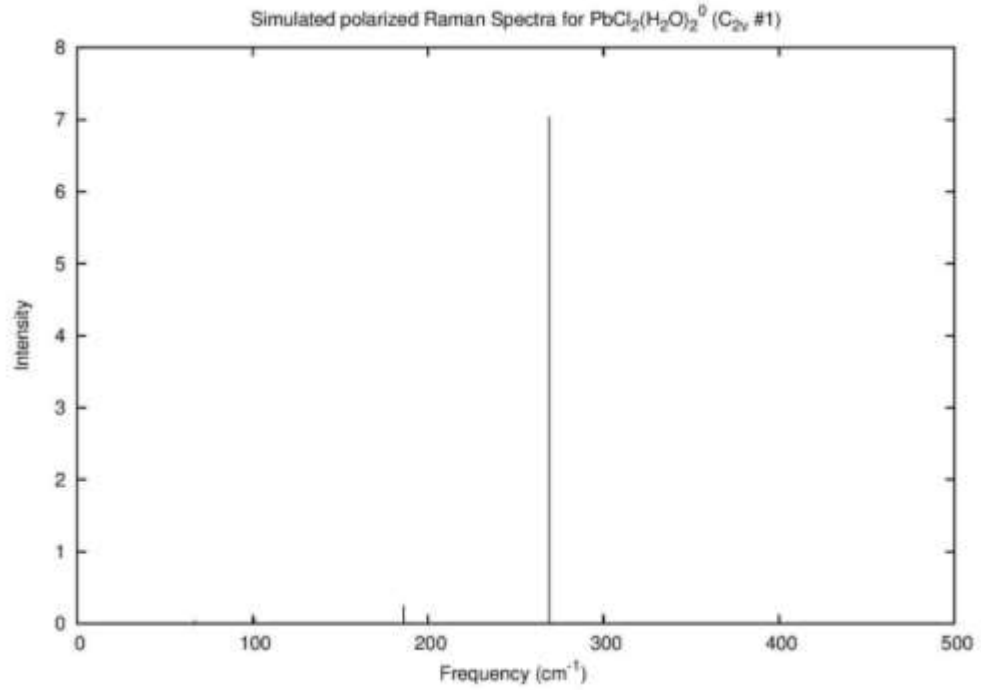
$[PbCl_2]^0$



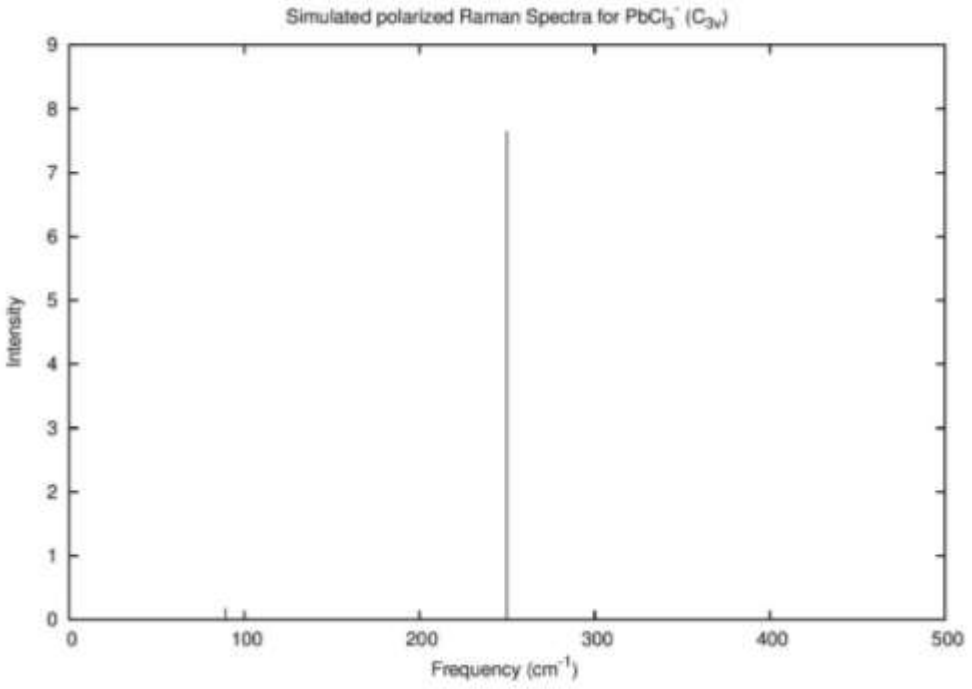
$[PbCl_2(H_2O)]^0$



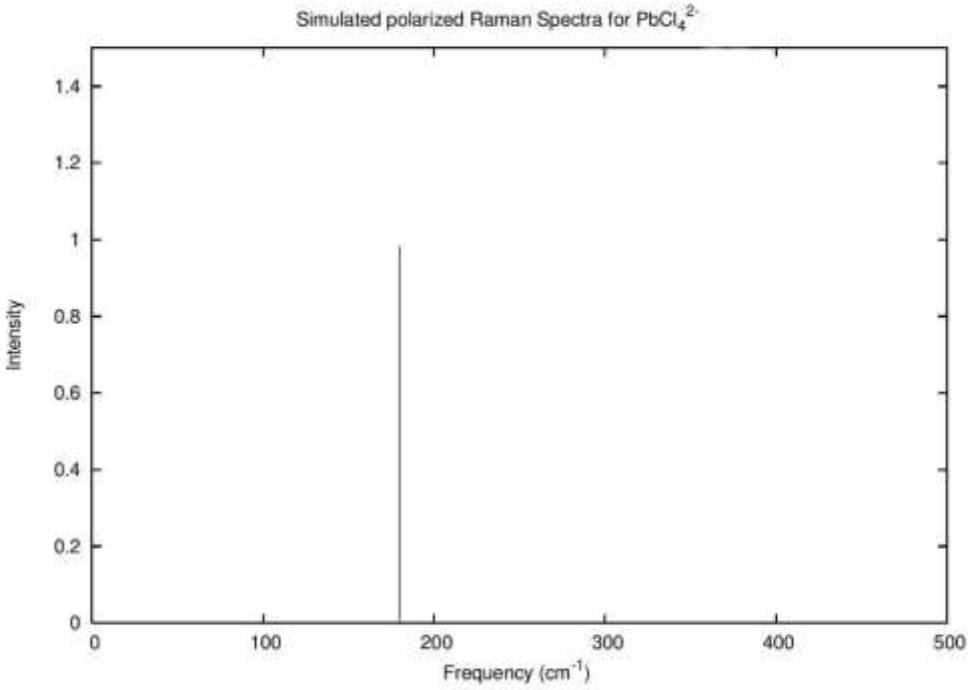
$[PbCl_2(H_2O)_2]^0$



$[PbCl_3]^-$



$[PbCl_4]^{2-}$


Simulated polarized Raman Spectra for $PbCl_4^{2-}$
Intensity
Frequency (cm^{-1})
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
100
200
300
400
500

CHAPTER 5 - APPENDIX A

SUPPLEMENTARY MATERIALS

Table 5A.1: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ CEP-121G**	**MP2/6-31G*/ CEP-121G**	**B3LYP/6-31G*/ CEP-121G**
1	0	$C_{\infty v}$	-78.5766515	-78.8027328	-79.0682646
		C_s	-78.5799072	-78.8052611	-79.0705353
1	1	C_{2v}	-154.6172670	-155.0339777	-155.5131372
		C_s #1	-154.6573262	-155.0721423	-155.5508892
		C_s #2	-154.6470003	-155.0614809	-155.5407031
		C_1	N/A	N/A	-155.5509286
1	2	C_{2v} #1	-230.7001185	-231.3014321	-231.9927067
		C_{2v} #2	-230.6888053	-231.2908212	-231.9833425
		C_s #1	-230.7223206	-231.3265142	-232.0172207
		C_s #2	-230.7100668	-231.3135128	-232.0041948
		C_1	N/A	-231.3269952	-232.0182483
1	3	C_{3v} #1	-306.7565542	-307.5481425	-308.4513260
		C_{3v} #2	-306.7375403	-307.5279325	-308.4338416
		C_s #1	-306.7709909	-307.5648708	-308.4662459
		C_s #2	-306.7685575	-307.5628326	-308.4662375
		C_1 #1	-306.7714873	-307.5680578	-308.4707754
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.8006398	-383.7831820	-384.8959429
		C_{4v} #2	-382.7751462	-383.7541654	-384.8703172
		C_4	-382.8011936	-383.7887915	-384.9086081
		C_s	-382.8136946	-383.7986953	-384.9121543
		C_1	-382.8160489	-383.8042179	-384.9183443
1	5	C_{2v} #1	-458.8253026	-460.0017548	-461.3281244
		C_{2v} #2	-458.7995679	-459.9721619	-461.3018133
		C_{2v} #3	-458.8179500	-459.9943731	-461.3226926
		C_{2v} #4	-458.8171006	-459.9936230	-461.3219247
		C_2	-458.8269052	-460.0113458	-461.3433114
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-458.8388406	-460.0163493	-461.3449173
		C_1	-458.8536947	-460.0318179	-461.3585428
2	0	$D_{\infty h}$	-154.2001690	-154.6314194	-155.1180610
		C_{2v}	-154.2850072	-154.7083527	-155.1905199
2	1	C_{2v} #1	-230.2983968	-230.9094823	-231.6041837
		C_{2v} #2	-230.2980991	-230.9092170	-231.6040344
2	2	D_{2h} #1	-306.2548462	-307.0601960	-307.9711159
		D_{2h} #2	-306.2667238	-307.0708891	-307.9806496

		C_{2h}	-306.2669748	-307.0727047	-307.9844938
		C_{2v} #1	-306.3694126	-307.1769274	-308.0568033
		C_{2v} #2	-306.2993691	-307.1040783	-308.0117449
		C_{2v} #3	-306.3784274	-307.1904455	-308.0980682
		C_{2v} #4	-306.2880424	-307.1000919	-308.0092468
		C_{2v} #5	-306.2993691	-307.1040782	-308.0117449
2	3	D_{3h} #1	-382.2779131	-383.2704210	-384.3929548
		D_{3h} #2	-382.2967388	-383.2888669	-384.4100421
		C_{2v} #1	-382.3817546	-383.3788308	-384.4979196
		C_{2v} #2	-382.3912627	-383.3922758	-384.5128477
		C_{2v} #3	-382.3904067	-383.3891633	-384.4723398
		C_{3h}	-382.2989964	-383.2949270	-384.4198913
		C_s	-382.3957474	-383.3970083	-384.5154918
2	4	D_{4h} #1	-458.2951954	-459.4756968	-460.8090130
		D_{4h} #2	-458.3188859	-459.4993915	-460.8311099
		C_{4h}	-458.3296723	-459.5172411	-460.8535024
		C_{2v}	-458.4021100	-459.5898467	-460.9197887
		C_s	-458.4148872	-459.5891859	Dissociation
3	0	D_{3h}	-229.6665384	-230.2889391	-230.9879422
		C_{3h}	-229.6821258	-230.3129377	-231.0153889
		C_{3v}	-229.7692730	-230.3862016	-231.0787370
		C_3	-229.7740101	-230.3933690	-231.0866174
3	1	C_{2v} #1	Dissociation	Dissociation	-307.4172291
		C_{2v} #2	-305.6931893	-306.5094073	-307.4206311
		C_2	N/A	N/A	N/A
		C_s #1	-305.8136303	Dissociation	Dissociation
		C_s #2	-305.8136302	Dissociation	Dissociation
3	2	C_{2v} #1	-381.7736261	Dissociation	Dissociation
		C_{2v} #2	-381.7988805	-382.8210712	-383.9391248
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.8609721	-459.0452870	-460.3722891
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.8782172	-459.0747737	-460.4052678
4	0	T_d	-304.9481196	-305.7595797	-306.6681413
		D_{2d}	N/A	-305.8060601	-306.7192302
		C_{3v}	Dissociation	-305.8089412	Dissociation
		C_3	Dissociation	-305.8237630	-306.7333168
		C_{2v}	-304.9428354	-305.7653302	-306.6779733
		C_s	-305.0337653	Dissociation	Dissociation
4	1	C_{2v}	Dissociation	-382.0057287	-383.1376558
		C_2	Dissociation	Dissociation	Dissociation
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-456.9124634	-458.0997458	-459.4345880

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.2: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ LANL2DZ**	**MP2/6-31G*/ LANL2DZ**	**B3LYP/6-31G*/ LANL2DZ**
1	0	$C_{\infty v}$	-78.5662254	-78.7897866	-79.0510617
1	0	C_s	N/A	N/A	N/A
1	1	C_{2v}	-154.5993221	-155.0127650	-155.4871418
		C_s #1	-154.6266116	-155.0390957	-155.5137539
		C_s #2	-154.6190149	-155.0309828	-155.50589
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.6638485	-231.2631661	-231.9501636
		C_{2v} #2	-230.6556646	-231.2556055	-231.9433991
		C_s #1	-230.6772858	-231.2791784	-231.9652601
		C_s #2	-230.6691169	-231.2702709	-231.9568659
		C_1	N/A	-231.2793642	-231.9657571
1	3	C_{3v} #1	-306.7059326	-307.4944024	-308.3928704
		C_{3v} #2	-306.6926061	-307.4805848	-308.3809019
		C_s #1	-306.7154451	-307.5066791	-308.4033843
		C_s #2	-306.7138262	-307.5052497	-308.4034893
		C_1 #1	-306.7156791	-307.5093934	N/A
		C_1 #2	N/A	N/A	-308.4071589
1	4	C_{4v} #1	-382.7391955	-383.7169228	-384.8251161
		C_{4v} #2	-382.7230051	-383.6992816	-384.8105328
		C_4	-382.7392035	-383.7186822	-384.8286863
		C_s	-382.7489451	-383.7303318	-384.8387462
		C_1	-382.7509504	-383.7341969	-384.8437996
1	5	C_{2v} #1	-458.7593019	-459.9272686	-461.2476564
		C_{2v} #2	-458.7426150	-459.9080387	-461.2315627
		C_{2v} #3	-458.7542582	-459.9220956	-461.2441521
		C_{2v} #4	-458.7534740	-459.9211594	-461.2431356
		C_2	-458.7595071	-459.9392926	-461.2516775
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	Dissociation	-459.9415854	-461.2621513
		C_1	-458.7825284	-459.9599931	-461.2822278
2	0	$D_{\infty h}$	-154.1711988	-154.6018435	-155.0847804
		C_{2v}	-154.2531656	-154.6719969	-155.1498243
2	1	C_{2v} #1	-230.2656603	-230.8713627	-231.5613196
		C_{2v} #2	-230.2654458	-230.8711582	-231.5611743
2	2	D_{2h} #1	-306.2079189	-307.0116109	-307.9180668
		D_{2h} #2	-306.2166701	-307.0198544	-307.9253689

		C_{2h}	-306.2168091	-307.0210634	-307.9278996
		C_{2v} #1	-306.3102776	-307.1122124	-307.9920838
		C_{2v} #2	-306.2661053	-307.0588211	-307.9546186
		C_{2v} #3	-306.3164967	-307.1243038	-308.0263322
		C_{2v} #4	-306.2370512	-307.0480105	-307.9526924
		C_{2v} #5	Dissociation	-307.0513238	-307.9546189
2	3	D_{3h} #1	-382.2229024	-383.2127263	-384.3303083
		D_{3h} #2	-382.2360823	-383.2261279	-384.3422650
		C_{2v} #1	-382.3214463	-383.3115157	-384.4242105
		C_{2v} #2	-382.3287150	-383.3242319	-384.4386596
		C_{2v} #3	-382.3303097	-383.3233610	-384.4063297
		C_{3h}	-382.2375704	-383.2303441	-384.3488927
		C_s	-382.3366746	Dissociation	-384.4448662
2	4	D_{4h} #1	-458.2351397	-459.4117531	-460.7404856
		D_{4h} #2	-458.2513895	-459.4285877	-460.7552208
		C_{4h}	-458.2598067	-459.4431528	-460.7727569
		C_{2v}	-458.3411175	-459.5219251	-460.8456025
		C_s	Dissociation	-459.5257167	Dissociation
3	0	D_{3h}	-229.6204871	-230.2420594	-230.9367028
		C_{3h}	-229.6821258	-230.2536798	-230.9517861
		C_{3v}	-229.7177512	-230.3298655	-231.0168291
		C_3	-229.7210982	-230.3349230	-231.0222994
3	1	C_{2v} #1	Dissociation	Dissociation	-307.3567224
		C_{2v} #2	-305.6324398	-306.4455455	-307.3524537
		C_2	N/A	N/A	N/A
		C_s #1	-305.7620110	Dissociation	Dissociation
		C_s #2	-305.7620110	Dissociation	Dissociation
3	2	C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	-381.7371262	-382.7522489	-383.8644778
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.8119454	-458.9931520	-460.3154699
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.8248836	-459.1656428	-460.339262
4	0	T_d	-304.8840035	-305.6931476	-306.5954949
		D_{2d}	N/A	-305.7279359	-306.6349311
		C_{3v}	Dissociation	-305.8089412	Dissociation
		C_3	Dissociation	Dissociation	-306.6501911
		C_{2v}	-304.8753039	-305.7127134	-306.6202503
		C_s	Dissociation	Dissociation	Dissociation
4	1	C_{2v}	Dissociation	-381.9213301	Dissociation
		C_2	Dissociation	Dissociation	Dissociation
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	Dissociation	-458.0180358	Dissociation

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.3: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ SDD**	**MP2/6-31G*/ SDD**	**B3LYP/6-31G*/ SDD**
1	0	$C_{\infty v}$	-78.5195662	-78.7523936	-79.0110640
1	0	C_s	-78.5206248	-78.7531730	-79.0115603
1	1	C_{2v}	-154.5534073	-154.9757902	-155.4468838
		C_s #1	-154.5773846	-155.0008944	-155.4709724
		C_s #2	-154.5707949	-154.9938194	-155.4641175
		C_1	N/A	N/A	-155.4709848
1	2	C_{2v} #1	-230.6115178	-231.2213485	-231.9038331
		C_{2v} #2	-230.6048938	-231.2157146	-231.8987101
		C_s #1	-230.6244555	-231.2376738	-231.9187686
		C_s #2	-230.6187786	-231.2315714	-231.9126877
		C_1	N/A	-231.2380079	N/A
1	3	C_{3v} #1	-306.6514402	-307.4497911	-308.3435102
		C_{3v} #2	-306.6408157	-307.4397982	-308.3350912
		C_s #1	-306.6617459	-307.4639819	-308.3553205
		C_s #2	-306.6609971	-307.4637599	-308.3565010
		C_1 #1	-306.6619618	-307.4674455	N/A
		C_1 #2	N/A	N/A	-308.3594078
1	4	C_{4v} #1	-382.6843038	-383.6717976	-384.7749665
		C_{4v} #2	-382.6711630	-383.6585201	-384.7644429
		C_4	N/A	-383.6744210	-384.7907646
		C_s	-382.6952948	-383.6880253	Dissociation
		C_1	-382.6970548	-383.6927217	-384.8122136
1	5	C_{2v} #1	-458.7061956	-459.8834260	-461.1996624
		C_{2v} #2	-458.6923910	-459.8679770	-461.1860759
		C_{2v} #3	-458.7024937	-459.8802468	-461.1975093
		C_{2v} #4	-458.7017747	-459.8793371	-461.1964966
		C_2	-458.7265957	-459.8995301	-461.2063882
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-458.7176738	-459.9004146	Dissociation
		C_1	-458.7280580	-459.9156801	-461.2323868
2	0	$D_{\infty h}$	-154.1221170	-154.5635598	-155.0396567
		C_{2v}	-154.1967489	-154.6325312	-155.1026682
2	1	C_{2v} #1	-230.2098652	-230.8324411	-231.5148260
		C_{2v} #2	-230.2096245	-230.8322110	-231.5146239
2	2	D_{2h} #1	-306.1597027	-306.9735101	-307.8730115
		D_{2h} #2	-306.1676177	-306.9807564	-307.8795137

		C_{2h}	-306.1677270	-306.9824072	-307.8821750
		C_{2v} #1	-306.2514344	-307.0693824	-307.9418879
		C_{2v} #2	-306.2109102	-307.0216404	-307.9176212
		C_{2v} #3	-306.2584646	-307.0823087	-307.9760645
		C_{2v} #4	-306.1880570	-307.0076884	-307.9076018
		C_{2v} #5	Dissociation	-307.0216259	-307.9176292
2	3	D_{3h} #1	-382.1749532	-383.1743799	-384.2855093
		D_{3h} #2	-382.1867085	-383.1855556	-384.2954931
		C_{2v} #1	-382.2634756	-383.2693323	-384.3741891
		C_{2v} #2	-382.2714286	-383.2826533	-384.3888880
		C_{2v} #3	-382.2714286	-383.4393134	-384.3568838
		C_{3h}	-382.1879653	-383.1903816	-384.3020989
		C_s	-382.2795394	Dissociation	Dissociation
2	4	D_{4h} #1	-458.1878735	-459.3735620	-460.6960499
		D_{4h} #2	-458.2027483	-459.3882906	-460.7088095
		C_{4h}	-458.2099374	-459.4027685	-460.7252873
		C_{2v}	-458.2830604	-459.4800779	-460.7956126
		C_s	Dissociation	-459.4735535	Dissociation
3	0	D_{3h}	-229.5665410	-230.1971847	-230.8849718
		C_{3h}	-229.6281890	-230.2183323	-230.9077041
		C_{3v}	-229.6546700	-230.2866807	-230.9637536
		C_3	-229.6578374	-230.2914762	-230.9687988
3	1	C_{2v} #1	Dissociation	Dissociation	-307.3116207
		C_{2v} #2	-305.5825465	-306.4071310	-307.3057281
		C_2	N/A	N/A	N/A
		C_s #1	Dissociation	-306.5258614	-307.4145228
		C_s #2	-305.6995865	Dissociation	Dissociation
3	2	C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	-381.6787035	-382.7121718	-383.8144136
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.7497182	-458.9503410	-460.2636172
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.7643181	-459.1145144	-460.2893112
4	0	T_d	-304.8334543	-305.6491324	-306.5445280
		D_{2d}	N/A	-305.6941885	-306.5919418
		C_{3v}	Dissociation	Dissociation	-306.7178043
		C_3	Dissociation	-305.8237630	-306.6008236
		C_{2v}	-304.8305043	-305.6793851	-306.5761572
		C_s	Dissociation	Dissociation	Dissociation
4	1	C_{2v}	Dissociation	Dissociation	-382.9925831
		C_2	Dissociation	Dissociation	Dissociation
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	Dissociation	-457.9833467	Dissociation

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.4: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ CEP-121G**	**MP2/6-31+G*/ CEP-121G**	**B3LYP/6-31+G*/ CEP-121G**
1	0	$C_{\infty v}$	-78.5880882	-78.8180840	-79.0800852
1	0	C_s	-78.5895782	-78.8192390	-79.0808212
1	1	C_{2v}	-154.6348673	-155.0608538	-155.5349727
		C_s #1	-154.6690893	-155.0929081	-155.5665750
		C_s #2	-154.6584366	-155.0818949	-155.5557875
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.7189395	-231.3355323	-232.0205580
		C_{2v} #2	-230.7072438	-231.3241970	-232.0100627
		C_s #1	-230.7366395	-231.3553588	-232.0390920
		C_s #2	-230.7261286	-231.3441855	-232.0285931
		C_1	N/A	N/A	-232.0391258
1	3	C_{3v} #1	-306.7781267	-307.5899708	-308.4854920
		C_{3v} #2	-306.7594570	-307.5703640	-308.4680887
		C_s #1	-306.7895205	-307.6031528	-308.4964872
		C_s #2	-306.7871973	-307.6013108	-308.4957640
		C_1 #1	-306.7895198	-307.6041818	-308.4976324
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.8267969	-383.8356442	-384.9385231
		C_{4v} #2	-382.8020150	-383.8078292	-384.9145521
		C_4	N/A	-383.8362496	-384.9398964
		C_s	-382.8365875	-383.8464180	-384.9490782
		C_1	-382.8379997	-383.8495391	-384.9525752
1	5	C_{2v} #1	-458.8573630	-460.0647799	-461.3789221
		C_{2v} #2	-458.8324654	-460.0364180	-461.3539149
		C_{2v} #3	-458.8506604	-460.0578856	-461.3738694
		C_{2v} #4	-458.8494939	-460.0565240	-461.3724532
		C_2	-458.8575160	-460.0662893	-461.3821497
		C_s #1	Dissociation	-460.0756450	Dissociation
		C_s #2	-458.8676194	-460.0793727	-461.3935081
		C_1	-458.8787287	-460.0914715	-461.4037199
2	0	$D_{\infty h}$	-154.2360647	-154.6850083	-155.1593430
		C_{2v}	-154.3022684	-154.7396578	-155.2136408
2	1	C_{2v} #1	-230.3229155	-230.9550183	-231.6408792
		C_{2v} #2	-230.3223755	-230.9543359	-231.6401904
2	2	D_{2h} #1	-306.3023909	-307.1385127	-308.0338432
		D_{2h} #2	-306.3167778	-307.1535926	-308.0476227

		C_{2h}	-306.3167779	-307.1535926	-308.0477872
		C_{2v} #1	-306.2514344	-307.2173463	-308.1114896
		C_{2v} #2	-306.3340942	-307.1677477	-308.0640965
		C_{2v} #3	-306.3981200	-307.2315455	-308.1271601
		C_{2v} #4	-306.3289187	-307.1696580	-308.0660001
		C_{2v} #5	-306.3340943	-307.1677477	-308.0640782
2	3	D_{3h} #1	-382.3312286	-383.3609444	-384.4671053
		D_{3h} #2	-382.3530493	-383.3846560	-384.4888500
		C_{2v} #1	-382.3533473	-383.4305022	-384.5368293
		C_{2v} #2	-382.4168201	Dissociation	Dissociation
		C_{2v} #3	-382.4153092	-383.3827004	-384.5440730
		C_{3h}	-382.3532897	-383.3854040	-384.4909497
		C_s	-382.3973487	-383.4367636	-384.5412761
2	4	D_{4h} #1	-458.3549107	-459.5791810	-460.8949393
		D_{4h} #2	-458.3833954	-459.6110911	-460.9239165
		C_{4h}	-458.3884430	-459.6179029	-460.9327712
		C_{2v}	-458.4328590	-459.6517216	-460.9685623
		C_s	-458.4444338	-459.6831941	Dissociation
3	0	D_{3h}	-229.7303211	-230.3877884	-231.0690601
		C_{3h}	-229.5789885	-230.3951381	-231.0801759
		C_{3v}	-229.8009023	-230.4464872	-231.1276867
		C_3	-229.8062157	-230.4532353	-231.1349023
3	1	C_{2v} #1	Dissociation	-306.6078289	-307.5006777
		C_{2v} #2	-305.7589901	-306.6164353	-307.5082531
		C_2	N/A	N/A	N/A
		C_s #1	Dissociation	-306.6942108	-307.5860516
		C_s #2	Dissociation	-306.6942108	-307.5860518
3	2	C_{2v} #1	-381.8158882	Dissociation	Dissociation
		C_{2v} #2	-381.8394479	-382.8958889	-383.9962892
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.9100443	-459.1417077	-460.4557931
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.9250049	-459.0663588	-460.4791675
4	0	T_d	-305.0476355	-305.9154686	-306.8014885
		D_{2d}	N/A	-305.9389461	-306.8311466
		C_{3v}	Dissociation	-305.9432970	-306.5908009
		C_3	Dissociation	-305.7093409	-306.8415377
		C_{2v}	-305.0376867	-305.9141207	-306.8013805
		C_s	Dissociation	Dissociation	-306.8513613
4	1	C_{2v}	-381.0812504	-382.1578846	-383.2564985
		C_2	Dissociation	-382.1752617	-383.2704437
		C_s	Dissociation	Dissociation	Dissociation

4	2	D_{2h}	-457.0337913	-458.2961183	- 459.6023222
		C_{2v} #1	Dissociation	Dissociation	-459.7035302
		C_{2v} #2	Dissociation	Dissociation	-459.7033324

Detached structure

Table 5A.5: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ LANL2DZ**	**MP2/6-31+G*/ LANL2DZ**	**B3LYP/6-31+G*/ LANL2DZ**
1	0	$C_{\infty v}$	-78.5744121	-78.8030576	-79.0617734
1	0	C_s	-78.5744509	-78.8031027	N/A
1	1	C_{2v}	-154.6143334	-155.0383645	-155.5089652
		C_s #1	-154.6385107	-155.0614816	-155.5314823
		C_s #2	-154.6307997	-155.0532001	-155.5236185
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.6814895	-231.2972329	-231.9788877
		C_{2v} #2	-230.6729895	-231.2888341	-231.9788877
		C_s #1	-230.6927874	-231.3106648	-231.9904970
		C_s #2	-230.6860507	-231.3033078	-231.9842249
		C_1	N/A	N/A	-231.9413340
1	3	C_{3v} #1	-306.7278759	-307.5385278	-308.4301496
		C_{3v} #2	-306.7148468	-307.5246348	-308.4183195
		C_s #1	-306.7361681	-307.5488149	-308.4386170
		C_s #2	-306.7345716	-307.5476327	-308.4378978
		C_1 #1	-306.7361657	-307.5495128	-308.4391061
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.7668724	-383.7728886	-384.8822252
		C_{4v} #2	-382.7511101	-383.7551437	-384.8590776
		C_4	N/A	-383.7728964	-384.8733716
		C_s	-382.7748273	-383.7828139	-384.8315995
		C_1	-382.7760569	-383.7858317	-384.8850292
1	5	C_{2v} #1	-458.7943469	-459.9964363	-461.3073038
		C_{2v} #2	-458.7782769	-459.9783313	-461.2922659
		C_{2v} #3	-458.7899329	-459.9921128	-461.3042872
		C_{2v} #4	-458.7888507	-459.9905569	-461.3028055
		C_2	-458.7850629	-459.9967005	-461.3079018
		C_s #1	N/A	N/A	N/A
		C_s #2	-458.8024482	-460.0148206	-461.3161461
		C_1	-458.8126432	-460.0196929	-461.3298034
2	0	$D_{\infty h}$	-154.2062451	-154.6549255	-155.1263710
		C_{2v}	-154.2715937	-154.7065846	-155.1766600
2	1	C_{2v} #1	-230.2912085	-230.9198409	-231.6018171
		C_{2v} #2	-230.2909034	-230.9194301	-231.6014178
2	2	D_{2h} #1	-306.2563475	-307.0912483	-307.9842549
		D_{2h} #2	-306.2675809	-307.1035921	-307.9951788

		C_{2h}	-306.2675809	-307.1035923	-307.9952818
		C_{2v} #1	-306.3896605	-307.1618249	-308.0505785
		C_{2v} #2	-306.2876124	-307.1193718	-308.0117867
		C_{2v} #3	-306.3408181	-307.1721434	-308.0625555
		C_{2v} #4	-306.2791316	-307.1198768	-308.0125062
		C_{2v} #5	-306.2876124	-307.1193718	-308.0117867
2	3	D_{3h} #1	-382.2783612	-383.3066738	-384.4099420
		D_{3h} #2	-382.2948025	-383.3259185	-384.4263854
		C_{2v} #1	-382.3533473	-383.3734753	-384.4742387
		C_{2v} #2	-382.3593701	-383.3827004	-384.4819091
		C_{2v} #3	-382.3604308	-383.3355032	-384.4819091
		C_{3h}	-382.2949911	-383.3264821	-384.4277852
		C_s	-382.3668676	-383.3898415	-384.4896330
2	4	D_{4h} #1	-458.2978478	-459.5202837	-460.8336018
		D_{4h} #2	-458.3188075	-459.5451399	-460.8546252
		C_{4h}	-458.3227412	-459.5505149	-460.8615158
		C_{2v}	-458.3781482	-459.5938929	-460.9051428
		C_s	Dissociation	Dissociation	Dissociation
3	0	D_{3h}	-229.6843322	-230.3427614	-231.0201818
		C_{3h}	-229.7330826	-230.3471072	-231.0276240
		C_{3v}	-229.7539590	-230.3980122	-231.1408627
		C_3	-229.7582617	-230.4031717	-231.0793682
3	1	C_{2v} #1	Dissociation	-306.5602649	-307.4493932
		C_{2v} #2	-305.7027716	-306.5601743	-307.4482343
		C_2	N/A	N/A	N/A
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-305.8016670	-306.6447098	Dissociation
3	2	C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	-381.7836667	-382.8370097	-383.9319886
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.8627687	-459.0929927	-460.4021793
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.8757774	-459.3907371	-460.4227262
4	0	T_d	-304.9894409	-305.8595677	-306.7401932
		D_{2d}	N/A	-305.8792139	-306.7653941
		C_{3v}	Dissociation	Dissociation	-306.8314214
		C_3	Dissociation	-305.9534738	-306.7333168
		C_{2v}	-304.9777065	-305.8535561	-306.7377067
		C_s	Dissociation	Dissociation	Dissociation
4	1	C_{2v}	Dissociation	-382.0910561	-383.1855568
		C_2	Dissociation	-382.0923654	-383.1866545
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-456.9670833	-458.2282414	-459.5304476

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.6: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ SDD**	**MP2/6-31+G*/ SDD**	**B3LYP/6-31+G*/ SDD**
1	0	$C_{\infty v}$	-78.5254595	-78.7623884	-79.0185533
1	0	C_s	-78.5260894	-78.7628505	-79.0187329
1	1	C_{2v}	-154.5651603	-154.9970861	-155.4645759
		C_s #1	-154.5868774	-155.0193601	-155.4854706
		C_s #2	-154.5798188	-155.0114522	-155.4781249
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.6273218	-231.2521467	-231.9296497
		C_{2v} #2	-230.6200702	231.2450368	-231.9233816
		C_s #1	-230.6382928	-231.2659028	-231.9413157
		C_s #2	-230.6333273	-231.2604411	-231.9366184
		C_1	N/A	N/A	N/A
1	3	C_{3v} #1	-306.6724995	-307.4916911	-308.3791795
		C_{3v} #2	-306.6611599	-307.4798864	-308.3692869
		C_s #1	-306.6811180	-307.5032406	-308.3883860
		C_s #2	-306.6802417	-307.5027711	-308.3883459
		C_1 #1	-306.6811180	-307.5045957	-308.3891282
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.7109856	-383.7254619	-384.8212131
		C_{4v} #2	-382.6971365	-383.7102285	-384.8092711
		C_4	N/A	-383.7254975	-384.8213043
		C_s	-382.7199143	-383.7372530	-384.8315995
		C_1	-382.7210178	-383.7403909	-384.8349155
1	5	C_{2v} #1	-458.7400844	-459.9495384	-461.2560851
		C_{2v} #2	-458.7253654	-459.9334954	-461.2428677
		C_{2v} #3	-458.7360800	-459.9458288	-461.2536526
		C_{2v} #4	-458.7350721	-459.9443715	-461.2522808
		C_2	Dissociation	-459.9967005	-461.2568479
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-458.7487017	-459.9613008	-461.2663064
		C_1	-458.7577077	-459.9742518	-461.2791878
2	0	$D_{\infty h}$	-154.1514322	-154.6090548	-155.0750399
		C_{2v}	-154.2122413	-154.6617581	-155.1256015
2	1	C_{2v} #1	-230.2326626	-230.8754342	-231.5512731
		C_{2v} #2	-230.2323388	-230.8750541	-231.5509007
2	2	D_{2h} #1	-306.2022617	-307.0452276	-307.9328214
		D_{2h} #2	-306.2125765	-307.0564945	-307.9426241

		C_{2h}	-306.2125765	-307.0565008	-307.9428560
		C_{2v} #1	-306.3357020	-307.1141654	-307.9971553
		C_{2v} #2	-306.2314174	-307.0759126	-307.9614574
		C_{2v} #3	-306.2811110	-307.1260664	-308.0103137
		C_{2v} #4	-306.2261140	-307.0737690	-307.9629455
		C_{2v} #5	-306.2314174	-307.0759126	-307.9614574
2	3	D_{3h} #1	-382.2244991	-383.2600523	-384.3584369
		D_{3h} #2	-382.2400581	-383.2775925	-384.3735437
		C_{2v} #1	-382.2938288	-383.3265181	-384.4217471
		C_{2v} #2	-382.2998674	-383.3397160	-384.4288266
		C_{2v} #3	-382.2998674	-383.6036830	-384.4288266
		C_{3h}	-382.2401215	-383.2782172	-384.3749918
		C_s	Dissociation	Dissociation	-384.4374913
2	4	D_{4h} #1	-458.2444000	-459.4735425	-460.7819671
		D_{4h} #2	-458.2642885	-459.4966914	-460.8012905
		C_{4h}	-458.2675649	-459.5019745	-460.8079462
		C_{2v}	-458.3181355	-459.5473948	-460.8529383
		C_s	Dissociation	Dissociation	Dissociation
3	0	D_{3h}	-229.6279813	-230.2941078	-230.9666148
		C_{3h}	-229.6865144	-230.3046087	-230.9791129
		C_{3v}	-229.6889989	-230.3501721	-231.0860307
		C_3	-229.6929045	-230.3555414	-231.0236147
3	1	C_{2v} #1	Dissociation	-306.5170508	-307.3995098
		C_{2v} #2	-305.7027716	-306.5161045	-307.3978228
		C_2	N/A	N/A	N/A
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-305.9287746	-306.5967115	Dissociation
3	2	C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	-381.7229967	-382.7910386	-383.8793216
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.7980551	-459.0439244	-460.3465499
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.8112959	-459.3397826	-460.3677303
4	0	T_d	-304.9376998	-305.8130798	-306.6900973
		D_{2d}	N/A	-305.8398632	-306.7202247
		C_{3v}	Dissociation	Dissociation	Dissociation
		C_3	Dissociation	-306.0969293	-306.6501911
		C_{2v}	-304.9279454	-305.8321021	-306.7086709
		C_s	Dissociation	-305.8624656	Dissociation
4	1	C_{2v}	-380.9680281	-382.0505637	-383.1393849
		C_2	Dissociation	-382.0517151	-383.1403548
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-456.9185149	-458.1843106	-459.4820671

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.7: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ CEP-121G**	**MP2/6-311+G*/ CEP-121G**	**B3LYP/6-311+G*/ CEP-121G**
1	0	$C_{\infty v}$	-78.6112299	-78.8574321	-79.1052307
1	0	C_s	-78.6112300	-78.8574445	N/A
1	1	C_{2v}	-154.6807725	-155.141266	-155.5851516
		C_s #1	-154.7134362	-155.1718578	-155.6155529
		C_s #2	-154.7021029	-155.1602893	-155.6037972
		C_1	N/A	-155.1718612	N/A
1	2	C_{2v} #1	-230.7896511	-231.4589413	-232.0971140
		C_{2v} #2	-230.7767041	-231.4462786	-232.0853755
		C_s #1	-230.8050649	-231.4773251	-232.1143290
		C_s #2	-230.7935236	-231.4643331	-232.1025103
		C_1	N/A	N/A	N/A
1	3	C_{3v} #1	-306.8722479	-307.7552767	-308.5876162
		C_{3v} #2	-306.8513350	-307.7329437	-308.5675476
		C_s #1	-306.8807008	-307.7660307	-308.5962399
		C_s #2	-306.8782227	-307.7641332	-308.5955779
		C_1 #1	-306.8807008	-307.7666384	-308.5966574
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.9432425	-384.0416365	-385.0646354
		C_{4v} #2	-382.9155299	-384.0100589	-385.0373965
		C_4	N/A	N/A	N/A
		C_s	-382.9498088	-384.0495275	-385.0726019
		C_1	-382.9507922	-384.0524203	-385.0756550
1	5	C_{2v} #1	-458.9948778	-460.3097070	-461.5283814
		C_{2v} #2	-458.9662720	-460.2773347	-461.4989448
		C_{2v} #3	-458.9868628	-460.3009717	-461.5218761
		C_{2v} #4	-458.9856556	-460.2993083	-461.5202455
		C_2	Dissociation	-459.9500888	-461.5287629
		C_s #1	Dissociation	-460.3188180	Dissociation
		C_s #2	-459.0092004	-460.3235835	-461.5355917
		C_1	-458.9466198	-460.3339093	-461.5455184
2	0	$D_{\infty h}$	-154.2830810	-154.7631265	-155.2106617
		C_{2v}	-154.3406515	-154.8111680	-155.1256015
2	1	C_{2v} #1	-230.3825445	-231.0664527	-231.7081730
		C_{2v} #2	-230.3818098	-231.0656635	-308.1330205
2	2	D_{2h} #1	-306.3935356	-307.2979039	-308.1330205
		D_{2h} #2	-306.4091380	-307.3144673	-308.1481783

		C_{2h}	-306.4091380	-307.3144670	-308.1481782
		C_{2v} #1	-306.2751170	-307.3682517	-308.2019811
		C_{2v} #2	-306.4197346	-307.3220909	-308.1585477
		C_{2v} #3	-306.4796200	-307.3824877	-308.2193671
		C_{2v} #4	-306.4199726	-307.3281158	-308.1657274
		C_{2v} #5	-306.4197346	-307.3220911	-308.1585477
2	3	D_{3h} #1	-382.4436875	-383.5602096	-384.5894706
		D_{3h} #2	-382.4673128	-383.5860446	-384.6134422
		C_{2v} #1	-382.5094250	-383.6203958	-384.6500699
		C_{2v} #2	-382.5191641	Dissociation	Dissociation
		C_{2v} #3	-382.5166129	-383.5713789	-384.627750
		C_{3h}	-382.4673129	Dissociation	-384.6136464
		C_s	-382.5044467	-383.6314562	Dissociation
2	4	D_{4h} #1	-458.4876409	-459.8173586	-461.0394559
		D_{4h} #2	-458.5183003	-459.8522153	-461.0709694
		C_{4h}	-458.5206369	-459.8551316	-461.0767164
		C_{2v}	-458.5594642	-459.8947465	-461.1171098
		C_s	-458.5696632	-459.8719924	Dissociation
3	0	D_{3h}	-229.7986863	-230.5040973	-231.1448896
		C_{3h}	N/A	-230.5053013	-231.1484841
		C_{3v}	-229.8588707	-230.5539051	-231.0738021
		C_3	-229.8632118	-230.5592975	-231.2006081
3	1	C_{2v} #1	Dissociation	-306.7579089	-307.5939626
		C_{2v} #2	-305.6492554	-306.7691618	-307.6043515
		C_2	N/A	-306.7693046	N/A
		C_s #1	-305.9287745	-306.8408956	-307.6761162
		C_s #2	-305.9287746	-306.8408955	-307.6761161
3	2	C_{2v} #1	-381.9197520	-383.0613016	-384.0906713
		C_{2v} #2	-381.9394850	-383.0811443	-384.1091640
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-458.0329721	-459.3690651	-460.5933748
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-458.0459499	-459.2936192	-460.6153508
4	0	T_d	-305.1357381	-306.0688934	-306.9006379
		D_{2d}	N/A	-306.0824831	-306.9213361
		C_{3v}	Dissociation	-306.0884701	-306.9227142
		C_3	Dissociation	-306.0969293	-306.6008236
		C_{2v}	-305.1206539	-306.0608331	-306.8950899
		C_s	-305.1804410	Dissociation	Dissociation
4	1	C_{2v}	Dissociation	-382.3447845	-383.3718603
		C_2	Dissociation	-382.3598578	-383.3849034
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-457.1627596	-458.5291958	-459.7459946

		C_{2v} #1	Dissociation	Dissociation	-459.8425206
		C_{2v} #2	Dissociation	Dissociation	-459.8434537

Detached structure

Table 5A.8: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ LANL2DZ**	**MP2/6-311+G*/ LANL2DZ**	**B3LYP/6-311+G*/ LANL2DZ**
1	0	$C_{\infty v}$	-78.5962570	-78.8414313	-79.0862088
1	0	C_s	N/A	N/A	N/A
1	1	C_{2v}	-154.6585140	-155.1174873	-155.5578893
		C_s #1	-154.6822490	-155.1400856	-155.5800060
		C_s #2	-154.6746567	-155.1319581	-155.5721440
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.7503270	-231.4190532	-232.0538751
		C_{2v} #2	-230.7407714	-231.4095637	-232.0454333
		C_s #1	-230.7600620	-231.4316326	-232.0646061
		C_s #2	-230.7524496	-231.4228436	-232.0573263
		C_1	N/A	N/A	N/A
1	3	C_{3v} #1	-306.8196028	-307.7017065	-308.5298770
		C_{3v} #2	-306.8047795	-307.6856101	-308.5162520
		C_s #1	-306.8257532	-307.7103713	-308.5368813
		C_s #2	-306.8239527	-307.7092696	-308.5361638
		C_1 #1	-306.8257532	-307.7109424	-308.5370763
		C_1 #2	N/A	N/A	N/A
1	4	C_{4v} #1	-382.8809689	-383.9768843	-384.9969480
		C_{4v} #2	-382.8627770	-383.9561600	-384.9803974
		C_4	N/A	N/A	N/A
		C_s	-382.8861664	-383.9845728	-385.0040584
		C_1	-382.8870312	-383.9874811	-385.0068769
1	5	C_{2v} #1	-458.9292977	-460.2400654	-461.4540137
		C_{2v} #2	-458.9106954	-460.2189257	-461.4361869
		C_{2v} #3	-458.9239126	-460.2344849	-461.4501966
		C_{2v} #4	-458.9228695	-460.2326434	-461.4486962
		C_2	Dissociation	-460.3097158	-461.4540155
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-458.8806805	-460.2479602	-461.4612090
		C_1	-458.9466198	-460.2627837	-461.4758326
2	0	$D_{\infty h}$	-154.2514364	-154.7315923	-155.1765370
		C_{2v}	-154.3099729	-154.7783790	-155.2576277
2	1	C_{2v} #1	-230.3503324	-231.0312288	-231.6687328
		C_{2v} #2	-230.3499304	-231.0307831	-231.6682155
2	2	D_{2h} #1	-306.3445516	-307.2480709	-308.0807888
		D_{2h} #2	-306.3569226	-307.2617837	-308.0929777

		C_{2h}	-306.3569226	-307.2617837	-308.0929777
		C_{2v} #1	-306.4711492	-307.3131091	-308.1413757
		C_{2v} #2	-306.3718078	-307.2729811	-308.1056127
		C_{2v} #3	-306.4213902	-307.3225274	-308.1543886
		C_{2v} #4	-306.3674691	-307.2763365	-308.1105947
		C_{2v} #5	-306.3718083	-307.2729811	-308.1056127
2	3	D_{3h} #1	-382.3875203	-383.5029159	-384.5291324
		D_{3h} #2	-382.4053338	-383.5239514	-384.5472541
		C_{2v} #1	-382.4549053	-383.5638191	-384.5872160
		C_{2v} #2	-382.4604477	Dissociation	Dissociation
		C_{2v} #3	-382.4613271	-383.5258364	-384.5944805
		C_{3h}	-382.4053338	-383.5239549	-384.5474706
		C_s	-382.4417030	Dissociation	Dissociation
2	4	D_{4h} #1	-458.4278971	-459.7564288	-460.9754625
		D_{4h} #2	-458.4506320	-459.7834924	-460.9986762
		C_{4h}	-458.4527082	-459.7861025	-461.0033453
		C_{2v}	-458.4988862	-459.8216155	-461.0398891
		C_s	Dissociation	Dissociation	Dissociation
3	0	D_{3h}	-229.7502819	-230.4569322	-231.0938980
		C_{3h}	N/A	-230.4575796	-231.0971288
		C_{3v}	-229.8119124	-230.5059658	-231.1408627
		C_3	-229.8149287	-230.5094935	-231.1452419
3	1	C_{2v} #1	Dissociation	-306.7093102	-307.5415417
		C_{2v} #2	-305.8456888	-306.7118150	-307.5431069
		C_2	N/A	-306.7119155	N/A
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	Dissociation	Dissociation	-307.6215305
3	2	C_{2v} #1	Dissociation	Dissociation	-384.0274300
		C_{2v} #2	-381.8833949	-383.0225369	-384.0449995
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.9855283	-459.3205354	-460.5400595
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.9964889	-459.2936192	-460.5592160
4	0	T_d	-305.0741292	-306.0099460	-306.8357187
		D_{2d}	N/A	-306.0242732	-306.8560000
		C_{3v}	Dissociation	Dissociation	Dissociation
		C_3	Dissociation	Dissociation	-306.8415377
		C_{2v}	-305.0589315	-305.9987375	-306.8295672
		C_s	Dissociation	Dissociation	Dissociation
4	1	C_{2v}	-381.1205296	-382.2772397	-383.3005597
		C_2	Dissociation	-382.2788697	-383.3011824
		C_s	Dissociation	Dissociation	Dissociation
4	2	D_{2h}	-457.092346	-458.4578438	-459.6696975

		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.9: Total energies for all stable geometries of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ SDD**	**MP2/6-311+G*/ SDD**	**B3LYP/6-311+G*/ SDD**
1	0	$C_{\infty v}$	-78.5759334	-78.8021175	-79.0431921
1	0	C_s	N/A	N/A	N/A
1	1	C_{2v}	-154.6098826	-155.0771741	-155.5132117
		C_s #1	-154.6306903	-155.0988155	-155.5337754
		C_s #2	-154.6231810	-155.0904899	-155.5258491
		C_1	N/A	N/A	N/A
1	2	C_{2v} #1	-230.6961097	-231.3748469	-232.0040851
		C_{2v} #2	-230.6879699	-231.3668700	-231.9969662
		C_s #1	-230.7052249	-231.3875372	-232.0149622
		C_s #2	-230.6995179	-231.3807216	-232.0092280
		C_1	N/A	N/A	N/A
1	3	C_{3v} #1	-306.7639059	-307.6556324	-308.4782310
		C_{3v} #2	-306.7511047	-307.6424250	-308.4668096
		C_s #1	-306.7701853	-307.6653480	-308.4859517
		C_s #2	-306.7692294	-307.6650460	-308.4860317
		C_1 #1	-306.7701854	-307.6662971	N/A
		C_1 #2	N/A	N/A	-308.4865111
1	4	C_{4v} #1	-382.8244878	-383.9300291	-384.9440249
		C_{4v} #2	-382.8086442	-383.9126503	-384.9300273
		C_4	N/A	N/A	N/A
		C_s	-382.8307315	-383.9396200	-384.9527315
		C_1	-382.8306625	-383.9427376	-384.9563834
1	5	C_{2v} #1	-458.8741849	-460.1932648	-461.4017970
		C_{2v} #2	-458.8573776	-460.1749475	-461.3860060
		C_{2v} #3	-458.8694272	-460.1885725	-461.3987242
		C_{2v} #4	-458.8684552	-460.1869989	-461.3973128
		C_2	Dissociation	-460.1932745	-461.4018428
		C_s #1	Dissociation	Dissociation	Dissociation
		C_s #2	-458.8806806	-460.2032399	Dissociation
		C_1	-458.8910877	-460.2178268	Dissociation.
2	0	$D_{\infty h}$	-154.1955995	-154.6851516	-155.1238358
		C_{2v}	-154.2510998	-154.7349879	-155.1700843
2	1	C_{2v} #1	-230.2922454	-230.9881111	-231.6183080
		C_{2v} #2	-230.2918388	-230.9876681	-231.6178262
2	2	D_{2h} #1	-306.2893842	-307.2016701	-308.0280931

		D_{2h} #2	-306.3006909	-307.2140960	-308.0390978
		C_{2h}	-306.3006910	-307.2140960	-308.0390979
		C_{2v} #1	-306.4170639	-307.2669911	-308.0880490
		C_{2v} #2	-306.3153280	-307.2304530	-308.0542805
		C_{2v} #3	-306.3622313	-307.2775360	-308.1023044
		C_{2v} #4	-306.3135746	-307.2297837	-308.0601476
		C_{2v} #5	-306.3153280	-307.2304529	-308.0542804
2	3	D_{3h} #1	-382.3326648	-383.4564976	-384.4764957
		D_{3h} #2	-382.3496134	-383.4755932	-384.4934775
		C_{2v} #1	-382.3956776	-383.5181812	-384.5348337
		C_{2v} #2	Dissociation	-383.5258364	-384.5417874
		C_{2v} #3	-382.4013103	-383.5258364	-384.5417874
		C_{3h}	-382.3496135	-383.4756137	-384.4937821
		C_s	-382.4067024	-383.5345525	-384.5515304
2	4	D_{4h} #1	-458.3733380	-459.7095473	-460.9225223
		D_{4h} #2	-458.3950598	-459.7347378	-460.9442842
		C_{4h}	-458.3966119	-459.7376195	-460.9487730
		C_{2v}	-458.4398345	-459.7765447	-460.9880753
		C_s	Dissociation	Dissociation	Dissociation
3	0	D_{3h}	-229.6926545	-230.4073627	-231.0388813
		C_{3h}	-229.6942237	-230.4154256	-231.0479498
		C_{3v}	-229.7477066	-230.4602019	-231.0860307
		C_3	-229.7506837	-230.4642310	-231.0903306
3	1	C_{2v} #1	Dissociation	-306.6669484	-307.4911742
		C_{2v} #2	-305.7334247	-306.6682228	-307.4916076
		C_2	N/A	-306.6682690	N/A
		C_s #1	-305.8167887	Dissociation	Dissociation
		C_s #2	-305.8167887	-306.7458240	-307.5667148
3	2	C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	-381.8236078	-382.9777308	-383.9927247
3	3	C_{3v} #1	Dissociation	Dissociation	Dissociation
		C_{3v} #2	-457.9213761	-459.2734358	-460.4848241
		C_{3v} #3	Dissociation	Dissociation	Dissociation
		C_{3v} #4	-457.9327677	Dissociation	-460.5047278
4	0	T_d	-305.0213993	-305.9625686	-306.7845572
		D_{2d}	N/A	-305.9862117	-306.8108494
		C_{3v}	Dissociation	Dissociation	Dissociation
		C_3	Dissociation	Dissociation	-306.9317415
		C_{2v}	-305.0084681	-305.958589	-306.7818252
		C_s	Dissociation	-306.0105191	-306.9403428
4	1	C_{2v}	-381.0701016	-382.2384069	-383.2545525
		C_2	Dissociation	-382.2399876	-383.2551867
		C_s	Dissociation	Dissociation	Dissociation

4	2	D_{2h}	-457.0430240	-458.4132138	-459.6206375
		C_{2v} #1	Dissociation	Dissociation	Dissociation
		C_{2v} #2	Dissociation	Dissociation	Dissociation

Detached structure

Table 5A.10: Pb-O bond lengths in Angstroms for lowest energy minimum structures of of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

		Optimized Pb-O Bond Lengths (Å)						
n	**m**	**Point Group Symmetry**	**HF SDD/6-311+G***		**MP2 SDD/6-311+G***		**B3LYP/ SDD/6-311+G***	
			OH	**H_2O**	**OH**	**H_2O**	**OH**	**H_2O**
1	0	$C_{\infty v}$	1.943	N/A	1.966	N/A	1.963	N/A
1	1	C_s #1	2.021	2.432	2.062	2.412	2.055	2.404
1	2	C_s	2.066	2.483	2.118	2.453	2.115	2.450
1	3	C_s #1	2.119	2.340 2.425	N/A	N/A	N/A	N/A
		C_1 #1	N/A	N/A	2.145	2.558 2.637 2.471	N/A	N/A
		C_1 #2	N/A	N/A	N/A	N/A	2.145	2.674 2.472 2.556
1	4	C_1	--	--	2.169	2.576 2.676 2.628 2.646	2.176	2.581 2.658 2.626 2.746
2	0	C_{2v}	2.089	N/A	2.132	N/A	2.125	N/A
2	2	C_{2v} #3	2.174	2.662	2.237	2.605	2.238	2.609
3	0	C_3	2.195	N/A	2.236	N/A	2.236	N/A

Table 5A.11: Pb-O vibrational stretching frequencies, in wavenumbers, calculated at HF/SDD/6-311+G* for minimum energy structures of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	OH/H_2O	Mixing
1	0	$C_{\infty v}$	646.9	σ_g	OH	
1	1	C_s #1	261.2 553.5	a' a'	OH/H_2O OH/H_2O	
1	2	C_s #1	217.4 243.5 519.7 540.8	a" a' a' a'	H_2O OH/H_2O OH OH	 H_2O twisting H_2O wagging
1	3	C_s #1	171.2 196.8 232.1 452.4 514.7	a" a' a' a' a'	OH H_2O H_2O OH OH	H_2O wagging H_2O rocking H_2O rocking
2	0	C_{2v}	487.7 520.8	b_2 a_1	OH OH	
2	2	C_{2v} #3	124.9 161.9 202.0 389.8 434.5 447.2	b_1 a_1 a_1 b_1 b_2 a_1	H_2O H_2O H_2O H_2O OH OH/H_2O	 H_2O rocking
3	0	C_3	402.1 448.9	e a	OH OH	

Table 5A.12: Pb-O vibrational stretching frequencies, in wavenumbers, calculated at MP2/SDD/6-311+G* for minimum energy structure of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

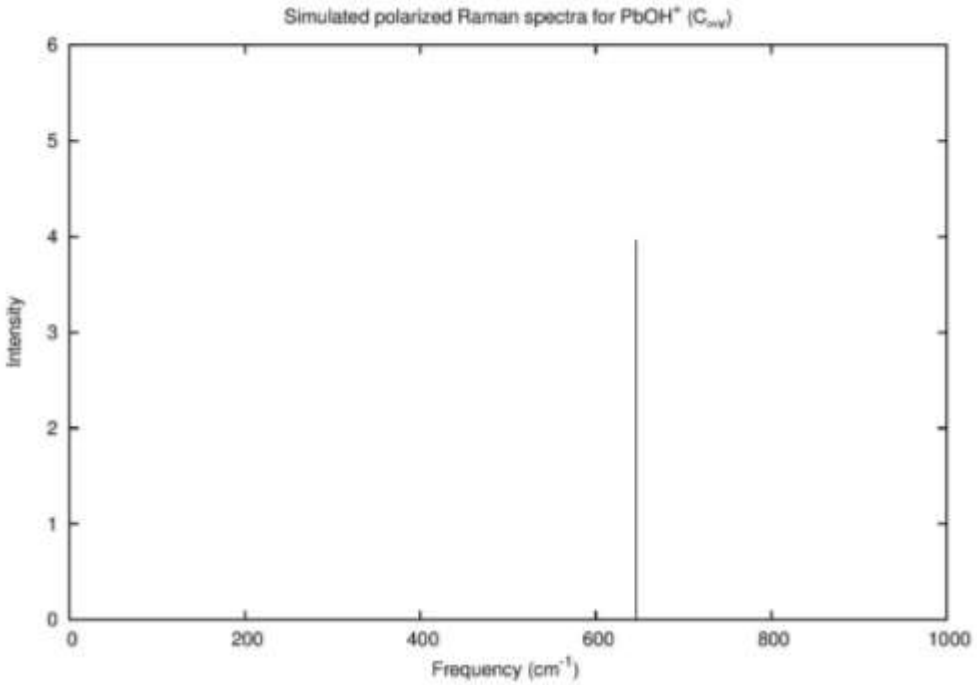
n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	OH/H_2O	Mixing
1	0	$C_{\infty v}$	618.9	σ_g	OH	
1	1	C_s #1	278.5 524.4	a' a'	OH/H_2O OH/H_2O	
1	2	C_s #1	225.6 253.9 262.3 487.9 527.5	a" a" a' a' a'	H_2O H_2O OH/H_2O OH OH	 H_2O wagging
1	3	C_1 #1	178.7 198.9 216.4 242.7 432.7 473.5 522.6	a a a a a a a	H_2O H_2O H_2O H_2O OH OH OH	H_2O twisting H_2O twist./wag. H_2O rocking H_2O wagging H_2O rocking
1	4	C_1	169.9 177.5 194.3 202.5 226.1 484.7	a a a a a a	H_2O H_2O H_2O H_2O OH/H_2O OH	H_2O twist./rock. H_2O twisting H_2O twisting H_2O twist./wag. H_2O twisting H_2O rocking
2	0	C_{2v}	462.3 488.7	b_2 a_1	OH OH	
2	2	C_{2v} #3	142.4 168.2 200.7 398.3 402.2 419.4	b_1 a_1 a_1 b_2 b_1 a_1	H_2O H_2O H_2O OH H_2O OH/H_2O	 H_2O rocking
3	0	C_3	384.9 423.6	e a	OH OH	

Table 5A.13: Pb-O vibrational stretching frequencies, in wavenumbers, calculated at B3LYP/SDD/6-311+G* for minimum energy structures of $[Pb(OH)_m(H_2O)_n]^{2-m}$, where m=1 – 4, n=0 – (6-m).

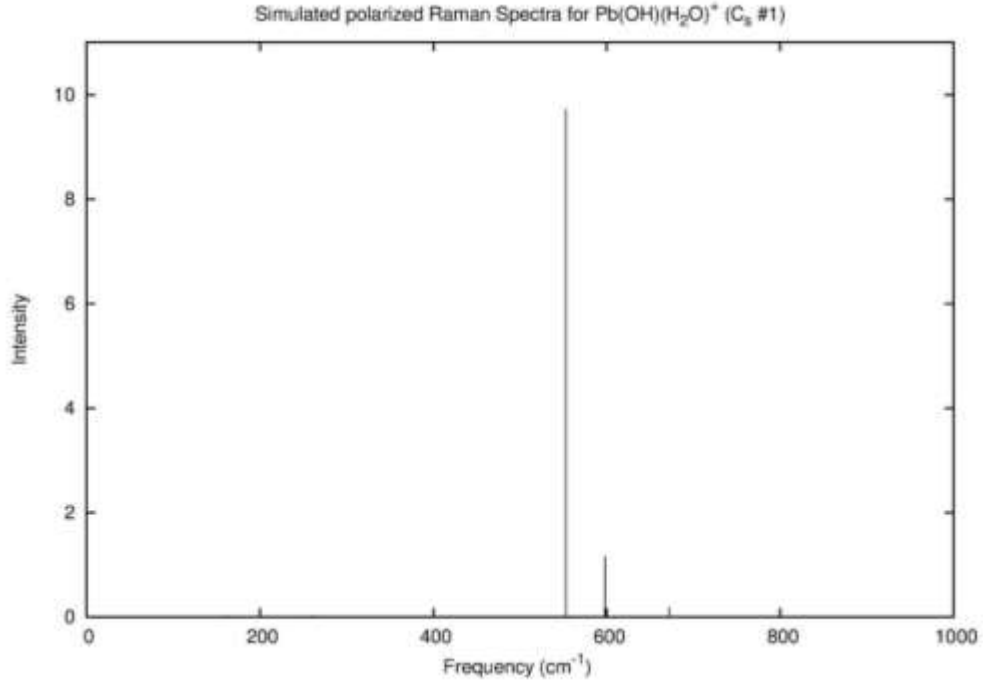
n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	OH/H_2O	Mixing
1	0	$C_{\infty v}$	614.8	σ_g	OH	
1	1	C_s #1	275.1 521.2	a' a'	OH/H_2O OH/H_2O	
1	2	C_s #1	235.7 255.2 483.5 533.6	a" a' a' a'	H_2O OH/H_2O OH OH	
1	3	C_1 #2	159.9 177.6 200.8 215.2 238.3 336.9 420.8 466.9	a a a a a a a a	H_2O H_2O H_2O H_2O OH/H_2O H_2O OH OH	H_2O twisting H_2O twist./wag. H_2O twisting H_2O rocking H_2O twisting H_2O rocking
1	4	C_1	170.2 185.9 193.3 202.5 209.3 455.6 463.6	a a a a a a a	H_2O H_2O OH/H_2O H_2O H_2O OH OH	H_2O twist./rock. H_2O twisting H_2O rock./wag. H_2O wagging H_2O twist./rock. H_2O rocking
2	0	C_{2v}	469.9 500.1	b_2 a_1	OH OH	
2	2	C_{2v} #3	147.2 170.5 200.7 392.8 412.3 413.0	b_1 a_1 a_1 b_2 b_1 a_1	H_2O H_2O H_2O OH H_2O OH/H_2O	 H_2O rocking
3	0	C_3	372.4 413.8	e a	OH OH	

Figure 5A-1: Simulated polarized Raman spectra for $[Pb(OH)_n(H_2O)_m]^{2-n}$, where n=1 – 4, m=0 – (6-n).

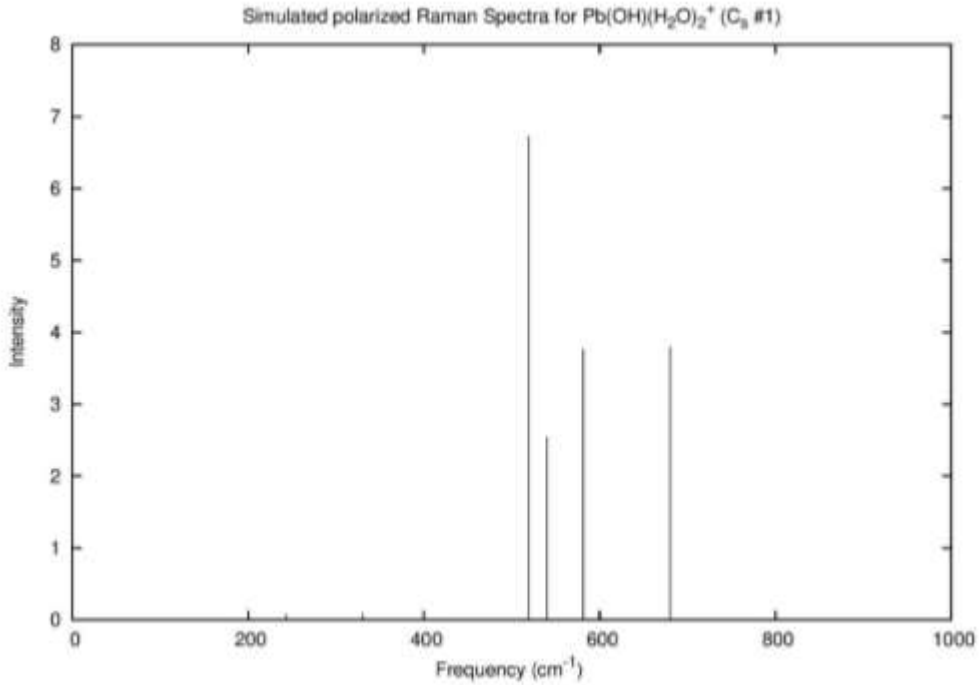
$[Pb(OH)]^+$



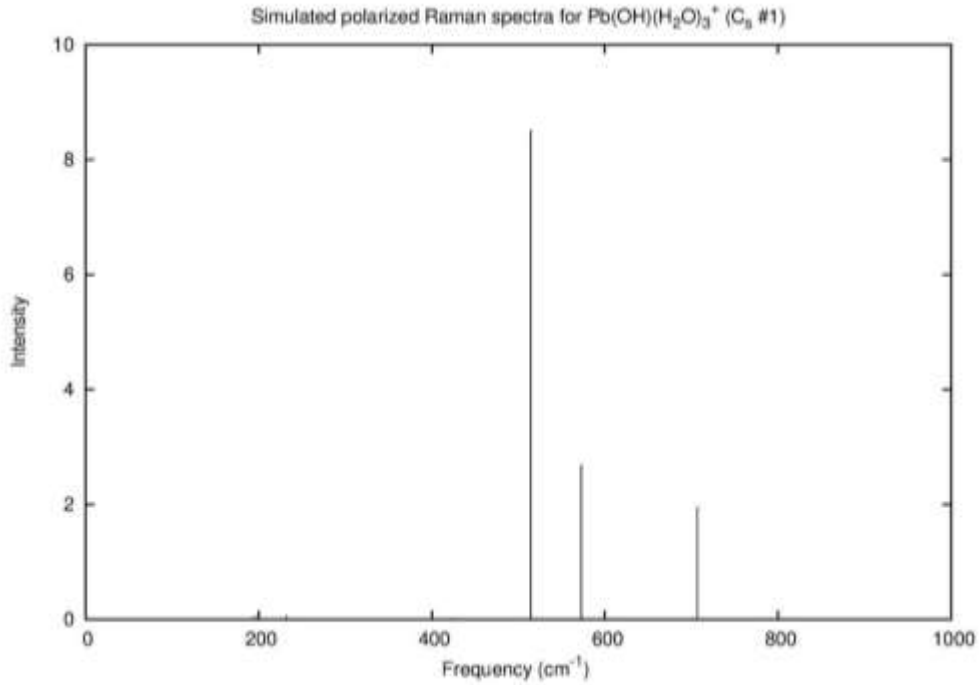
$[Pb(OH)(H_2O)]^+$



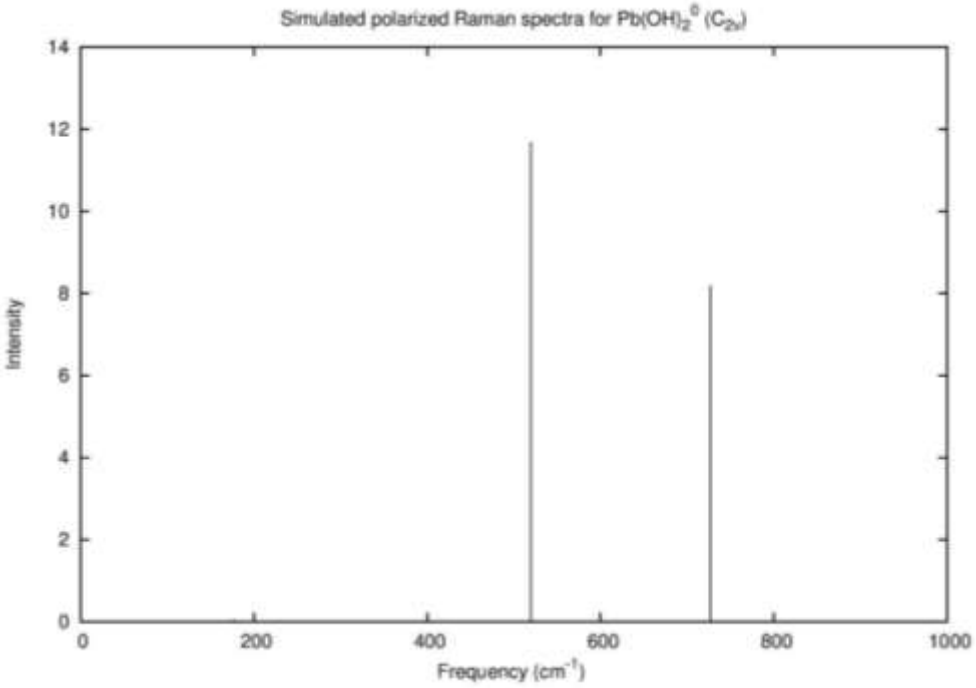
$[Pb(OH)(H_2O)_2]^+$



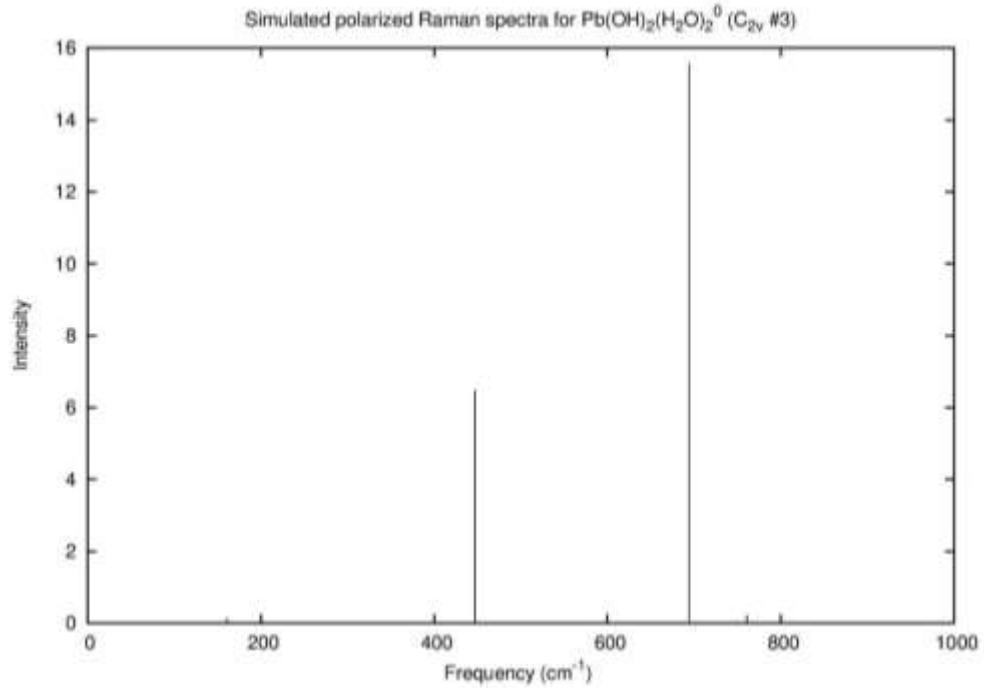
$[Pb(OH)(H_2O)_3]^+$



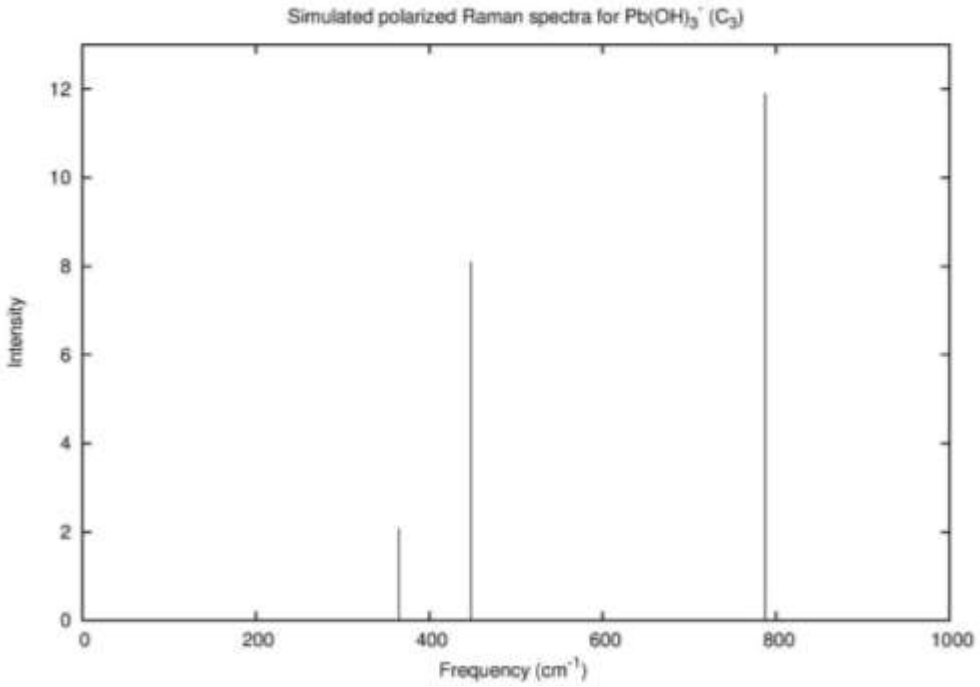
$[Pb(OH)_2]^0$



$[Pb(OH)_2(H_2O)_2]^0$



$[Pb(OH)_3]^-$


Simulated polarized Raman spectra for Pb(OH)3- (C3)
Intensity
Frequency (cm-1)
0
2
4
6
8
10
12
0
200
400
600
800
1000

CHAPTER 6 - APPENDIX A

SUPPLEMENTARY MATERIALS

Table 6A.1: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ CEP-121G**	**MP2/6-31G*/ CEP-121G**	**B3LYP/6-31G*/ CEP-121G**
1	0	C_{3v}	-58.9332771	-59.1279054	-59.3693047
1	1	C_s #1	-135.0318999	-135.4192365	-135.8764195
		C_s #2	-135.0317401	-135.4187487	-135.8755128
		C_1	-135.0324977	-135.4197939	-135.8769014
1	2	C_s	-211.1191558	-211.6978829	-212.3683475
		C_1	-211.1205194	-211.6994958	-212.3697297
1	3	C_{3v} #1	-287.1835780	-287.9534801	-288.8372356
		C_{3v} #2	-287.1823014	-287.9525895	-288.8359131
		C_{3v} #3	-287.1827412	-287.9522854	-288.8358525
		C_{3v} #4	-287.1848594	-287.9550586	-288.8378742
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	N/A	N/A
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.1853114	-287.9554991	-288.8386480
		C_1	N/A	N/A	N/A
1	4	C_s #1	-363.2483981	-364.2090252	-365.3017556
		C_s #2	-363.2478287	-364.2084798	-365.3013820
		C_1	-363.2488194	-364.2099382	-365.3025693
1	5	C_s #1	-439.2911101	-440.4422834	-441.7466918
		C_s #2	-439.2906178	-440.4430805	-441.7477036
		C_1	-439.2981935	-440.4507015	-441.7554670
2	0	D_{3h}	-115.1915790	-115.5623054	-116.0006826
		D_{3d}	-115.1915798	-115.5623059	-116.0006828
		D_3	-115.1915798	-115.5623055	-116.0006967
		C_{2v}	-115.2229687	-115.5955871	-116.0353952
		C_2	-115.2237351	-115.5962863	-116.0359474
2	1	C_{2v} #1	-191.2818282	-191.8456626	-192.5007621
		C_{2v} #2	-191.2822432	-191.8460208	-192.5009449
		C_{2v} #3	-191.2818993	-191.8456447	-192.4999458
		C_{2v} #4	-191.2823729	-191.8460635	-192.5002052
		C_2	-191.2823729	-191.8460635	-192.5009484
		C_s #1	-191.3088494	-191.8732534	-192.5261301
		C_s #2	-191.2900475	-191.8531595	-192.5053273
		C_1	N/A	N/A	N/A
2	2	C_{2h} #1	-267.3409426	-268.0940285	-268.9758070
		C_{2h} #2	-267.3415580	-268.0942814	-268.9587911

		C_{2v} #1	-267.3419115	-268.0949542	-268.9595660
		C_{2v} #2	-267.3419210	-268.0953210	-268.9605901
		C_{2v} #3	-267.3430536	-268.0965970	-268.9614070
		C_{2v} #4	-267.3414424	-268.0948684	-268.9594952
		C_s #1	-267.3750036	-268.1300154	-268.9936811
		C_1	-267.3761243	-268.1309976	-268.9947806
2	3	D_{3h} #1	-343.4085534	-344.3525919	-345.4311848
		D_{3h} #2	-343.4078493	-344.3519806	-345.4305918
		D_{3h} #3	-343.4069464	-344.3516239	-345.4304057
		D_{3h} #4	-343.4086752	-344.3534710	-345.4321985
		D_3	-343.4093307	-344.3539591	-345.4326891
		C_{3v}	-343.4088086	-344.3535135	-345.4322116
		C_3	-343.4095655	-344.3541351	-345.4327054
		C_{2v}	-343.4163317	-344.3620263	-345.4395857
		C_2	-343.4194152	-344.3652424	-345.4424517
		C_s	-343.4257265	-344.3721153	-345.4485270
2	4	C_{2h} #1 (trans)	-419.4625664	-420.5969055	-421.8857181
		C_{2h} #2 (trans)	-419.4625997	-420.5969329	-421.8857985
		C_{2v} #1 (cis)	-419.4662721	-420.6018049	-421.8896625
		C_{2v} #2 (cis)	-419.4662087	-420.6011288	-421.8886418
		C_{2v} #3 (cis)	-419.4694540	-420.6046759	-421.8910268
		C_{2v} #4 (cis)	-419.4731852	-420.6091307	-421.8949579
		C_2	-419.4783690	-420.6169231	-421.9037472
3	0	C_{3v} #1	-171.4952340	-172.0447596	-172.6804855
		C_{3v} #2	-171.4971830	-172.0467018	-172.6821310
		C_3	-171.4971832	-172.0467019	-172.6821701
3	1	C_s #1	-247.5521484	-248.2921532	-249.1398694
		C_s #2	-247.5523293	-248.2924295	-249.1399532
		C_s #3	-247.5507222	-248.2908080	-249.1386446
		C_s #4	-247.5522263	-248.2926066	-249.1405772
		C_1	-247.5582173	-248.2980968	-249.1440834
3	2	C_s #1	-323.6037299	-324.5348596	-325.5931301
		C_s #2	-323.6041935	-324.5340618	-325.5910356
		C_s #3	-323.6009001	-324.5310452	-325.5884863
		C_s #4	-323.6046406	-324.5346279	-325.5916685
		C_1	-323.6046444	-324.5356135	-325.7121240

3	3	C_{3v} #1	-399.6439602	-400.7649481	-402.0343249
		C_{3v} #2	-399.6450511	-400.7653510	-402.0355558
		C_{3v} #3	-399.6581528	-400.7799205	-402.0473534
		C_{3v} #4	-399.6549156	-400.7759551	-402.0434674
		C_3	-399.6581895	-400.7799493	-402.0478759
		C_s	-399.6579916	N/A	N/A
		C_1	-399.6564974	N/A	N/A
4	0	T_d #1	-227.7143271	-228.4403209	-229.2762622
		T_d #2	-227.7138892	-228.4397054	-229.2754185
		C_3	-227.7184049	-228.4429062	-229.2765625
		C_s	-227.7309763	-228.4559648	-229.2896257
		C_1	-227.7374408	-228.4619958	-229.2899432
4	1	C_{2v} #1	-303.7812863	-304.6955743	-305.7347580
		C_{2v} #2	-303.7804250	-304.6949603	-305.7343821
		C_{2v} #3	-303.7808286	-304.6952513	-305.7344880
		C_{2v} #4	-303.7821263	-304.6965375	-305.7356722
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	-305.7357509
4	2	C_{2h} #1	-379.8179004	-380.9212337	-382.1742550
		C_{2h} #2	-379.8184659	-380.9218598	-382.1748268
		C_2	-379.8223864	-380.9266431	-382.1785789
		C_s	-379.8222008	-380.9265253	-382.1784893
		C_1	-379.8276585	-380.9328806	-382.1828973
5	0	C_{3h} #1	-283.9481872	-284.8472837	-285.8739976
		C_{3h} #2	-283.9481843	-284.8472837	-285.8740044
		C_{3v} #1	-283.9478987	-284.8467405	-285.8730735
		C_{3v} #2	-283.9478987	-284.8467405	-285.8730725
		C_3	-283.9489992	-284.8479641	-285.8741892
		C_s	-283.9657901	-284.8649255	-285.8858089
		C_1	-283.9661755	-284.8653055	-285.8861530
5	1	C_s #1	-360.0057812	-361.0951455	-362.3269855
		C_s #2	-360.0054117	-361.0946126	-362.3267262
		C_s #3	-360.0054115	-361.0946124	-362.3267264
		C_s #4	-360.0057813	-361.0951455	-362.2602004
		C_1	-360.0034734	-361.0988208	-362.3320207
6	0	C_s #1	-340.0002785	-341.1089228	-342.3192391
		C_s #2	-340.0001162	-341.2533462	-342.4671857
		C_s #3	-340.0043086	-341.0941037	-342.3194016
		C_1	-340.1826712	-341.2561164	-342.4693006

Detached structure

Table 6A.2: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ LANL2DZ**	**MP2/6-31G*/ LANL2DZ**	**B3LYP/6-31G*/ LANL2DZ**
1	0	C_{3v}	-58.9088501	-59.1046150	-59.3418624
1	1	C_s #1	-134.9971293	-135.3853180	-135.8385565
		C_s #2	-134.9969765	-135.3847662	-135.8375329
		C_1	-134.9977433	-135.3858962	-135.8390527
1	2	C_s #1	-211.0731014	-211.6523639	-212.3188386
		C_1	-211.0744558	-211.6538983	-212.3200406
1	3	C_{3v} #1	-287.1285117	-287.8982590	-288.7773096
		C_{3v} #2	-287.1267125	-287.8970481	-288.7760400
		C_{3v} #3	-287.1275301	-287.8969599	-288.7758844
		C_{3v} #4	-287.1289983	-287.8993281	-288.7778992
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	N/A	N/A
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.1296107	-287.8997842	-288.7784996
		C_1	-287.1346214	N/A	N/A
1	4	C_s #1	-363.1844516	-364.1445933	-365.2333257
		C_s #2	-363.1840061	-364.1441215	-365.2330744
		C_1	-363.1846421	-364.1451092	-365.2338947
1	5	C_s #1	-439.2217098	-440.3711399	-441.6713304
		C_s #2	-439.2219767	-440.3726408	-441.6728806
		C_1	-439.2295397	-440.3906541	-441.6834257
2	0	D_{3h}	-115.1610842	-115.5331454	-115.9677097
		D_{3d}	-115.1610856	-115.5331469	-115.9677112
		D_3	-115.1610857	-115.5331470	-115.9677298
		C_{2v}	-115.1894279	-115.5626777	-115.9985296
		C_2	-115.1901604	-115.5633777	-115.9991146
2	1	C_{2v} #1	-191.2402609	-191.8044138	-192.4548061
		C_{2v} #2	-191.2408113	-191.8049278	-192.4551692
		C_{2v} #3	-191.2404690	-191.8045864	-192.4542770
		C_{2v} #4	-191.2410597	-191.8051387	-192.4546926
		C_2	-191.2410597	-191.8051387	-192.4551692
		C_s #1	-191.2637006	-191.8284425	-192.4772715
		C_s #2	-191.2476920	-191.8113568	-192.4597527
		C_1	N/A	N/A	-192.4772471
2	2	C_{2h} #1	-267.2925830	-268.0463424	-268.9297790
		C_{2h} #2	-267.2929869	-268.0462297	-268.9068167

		C_{2v} #1	-267.2930890	-268.0464669	-268.9070405
		C_{2v} #2	-267.2929779	-268.0468044	-268.9083420
		C_{2v} #3	-267.2939347	-268.0477916	-268.9087286
		C_{2v} #4	-267.2926803	-268.0464017	-268.9075782
		C_s #1	-267.3204256	-268.0754345	-268.9351915
		C_1	-267.3212650	-268.0764636	-268.9363613
2	3	D_{3h} #1	-343.3496669	-344.2933097	-345.3671196
		D_{3h} #2	-343.3489828	-344.2926730	-345.3665351
		D_{3h} #3	-343.3484294	-344.2929212	-345.3672526
		D_{3h} #4	-343.3500249	-344.2946623	-345.3689800
		D_3	-343.3504519	-344.2948553	-345.3690977
		C_{3v}	-343.3500264	-344.2946623	-345.3689800
		C_3	-343.3505425	-344.2948577	-345.3691031
		C_{2v}	-343.3567630	-344.3013758	-345.3741777
		C_2	-343.3598322	-344.3047029	-345.3773203
		C_s	-343.3676690	-344.3140783	-345.4470552
2	4	C_{2h} #1 (trans)	-419.3977591	-420.5312787	-421.8157431
		C_{2h} #2 (trans)	-419.3978095	-420.5313264	-421.8158311
		C_{2v} #1 (cis)	-419.4001679	-420.5344418	-421.8179500
		C_{2v} #2 (cis)	-419.3995477	-420.5331717	-421.8165477
		C_{2v} #3 (cis)	-419.4037977	-420.5377218	-421.8199994
		C_{2v} #4 (cis)	-419.4052547	-420.5393532	-421.8210651
		C_2	-419.4089609	-420.5441074	-421.8270049
3	0	C_{3v} #1	-171.4511234	-172.0010195	-172.6326758
		C_{3v} #2	-171.4528265	-172.0027657	-172.6342327
		C_3	-171.4528265	-172.0027657	-172.6821701
3	1	C_s #1	-247.5000166	-248.2399626	-249.0831902
		C_s #2	-247.4996103	-248.2396545	-249.0828954
		C_s #3	-247.4984369	-248.2383570	-249.0818184
		C_s #4	-247.5006406	-248.2409806	-249.0845460
		C_1	-247.5048389	-248.2448065	-249.0869719
3	2	C_s #1	-323.5463201	-324.4769269	-325.5309971
		C_s #2	-323.5433421	-324.4727450	-325.5260377
		C_s #3	-323.5410007	-324.4705084	-325.5241486
		C_s #4	-323.5437979	-324.4733095	-325.5266014
		C_1	-323.5450869	-324.4829678	-325.5265065

3	3	C_{3v} #1	-399.5792132	-400.6981528	-401.9629936
		C_{3v} #2	-399.5817242	-400.7004477	-401.9658522
		C_{3v} #3	-399.5920027	-400.7118903	-401.9753649
		C_{3v} #4	-399.5898201	-400.7092859	-401.9729078
		C_3	-399.5922727	-400.7126021	-401.9774597
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.6657222	-228.3917585	-229.2224785
		T_d #2	-227.6652371	-228.3911094	-229.2216137
		C_3	-227.6313673	-228.3944905	-229.2230402
		C_s	-227.6793960	-228.4044347	-229.2343223
		C_1	-227.6852696	-228.4099828	-229.2344112
4	1	C_{2v} #1	-303.7223665	-304.6363752	-305.6721605
		C_{2v} #2	-303.7217651	-304.6359799	-305.6718512
		C_{2v} #3	-303.7218628	-304.6359582	-305.6717426
		C_{2v} #4	-303.7231536	-304.6373056	-305.6729630
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.7577386	-380.8606363	-382.1094954
		C_{2h} #2	-379.7582717	-380.8612585	-382.1101057
		C_2	-379.7600396	-380.8632037	-382.1111713
		C_s	-379.7598676	-380.8630825	-382.1110447
		C_1	-379.7626827	-380.8666613	-382.1136435
5	0	C_{3h} #1	-283.8950859	-284.7942791	-285.8163260
		C_{3h} #2	-283.8950860	-284.7942791	-285.8163331
		C_{3v} #1	-283.8944948	-284.7934138	-285.8153135
		C_{3v} #2	-283.8944948	-284.7934138	-285.8153193
		C_3	-283.8953430	-284.7944080	-285.8163513
		C_s	-283.9081746	-284.8072042	-285.8249076
		C_1	-283.9084640	-284.8074788	-285.8251590
5	1	C_s #1	-359.9436053	-361.0317092	-362.2601486
		C_s #2	-359.9434990	-361.0314773	-362.2601476
		C_s #3	-359.9434990	-361.0314773	-362.2601476
		C_s #4	-359.9436053	-361.0951455	-362.2193183
		C_1	-359.9491573	-361.0400551	-362.2699803
6	0	C_s #1	-339.9350496	-341.0360640	-342.2398047
		C_s #2	-339.9348873	-341.1923555	-342.4033962
		C_s #3	-339.9315109	-341.0306641	-342.2392151
		C_1	-340.1210615	-341.1934340	-342.4037931

Detached structure

Table 6A.3: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31G*/ SDD**	**MP2/6-31G*/ SDD**	**B3LYP/6-31G*/ SDD**
1	0	C_{3v}	-58.8821178	-59.0808636	-59.3184726
1	1	C_s #1	-134.9625308	-135.3559149	-135.8069249
		C_s #2	-134.9623613	-135.3552609	-135.8058795
		C_1	-134.9629503	-135.3563298	-135.8073299
1	2	C_s #1	-211.0326720	-211.6187987	-212.2815915
		C_1	-211.0336982	-211.6198992	-212.2823812
1	3	C_{3v} #1	-287.0877314	-287.8641265	-288.7388546
		C_{3v} #2	-287.0855929	-287.8620115	-288.7367752
		C_{3v} #3	-287.0863933	-287.8623810	-288.7371136
		C_{3v} #4	-287.0871142	-287.8637069	-288.7380171
		C_s #1	-287.0878304	-287.8645247	-288.7389984
		C_s #2	N/A	N/A	N/A
		C_3 #1	-287.0880932	-287.8647006	-288.7392165
		C_3 #2	N/A	N/A	N/A
		C_1	-287.0909607	-287.8684711	-288.7414920
1	4	C_s #1	-363.1405490	-364.1077233	-365.1915773
		C_s #2	-363.1404432	-364.1076544	-365.1916457
		C_1	-363.1407849	-364.1082814	-365.1923850
1	5	C_s #1	-439.1788233	-440.3344040	-441.6304181
		C_s #2	-439.1788294	-440.3353956	-441.6304749
		C_1	-439.1843431	-440.3440124	-441.6556759
2	0	D_{3h}	-115.1306339	-115.5065633	-115.9392072
		D_{3d}	-115.1306348	-115.5065639	-115.9392081
		D_3	-115.1306348	-115.5065633	-115.9392203
		C_{2v}	-115.1544592	-115.5344206	-115.9666231
		C_2	-115.1549536	-115.5349134	-115.9670148
2	1	C_{2v} #1	-191.2053214	-191.7753093	-192.4219262
		C_{2v} #2	-191.2056173	-191.7756115	-192.4221216
		C_{2v} #3	-191.2052944	-191.7750767	-192.4210888
		C_{2v} #4	-191.2056525	-191.7754546	-192.4213674
		C_2	-191.2056525	-191.7756116	-192.4221225
		C_s #1	-191.2229235	-191.7958791	-192.4397591
		C_s #2	-191.2100191	-191.7804968	-192.4245185
		C_1	-191.2230441	N/A	-192.4397527
2	2	C_{2h} #1	-267.2555210	-268.0149297	-268.8905140
		C_{2h} #2	-267.2557878	-268.0146287	-268.8709791

		C_{2v} #1	-267.2558178	-268.0146833	-268.8710990
		C_{2v} #2	-267.2556628	-268.0151200	-268.8724386
		C_{2v} #3	-267.2563071	-268.0156606	-268.8724409
		C_{2v} #4	-267.2554511	-268.0146384	-268.8715439
		C_s #1	-267.2775479	-268.0411471	-268.8953179
		C_1	-267.2783308	-268.0421835	-268.8965086
2	3	D_{3h} #1	-343.3106151	-344.2601901	-345.3291928
		D_{3h} #2	-343.3098884	-344.2593845	-345.3284745
		D_{3h} #3	-343.3090888	-344.2589876	-345.3285822
		D_{3h} #4	-343.3104132	-344.2604674	-345.3300439
		D_3	-343.3109894	-344.2608933	-345.3302970
		C_{3v}	-343.3104133	-344.2604675	-345.3300440
		C_3	-343.3109893	-344.2608933	-345.3302997
		C_{2v}	-343.3157451	-344.2673625	-345.3351558
		C_2	-343.3184423	-344.2704981	-345.3380590
		C_s	-343.3233736	-344.2784450	-345.3874473
2	4	C_{2h} #1 (trans)	-419.3575967	-420.4970250	-421.7763330
		C_{2h} #2 (trans)	-419.3576491	-420.4970942	-421.7764359
		C_{2v} #1 (cis)	-419.3581339	-420.4983249	-421.7767429
		C_{2v} #2 (cis)	-419.3579245	-420.4977394	-421.7764692
		C_{2v} #3 (cis)	-419.3608899	-420.5023577	-421.7788039
		C_{2v} #4 (cis)	-419.3618987	-420.5034725	-421.7794184
		C_2	-419.3656779	-420.5091085	-421.7859438
3	0	C_{3v} #1	-171.4107380	-171.9702644	-172.5957634
		C_{3v} #2	-171.4119439	-171.9716063	-172.5969055
		C_3	-171.4119441	-171.9716064	-172.5969410
3	1	C_s #1	-247.5000166	-248.2077765	-249.0446743
		C_s #2	-247.4578962	-248.2069851	-249.0439477
		C_s #3	-247.4571382	-248.2060374	-249.0432153
		C_s #4	-247.4594040	-248.2092906	-249.0465055
		C_1	-247.4619347	-248.2117184	-249.0474797
3	2	C_s #1	-323.5039786	-324.4439346	-325.4912442
		C_s #2	-323.4994432	-324.4374558	-325.4839879
		C_s #3	-323.4974776	-324.4354873	-325.4824617
		C_s #4	-323.4998907	-324.4380505	-325.4844732
		C_1	-323.4999293	-324.4477400	-325.4848655
3	3	C_{3v} #1	-399.5373770	-400.6635646	-401.9224806

		C_{3v} #2	-399.5399282	-400.6669973	-401.9261867
		C_{3v} #3	-399.5478068	-400.6776458	-401.9338699
		C_{3v} #4	-399.5461554	-400.6746404	-401.9312115
		C_3	-399.5484651	-400.6786113	-401.9365456
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.6291357	-228.3625334	-229.1875051
		T_d #2	-227.6287711	-228.3620157	-229.1868236
		C_3	-227.7227200	-228.3644437	-229.1875887
		C_s	-227.6380966	-228.3727002	-229.1943370
		C_1	-227.6422615	-228.3772827	-229.1943192
4	1	C_{2v} #1	-303.6786705	-304.6019692	-305.6303017
		C_{2v} #2	-303.6784079	-304.6018433	-305.6302266
		C_{2v} #3	-303.6782602	-304.6015690	-305.6299056
		C_{2v} #4	-303.6794882	-304.6029758	-305.6311029
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.7175154	-380.8277022	-382.0701061
		C_{2h} #2	-379.7179616	-380.8282349	-382.0706261
		C_2	-379.7185355	-380.8293990	-382.0710841
		C_s	-379.7183185	-380.8291710	-382.0708755
		C_1	-379.7197790	-380.8324630	-382.0723148
5	0	C_{3h} #1	-283.8561953	-284.7635389	-285.7788279
		C_{3h} #2	-283.8561953	-284.7635389	-285.7788342
		C_{3v} #1	-283.8555528	-284.7627433	-285.7779651
		C_{3v} #2	-283.8555528	-284.7627433	-285.7779760
		C_3	-283.8561975	-284.7635465	-285.7788266
		C_s	-283.8646853	-284.7741234	-285.7836779
		C_1	-283.8649105	-284.7743348	-285.7838823
5	1	C_s #1	-359.9007904	-360.9982282	-362.2194049
		C_s #2	-359.9007536	-360.9981601	-362.2193391
		C_s #3	-359.9007536	-360.9981601	-362.2193051
		C_s #4	-359.9007904	-360.9982282	-362.3470166
		C_1	-359.9047995	-361.0063589	-362.2278695
6	0	C_s #1	-339.8532302	-340.9705835	-342.1671014
		C_s #2	-339.8530727	-341.1594777	-342.3639229
		C_s #3	-339.8595115	-340.9710174	-342.1710136
		C_1	-340.0783018	-341.1603120	-342.3639311

Detached structure

Table 6A.4: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**M**	**Point Group**	**HF/6-31+G*/ CEP-121G**	**MP2/6-31+G*/ CEP-121G**	**B3LYP/6-31+G*/ CEP-121G**
1	0	C_{3v}	-58.9346827	-59.1301714	-59.3708375
1	1	C_s #1	-135.0357616	-135.4278391	-135.8824647
		C_s #2	-135.0353824	-135.4270038	-135.8813004
		C_1	-135.0365233	-135.4283009	-135.8830708
1	2	C_s	-211.1258162	-211.7134589	-212.3797153
		C_1	-211.1269899	-211.7149277	-212.3808080
1	3	C_{3v} #1	-287.1936547	-287.1895222	-288.8549082
		C_{3v} #2	-287.1925772	-287.9766236	-288.8537016
		C_{3v} #3	-287.1936506	-287.9769766	-288.8544814
		C_{3v} #4	-287.1961823	-287.9793214	-288.8565553
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	N/A	N/A
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.1963466	-287.9797186	-288.8569912
		C_1	N/A	N/A	N/A
1	4	C_s #1	-363.2643231	-364.2447366	-365.3292364
		C_s #2	-363.2640432	-364.2443771	-365.3290200
		C_1	-363.2644277	-364.2448811	-365.3292673
1	5	C_s #1	-439.3121854	-440.4886806	-441.7837550
		C_s #2	-439.3107100	-440.4886006	-441.7830713
		C_1	-439.3179915	-440.4959733	-441.7899847
2	0	D_{3h}	-115.1929442	-115.5666240	-116.0031170
		D_{3d}	-115.1929457	-115.5666250	-116.0031182
		D_3	-115.1929457	-115.5666242	-116.0031315
		C_{2v}	-115.2245836	-115.5997854	-116.0374193
		C_2	-115.2255440	-115.6004693	-116.0381280
2	1	C_{2v} #1	-191.2868636	-191.8579729	-192.5090615
		C_{2v} #2	-191.2874232	-191.8583377	-192.5093215
		C_{2v} #3	-191.2866167	-191.8575063	-192.5079055
		C_{2v} #4	-191.2872383	-191.8579341	-192.5082796
		C_2	-191.2874230	-191.8584033	-192.5093245
		C_s #1	-191.3130911	-191.8842301	-192.5330120
		C_s #2	-191.2954302	-191.8658983	-192.5141476
		C_1	-191.3133090	-191.8844911	-192.5331353
2	2	C_{2h} #1	-267.3502276	-268.1158018	-269.0615717

		C_{2h} #2	-267.3505793	-268.1154837	-268.9748705
		C_{2v} #1	-267.3506469	-268.1156350	-268.9749494
		C_{2v} #2	-267.3512066	-268.1167870	-268.9767888
		C_{2v} #3	-267.3519830	-268.1174067	-268.9770985
		C_{2v} #4	-267.3502431	-268.1159394	-268.9754649
		C_s #1	-267.3833062	-268.1507565	-269.0081637
		C_1	-267.3847237	-268.1520726	-268.8965086
2	3	D_{3h} #1	-343.4218285	-344.3829647	-345.4543518
		D_{3h} #2	-343.4212752	-344.3820521	-345.4538103
		D_{3h} #3	-343.4197666	-344.3815459	-345.4525681
		D_{3h} #4	-343.4218094	-344.3830168	-345.4548480
		D_3	-343.4223983	-344.3839530	-345.4553224
		C_{3v}	-343.4219428	-344.3830377	-345.4548480
		C_3	-343.4224637	-344.3839536	-345.4553261
		C_{2v}	-343.4294523	-344.3924073	-345.4621263
		C_2	-343.4335508	-344.3967088	-345.4662662
		C_s	-343.4392369	-344.4036721	-345.3458149
2	4	C_{2h} #1 (trans)	-419.4832214	-420.6408698	-421.9205654
		C_{2h} #2 (trans)	-419.4832255	-420.6409542	-421.9205711
		C_{2v} #1 (cis)	-419.4847813	-420.6434209	-421.9217350
		C_{2v} #2 (cis)	-419.4855739	-420.6440071	-421.9222318
		C_{2v} #3 (cis)	-419.4879239	-420.6469849	-421.9235725
		C_{2v} #4 (cis)	-419.4919948	-420.6515496	-421.9273855
		C_2	-419.4963761	-420.6582865	-421.9335910
3	0	C_{3v} #1	-171.4971234	-172.0518871	-172.6833161
		C_{3v} #2	-171.4993747	-172.0534625	-172.6852426
		C_3	-171.4993745	-172.0536416	-172.6852813
3	1	C_s #1	-247.5587019	-248.3085622	-249.1506215
		C_s #2	-247.5590944	-248.3087958	-249.1508120
		C_s #3	-247.5570095	-248.3074299	-249.1490706
		C_s #4	-247.5582196	-248.3087150	-249.1505590
		C_1	-247.5643869	-248.3147158	-249.1545350
3	2	C_s #1	-323.6141659	-324.5611977	-325.6111593
		C_s #2	-323.6152316	-324.5611734	-325.6098349
		C_s #3	-323.6115296	-324.5574722	-325.6063005
		C_s #4	-323.6156521	-324.5616974	-325.6103451
		C_1	N/A	N/A	-325.6102884

3	3	C_{3v} #1	-399.6596419	-400.8010162	-402.0613082
		C_{3v} #2	-399.6606335	-400.8024317	-402.0631877
		C_{3v} #3	-399.6733136	-400.8171518	-402.0737195
		C_{3v} #4	-399.6699956	-400.8129627	-402.0700586
		C_3	-399.6733567	-400.8171610	-402.0740635
		C_s	-399.6735569	-400.8171371	-402.0737869
		C_1	-399.6723970	-400.8167354	-402.0742016
4	0	T_d #1	-227.7186155	-228.4516148	-229.2823765
		T_d #2	-227.7184184	-228.4511262	-229.2817602
		C_3	-227.6770981	-228.4549863	-229.2830343
		C_s	-227.7353079	-228.4732928	-229.2954312
		C_1	-227.7410444	-228.4738832	-229.2956301
4	1	C_{2v} #1	-303.7898168	-304.7181744	-305.7489792
		C_{2v} #2	-303.7885210	-304.7175792	-305.7481213
		C_{2v} #3	-303.7891145	-304.6600867	-305.7484553
		C_{2v} #4	-303.7905404	-304.7195245	-305.7498081
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.8338942	-380.9568458	-382.2002685
		C_{2h} #2	-379.8345213	-380.9575382	-382.2010412
		C_2	-379.8370372	-380.9612472	-382.2031952
		C_s	-379.8365389	-380.9609373	-382.2026768
		C_1	-379.8408123	-380.9662289	-382.2053454
5	0	C_{3h} #1	-283.9558614	-284.8660492	-285.8854239
		C_{3h} #2	-283.9558614	-284.8660492	-285.8854308
		C_{3v} #1	-283.9554349	-284.8656358	-285.8845191
		C_{3v} #2	-283.9554349	-284.8656358	-285.8845179
		C_3	-283.9566278	-284.8663284	-285.8856143
		C_s	-283.9724278	-284.8837691	-285.8962030
		C_1	-283.9728177	-284.8843682	-285.8965866
5	1	C_s #1	-360.0180553	-361.1253319	-362.3472420
		C_s #2	-360.0177307	-361.1247382	-362.3468099
		C_s #3	-360.0177307	-361.1247382	-362.3468181
		C_s #4	-360.0180553	-361.1253319	-362.2838211
		C_1	-360.0184669	-361.1277026	-362.3498201
6	0	C_s #1	-340.0184106	-341.1365910	-342.3335777
		C_s #2	-340.0183383	-341.2790997	-342.4827063
		C_s #3	-340.0119744	-341.1349579	-342.3331641
		C_1	-340.1916797	-341.2819493	-342.4840687

Detached structure

Table 6A.5: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ LANL2DZ**	**MP2/6-31+G*/ LANL2DZ**	**B3LYP/6-31+G*/ LANL2DZ**
1	0	C_{3v}	-58.9147437	-59.1116571	-59.3487221
1	1	C_s #1	-135.0046460	-135.3978960	-135.8489573
		C_s #2	-135.0042829	-135.3970259	-135.8477663
		C_1	-135.0052821	-135.3982739	-135.8494903
1	2	C_s	-211.0829342	-211.6715524	-212.3342920
		C_1	-211.0840461	-211.6728710	-212.3808080
1	3	C_{3v} #1	-287.1422687	-287.9263492	-288.8000022
		C_{3v} #2	-287.1407630	-287.9256100	-288.7988995
		C_{3v} #3	-287.1416838	-287.9253918	-288.7991681
		C_{3v} #4	-287.1433018	-287.9274367	-288.8009094
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	N/A	N/A
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.1437151	-287.9279459	-288.8014361
		C_1	-287.1478825	-287.9326857	-288.8047267
1	4	C_s #1	-363.2030709	-364.1833812	-365.2651860
		C_s #2	-363.2029034	-364.1831048	-365.2651534
		C_1	-363.2031137	-364.1834478	-365.2652603
1	5	C_s #1	-439.2462245	-440.4217047	-441.7141422
		C_s #2	-439.2464337	-440.4222077	-441.7140729
		C_1	-439.2526124	-440.4361302	-441.7233706
2	0	D_{3h}	-115.1670530	-115.5420232	-115.9754075
		D_{3d}	-115.1670544	-115.5420243	-115.9754090
		D_3	-115.1670544	-115.5420243	-115.9754280
		C_{2v}	-115.1940055	-115.5701526	-116.0043497
		C_2	-115.1947509	-115.5707822	-116.0048909
2	1	C_{2v} #1	-191.2497297	-191.8215620	-192.4684933
		C_{2v} #2	-191.2502293	-191.8221168	-192.4688271
		C_{2v} #3	-191.2497304	-191.8215662	-192.5079055
		C_{2v} #4	-191.2502903	-191.8221510	-192.4682948
		C_2	-191.2502903	-191.8221646	-192.4688274
		C_s #1	-191.2705312	-191.8424738	-192.4877676
		C_s #2	-191.2561877	-191.8275217	-192.4726273
		C_1	-191.2706911	-191.8426849	-192.4878984
2	2	C_{2h} #1	-267.3065113	-268.0726989	-269.0146658
		C_{2h} #2	-267.3064488	-268.0718089	-268.9283632

		C_{2v} #1	-267.3064401	-268.0718482	-268.9283535
		C_{2v} #2	-267.3067965	-268.0729209	-268.9299990
		C_{2v} #3	-267.3073948	-268.0734242	-268.9300641
		C_{2v} #4	-267.3062885	-268.0723068	-268.9289723
		C_s #1	-267.3313411	-268.0991031	-268.9536437
		C_1	-267.3322646	-268.0999698	-269.0094400
2	3	D_{3h} #1	-343.3675912	-344.3286317	-345.3962832
		D_{3h} #2	-343.3669919	-344.3279489	-345.3957507
		D_{3h} #3	-343.3661885	-344.3284555	-345.3956726
		D_{3h} #4	-343.3679360	-344.3299422	-345.3976848
		D_3	-343.3682927	-344.3304312	-345.3978572
		C_{3v}	-343.3679361	-344.3299422	-345.3976848
		C_3	-343.3682927	-344.3304310	-345.3978649
		C_{2v}	-343.3692676	-344.3362254	-345.4022090
		C_2	-343.3769227	-344.3399565	-345.4059595
		C_s	-343.3833662	-344.3481769	-345.4718546
2	4	C_{2h} #1 (trans)	-419.4218282	-420.5795135	-421.8555455
		C_{2h} #2 (trans)	-419.4218523	-420.5795930	-421.8555670
		C_{2v} #1 (cis)	-419.4221514	-420.5800312	-421.8556047
		C_{2v} #2 (cis)	-419.4224175	-420.5801004	-421.8557296
		C_{2v} #3 (cis)	-419.4252354	-420.5834625	-421.8574292
		C_{2v} #4 (cis)	-419.4268749	-420.5853629	-421.8588659
		C_2	-419.4317304	-420.5888791	-421.8625735
3	0	C_{3v} #1	-171.4552028	-172.0105964	-172.6387152
		C_{3v} #2	-171.4571342	-172.0119708	-172.6403094
		C_3	-171.4571342	-172.0121172	-172.6403579
3	1	C_s #1	-247.5089657	-248.2592350	-249.0975478
		C_s #2	-247.5088064	-248.2589857	-249.0973291
		C_s #3	-247.5074656	-248.2582481	-249.0962570
		C_s #4	-247.5092291	-248.2601570	-249.0983065
		C_1	-247.5131457	-248.2637755	-249.1007485
3	2	C_s #1	-323.5592877	-324.5060469	-325.5528270
		C_s #2	-323.5563394	-324.5017251	-325.5482902
		C_s #3	-323.5538596	-324.4992164	-325.5460216
		C_s #4	-323.5567066	-324.5022484	-325.5486937
		C_1	N/A	-324.5105613	-325.5487424
3	3	C_{3v} #1	-399.5989558	-400.7392627	-401.9962375

		C_{3v} #2	-399.6009536	-400.7417677	-401.9989873
		C_{3v} #3	-399.6097714	-400.7520766	-402.0064092
		C_{3v} #4	-399.6078634	-400.7495439	-402.0045213
		C_3	-399.6101379	-400.7525426	-402.0078919
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.6732722	-228.4074087	-229.2328843
		T_d #2	-227.6730128	-228.4067406	-229.2322026
		C_3	-227.6367213	-228.4101279	-229.2335171
		C_s	-227.6856174	-228.4236357	-229.2431987
		C_1	-227.6908612	-228.4240493	-229.2432234
4	1	C_{2v} #1	-303.7325052	-304.6603182	-305.6892767
		C_{2v} #2	-303.7313216	-304.6598784	-305.6884337
		C_{2v} #3	-303.7317446	-304.6600867	-305.6886421
		C_{2v} #4	-303.7330742	-304.6614590	-305.6898894
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.7759537	-380.8986587	-382.1389921
		C_{2h} #2	-379.7764345	-380.8992723	-382.1396452
		C_2	-379.7771555	-380.9000934	-382.1401152
		C_s	-379.7767389	-380.8999925	-382.1396571
		C_1	-379.7785133	-380.9024787	-382.1403805
5	0	C_{3h} #1	-283.9048958	-284.8155526	-285.8308712
		C_{3h} #2	-283.9048958	-284.8155526	-285.8308762
		C_{3v} #1	-283.9041170	-284.8148322	-285.8297675
		C_{3v} #2	-283.9041170	-284.8148322	-285.8297737
		C_3	-283.9050211	-284.8155561	-285.8308918
		C_s	-283.9161302	-284.8270104	-285.8376989
		C_1	-283.9164485	-284.8275029	-285.8379896
5	1	C_s #1	-359.9575837	-361.0636489	-362.2838926
		C_s #2	-359.9576011	-361.0634171	-362.2838339
		C_s #3	-359.9576011	-361.0634170	-362.2838339
		C_s #4	-359.9575838	-361.0636489	-362.2423021
		C_1	-359.9613966	-361.0699607	-362.2902489
6	0	C_s #1	-339.9453514	-341.0631961	-342.2551735
		C_s #2	-339.9453636	-341.2193801	-342.4228901
		C_s #3	-339.9476400	-341.0611488	-342.2547408
		C_1	-340.1320284	-341.2207361	-342.4228719

Detached structure

Table 6A.6: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-31+G*/ SDD**	**MP2/6-31+G*/ SDD**	**B3LYP/6-31+G*/ SDD**
1	0	C_{3v}	-58.8838967	-59.0837316	-59.3207509
1	1	C_s #1	-134.9667874	-135.3646682	-135.8136843
		C_s #2	-134.9666097	-135.3640757	-135.8127518
		C_1	-134.9672656	-135.3650759	-135.8141353
1	2	C_s	-211.0399702	-211.6346071	-212.2941265
		C_1	-211.0410174	-211.6359294	-212.4503535
1	3	C_{3v} #1	-287.0991885	-287.8892107	-288.7591169
		C_{3v} #2	-287.0973410	-287.8874673	-288.7575973
		C_{3v} #3	-287.0983829	-287.8880753	-288.7581633
		C_{3v} #4	-287.0990828	-287.8891907	-288.7590105
		C_s #1	-287.0992895	-287.8896301	-288.8516128
		C_s #2	N/A	N/A	N/A
		C_3 #1	-287.0997758	-287.8900898	-288.7592697
		C_3 #2	N/A	N/A	N/A
		C_1	-287.1023615	-287.8937113	N/A
1	4	C_s #1	-363.1570616	-364.1436345	-365.2212863
		C_s #2	-363.1569788	-364.1434722	-365.2212780
		C_1	-363.1571216	-364.1437811	-365.2213487
1	5	C_s #1	-439.2008910	-440.3815781	-441.6702296
		C_s #2	-439.2011100	-440.3821169	-441.6702301
		C_1	-439.2053417	-440.3894767	-441.6784138
2	0	D_{3h}	-115.1335633	-115.5123609	-115.9436874
		D_{3d}	-115.1335646	-115.5123630	-115.9436886
		D_3	-115.1335637	-115.5123613	-115.9437010
		C_{2v}	-115.1566759	-115.5393550	-115.9699618
		C_2	-115.1572303	-115.5398364	-115.9703846
2	1	C_{2v} #1	-191.2118710	-191.7891457	-192.4325787
		C_{2v} #2	-191.2121981	-191.7894638	-192.4328000
		C_{2v} #3	-191.2497304	-191.7889871	-192.4678692
		C_{2v} #4	-191.2122374	-191.7893567	-192.4322836
		C_2	-191.2122374	-191.7894824	-192.4328010
		C_s #1	-191.2281664	-191.8078705	-192.4486136
		C_s #2	-191.2162141	-191.7938824	-192.4350091
		C_1	-191.2282822	-191.8079539	-192.4486096
2	2	C_{2h} #1	-267.2661480	-268.0374611	-268.9746384
		C_{2h} #2	-267.2662847	-268.0369860	-268.8894604

		C_{2v} #1	-267.2662817	-268.0370082	-268.8894740
		C_{2v} #2	-267.2663073	-268.0376461	-268.8907113
		C_{2v} #3	-267.2668575	-268.0380536	-268.8907747
		C_{2v} #4	-267.2660274	-268.0370999	-268.8898881
		C_s #1	-267.2869694	-268.0625348	-268.9121630
		C_1	-267.2876610	-268.0633905	-268.9544706
2	3	D_{3h} #1	-343.3254304	-344.2920359	-345.3553370
		D_{3h} #2	-343.3247994	-344.2913866	-345.3547740
		D_{3h} #3	-343.3239003	-344.2908500	-345.3544407
		D_{3h} #4	-343.3253341	-344.2924167	-345.3561991
		D_3	-343.3258246	-344.2929987	-345.3564486
		C_{3v}	-343.3253341	-344.2924167	-345.3561946
		C_3	-343.3258246	-344.2929986	-345.3564506
		C_{2v}	-343.3303779	-344.2995334	-345.3612955
		C_2	-343.3333297	-344.3029344	-345.4059595
		C_s	-343.3373071	-344.3104963	-345.3458149
2	4	C_{2h} #1 (trans)	-419.3778370	-420.5404679	-421.8123524
		C_{2h} #2 (trans)	-419.3778672	-420.5405315	-421.8123803
		C_{2v} #1 (cis)	-419.3779251	-420.5412021	-421.8123824
		C_{2v} #2 (cis)	-419.3780566	-420.5410942	-421.8124942
		C_{2v} #3 (cis)	-419.3805807	-420.5455065	-421.8145644
		C_{2v} #4 (cis)	-419.3815435	-420.5467484	-421.8154214
		C_2	-419.3844988	Dissociation	-421.8194048
3	0	C_{3v} #1	-171.4135971	-171.9781978	-172.6006480
		C_{3v} #2	-171.4150359	-171.9794034	-172.6018925
		C_3	-171.4150360	-171.9794793	-172.6019286
3	1	C_s #1	-247.4660660	-248.2251680	-249.0577957
		C_s #2	-247.4656647	-248.2245691	-249.0572909
		C_s #3	-247.4647495	-248.2238517	-249.0565056
		C_s #4	-247.4665790	-248.2263251	-249.0588547
		C_1	-247.4690784	-248.2289241	-249.0599060
3	2	C_s #1	-323.5156569	-324.4709013	-325.5119157
		C_s #2	-323.5112685	-324.4645167	-325.5053542
		C_s #3	-323.5092848	-324.4622175	-325.5035628
		C_s #4	-323.5116453	-324.4650743	-325.5057091
		C_1	N/A	-324.4734687	-325.5056369
3	3	C_{3v} #1	-399.5554818	-400.7028267	-401.9548284

		C_{3v} #2	-399.5576172	-400.7059077	-401.9579647
		C_{3v} #3	-399.5642314	-400.7151336	-401.9635110
		C_{3v} #4	-399.5629463	-400.7125948	-401.9618726
		C_3	-399.5649401	-400.7158818	-401.9656183
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.6344722	-228.3755326	-229.1962851
		T_d #2	-227.6342275	-228.3750027	-229.1956725
		C_3	-227.7856567	-228.3775929	-229.1964062
		C_s	-227.6430755	-228.3896237	-229.2025946
		C_1	-227.6470122	-228.3899537	-229.2026035
4	1	C_{2v} #1	-303.6879352	-304.6242333	-305.6468843
		C_{2v} #2	-303.6871275	-304.6241078	-305.6463222
		C_{2v} #3	-303.6873409	-304.6240817	-305.6463873
		C_{2v} #4	-303.6885706	-304.6254797	-305.6475140
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.7329355	-380.8621994	-382.0972221
		C_{2h} #2	-379.7333665	-380.8627328	-382.0978063
		C_2	-379.7337988	-380.8637996	-382.0981950
		C_s	-379.7334207	-380.8636253	-382.0978481
		C_1	-379.7342459	-380.8657159	-382.0979351
5	0	C_{3h} #1	-283.8639684	-284.7822877	-285.7919550
		C_{3h} #2	-283.8639680	-284.7822877	-285.7919601
		C_{3v} #1	-283.8632609	-284.7815520	-285.7909795
		C_{3v} #2	-283.8632609	-284.7815520	-285.7909890
		C_3	-283.8639684	-284.7822877	-285.7919597
		C_s	-283.8717415	-284.7922686	-285.7960019
		C_1	-283.8720165	-284.7926820	-285.7962651
5	1	C_s #1	-359.9134955	-361.0280222	-362.2423366
		C_s #2	-359.9135353	-361.0277940	-362.2423962
		C_s #3	-359.9135353	-361.0277940	-362.2423129
		C_s #4	-359.9134955	-361.0280222	-362.4570631
		C_1	-359.9162305	-361.0344693	-362.2478861
6	0	C_s #1	-339.8634672	-340.9978298	-342.1827787
		C_s #2	-339.8633788	-341.1843767	-342.3820717
		C_s #3	-339.8712775	-340.9991734	-342.1864289
		C_1	-340.0882515	-341.1852469	-342.3822281

Detached structure

Table 6A.7: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ CEP-121G**	**MP2/6-311+G*/ CEP-121G**	**B3LYP/6-311+G*/ CEP-121G**
1	0	C_{3v}	-58.9512660	-59.1569366	-59.3888358
1	1	C_s #1	-135.0764399	-135.4970502	-135.9264682
		C_s #2	-135.0759009	-135.4958318	-135.9251350
		C_1	-135.0772360	-135.4973970	-135.9270943
1	2	C_s #1	-211.1902797	-211.8246710	-212.4493975
		C_1	-211.1914061	-211.8260177	-212.4503535
1	3	C_{3v} #1	-287.2805030	-288.1289969	-288.9488076
		C_{3v} #2	-287.2800880	-288.1292702	-288.9482992
		C_{3v} #3	-287.2809199	-288.1290539	-288.9489109
		C_{3v} #4	-287.2839944	-288.1317508	-288.9516069
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	N/A	N/A
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.2839946	-288.1320110	-288.9517194
		C_1	N/A	-288.0839731	N/A
1	4	C_s #1	-363.3742940	-364.4381562	-365.4481015
		C_s #2	-363.3740184	-364.4377521	-365.4478642
		C_1	-363.3743586	-364.4382338	-365.4481507
1	5	C_s #1	-439.4438097	-440.7219810	-441.9259486
		C_s #2	-439.4429316	-440.7212816	-441.9248888
		C_1	-439.4500848	-440.7299490	-441.9330917
2	0	D_{3h}	-115.2251701	-115.6196854	-116.0385112
		D_{3d}	-115.2251726	-115.6196858	-116.0385138
		D_3	-115.2251725	-115.6196854	-116.0385269
		C_{2v}	-115.2570634	-115.6529014	-116.0727280
		C_2	-115.2583519	-115.6539580	-116.0737587
2	1	C_{2v} #1	-191.3424851	-191.9525839	-192.5696941
		C_{2v} #2	-191.3431896	-191.9530565	-192.5700738
		C_{2v} #3	-191.2118509	-191.9519939	-192.4319763
		C_{2v} #4	-191.3428916	-191.9525258	-192.5689914
		C_2	-191.3431901	-191.9532347	-192.5700740
		C_s #1	-191.3692712	-191.9792574	-192.5938205
		C_s #2	-191.3516882	-191.9611464	-192.5752529
		C_1	-191.3698571	-191.9799901	-192.5944211
2	2	C_{2h} #1	-267.4290941	-268.2518887	-268.9758074
		C_{2h} #2	-267.4293237	-268.2514852	-269.0606612

		C_{2v} #1	-267.4294166	-268.2515383	-269.0609138
		C_{2v} #2	-267.4301260	-268.2528754	-269.0626683
		C_{2v} #3	-267.4308992	-268.2535303	-269.0630256
		C_{2v} #4	-267.4291787	-268.2524198	-269.0613126
		C_s #1	-267.4624118	-268.2872316	-269.0938205
		C_1	-267.4641874	-268.2888596	-268.9128972
2	3	D_{3h} #1	-343.5230681	-344.5595250	-345.5643066
		D_{3h} #2	-343.5226529	-344.5587512	-345.5640327
		D_{3h} #3	-343.5213306	-344.5587189	-345.5628756
		D_{3h} #4	-343.5233287	-344.5595842	-345.5651190
		D_3	-343.5238213	-344.5607767	-345.5655403
		C_{3v}	-343.5238267	-344.5598271	-345.5651296
		C_3	-343.5241157	-344.5608110	-345.5655467
		C_{2v}	-343.5301982	-344.5688501	-345.5715188
		C_2	-343.5346535	-344.5734851	-345.5760397
		C_s	-343.5411052	-344.5813276	-345.4718546
2	4	C_{2h} #1 (trans)	-419.6068306	-420.8581465	-422.0545292
		C_{2h} #2 (trans)	-419.6068245	-420.8582536	-422.0545353
		C_{2v} #1 (cis)	-419.6084541	-420.8608509	-422.0557183
		C_{2v} #2 (cis)	-419.6092631	-420.8614294	-422.0563570
		C_{2v} #3 (cis)	-419.6109755	-420.8639312	-422.0570097
		C_{2v} #4 (cis)	-419.6153118	-420.8688309	-422.0611424
		C_2	-419.6202514	Dissociation	-422.0680772
3	0	C_{3v} #1	-171.5451330	-172.1312681	-172.7355425
		C_{3v} #2	-171.5477786	-172.1331685	-172.7379250
		C_3	-171.5477784	-172.1336254	-172.7379599
3	1	C_s #1	-247.6297723	-248.4293740	-249.2280680
		C_s #2	-247.6302406	-248.4295014	-249.2283758
		C_s #3	-247.6279057	-248.4282230	-249.2261999
		C_s #4	-247.6290430	-248.4292989	-249.2276724
		C_1	-247.6356443	-248.4358383	-249.2319509
3	2	C_s #1	-323.7070019	-324.7221485	-325.7122750
		C_s #2	-323.7089023	-324.7230263	-325.7117078
		C_s #3	-323.7048599	-324.7189450	-325.7076637
		C_s #4	-323.7092844	-324.7235053	-325.7121377
		C_1	N/A	N/A	-325.7121241
3	3	C_{3v} #1	-399.7744455	-401.0016935	-402.1865602

		C_{3v} #2	-399.7756616	-401.0039099	-402.1885140
		C_{3v} #3	-399.7887080	-401.0193435	-402.1991481
		C_{3v} #4	-399.7847714	-401.0142328	-402.1948414
		C_3	-399.7888332	-401.0193444	-402.1995338
		C_s	-399.7890360	N/A	-402.1991733
		C_1	-399.7880362	N/A	-402.1996797
4	0	T_d #1	-227.7809233	-228.5558319	-229.3507609
		T_d #2	-227.7807545	-228.5555938	-229.3501704
		C_3	-227.7393369	-228.5599806	-229.3517415
		C_s	-227.7984024	-228.5790413	-229.3646834
		C_1	-227.8044704	-228.5797831	-229.3649740
4	1	C_{2v} #1	-303.8757288	-304.8643427	-305.8427378
		C_{2v} #2	-303.8746425	-304.8642465	-305.8419002
		C_{2v} #3	-303.8751028	-304.8648697	-305.8421993
		C_{2v} #4	-303.8765018	-304.8658919	-305.8435359
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.9423024	-381.1440643	-382.3182821
		C_{2h} #2	-379.9428998	-381.1445167	-382.3190392
		C_2	-379.9451976	-381.1478313	-382.3210363
		C_s	-379.9447175	-381.1475100	-382.3205229
		C_1	-379.9492487	-381.1534288	-382.3230716
5	0	C_{3h} #1	-284.0339106	-284.9970099	-285.9710336
		C_{3h} #2	-284.0339106	-284.9970099	-285.9710392
		C_{3v} #1	-284.0335240	-284.9964898	-285.9700482
		C_{3v} #2	-284.0335240	-284.9964898	-285.9700478
		C_3	-284.0346679	-284.9973158	-285.9712487
		C_s	-284.0506474	-285.0150899	-285.9818979
		C_1	-284.0509999	-285.0157768	-285.9822195
5	1	C_s #1	-360.1185827	-361.2970341	-362.4570631
		C_s #2	-360.1181806	-361.2964689	-362.4569093
		C_s #3	-360.1181806	-361.2964689	-362.4566209
		C_s #4	-360.1185826	-361.2970341	-362.3927496
		C_1	-360.1191568	-361.3003535	-362.4601395
6	0	C_s #1	-340.1125309	-341.2936075	-342.4357782
		C_s #2	-340.1123728	-341.4363269	-342.5851997
		C_s #3	-340.1064129	-341.2915572	-342.4350462
		C_1	-340.2850501	-341.4392264	-342.5864965

Detached structure

Table 6A.8: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ LANL2DZ**	**MP2/6-311+G*/ LANL2DZ**	**B3LYP/6-311+G*/ LANL2DZ**
1	0	C_{3v}	-58.9305659	-59.1378685	-59.3660524
1	1	C_s #1	-135.0443398	-135.4663105	-135.8920928
		C_s #2	-135.0438879	-135.4651560	-135.8908249
		C_1	-135.0449609	-135.4665566	-135.8926263
1	2	C_s	-211.1461117	-211.7816468	-212.4028459
		C_1	-211.1471831	-211.7828760	-212.4036938
1	3	C_{3v} #1	-287.2278349	-288.0769236	-288.8928105
		C_{3v} #2	-287.2264142	-288.0768083	-288.8918423
		C_{3v} #3	-287.2272106	-288.0759971	-288.8920639
		C_{3v} #4	-287.2289355	-288.0780601	-288.8938988
		C_s #1	N/A	N/A	N/A
		C_s #2	N/A	-288.0817876	-288.8960368
		C_3 #1	N/A	N/A	N/A
		C_3 #2	-287.2292458	-288.0786541	-288.8943010
		C_1	-287.1663429	N/A	-288.8978875
1	4	C_s #1	-363.3113722	-364.3753121	-365.3824508
		C_s #2	-363.3112181	-364.3749837	-365.3824197
		C_1	-363.3113909	-364.3753280	-365.3824808
1	5	C_s #1	-439.3762254	-440.6537658	-441.8549720
		C_s #2	-439.3762375	-440.6540323	-441.8549121
		C_1	-439.3835541	-440.6686475	-441.8652914
2	0	D_{3h}	-115.1984564	-115.5944945	-116.0100201
		D_{3d}	-115.1984575	-115.5944941	-116.0100224
		D_3	-115.1984575	-115.5944945	-116.0100418
		C_{2v}	-115.2253662	-115.6223001	-116.0386011
		C_2	-115.2261143	-115.6230687	-116.0391848
2	1	C_{2v} #1	-191.3040443	-191.9149600	-192.5279125
		C_{2v} #2	-191.3045295	-191.9155416	-192.5282388
		C_{2v} #3	-191.3421198	-191.9151001	-192.5685165
		C_{2v} #4	-191.3045921	-191.9156811	-192.5277279
		C_2	-191.3045927	-191.9157885	-192.5282414
		C_s #1	-191.3252777	-191.9361609	-192.5473190
		C_s #2	-191.3107912	-191.9213501	-192.5321516
		C_1	-191.3256734	-191.9368373	-192.5477092
2	2	C_{2h} #1	-267.3844839	-268.2081918	-268.9297796
		C_{2h} #2	-267.3842809	-268.2070840	-269.0131735

		C_{2v} #1	-267.3842723	-268.2070826	-269.0131660
		C_{2v} #2	-267.3847105	-268.2082751	-269.0148592
		C_{2v} #3	-267.3853030	-268.2088771	-269.0149113
		C_{2v} #4	-267.3842137	-268.2079532	-269.0138497
		C_s #1	-267.4089246	-268.2340516	-269.0378959
		C_1	-267.4101654	-268.2352396	-269.0954546
2	3	D_{3h} #1	-343.4678567	-344.5046401	-345.5054678
		D_{3h} #2	-343.4673242	-344.5038017	-345.5050055
		D_{3h} #3	-343.4664957	-344.5049175	-345.5048289
		D_{3h} #4	-343.4682144	-344.5058274	-345.5067805
		D_3	-343.4686276	-344.5068798	-345.5070256
		C_{3v}	-343.4682145	-344.5058274	-345.5067805
		C_3	-343.4686276	-344.5068798	-345.5070319
		C_{2v}	-343.4728714	-344.5115379	-345.5071209
		C_2	-343.4767781	-344.5156767	-345.5145621
		C_s	-343.4840155	-344.5249562	-345.4145084
2	4	C_{2h} #1 (trans)	-419.5445473	-420.7965570	-421.9888590
		C_{2h} #2 (trans)	-419.5445635	-420.7966994	-421.9888857
		C_{2v} #1 (cis)	-419.5449762	-420.7970724	-421.9889390
		C_{2v} #2 (cis)	-419.5450409	-420.7969541	-421.9889902
		C_{2v} #3 (cis)	-419.5470861	-420.7994963	-421.9898850
		C_{2v} #4 (cis)	-419.5487215	-420.8013419	-421.9912744
		C_2	-419.5517032	-420.8761435	-421.9952212
3	0	C_{3v} #1	-171.5021249	-172.0888301	-172.6898904
		C_{3v} #2	-171.5039491	-172.0900485	-172.6915191
		C_3	-171.5039491	-172.0905076	-172.6915668
3	1	C_s #1	-247.5783406	-248.3783568	-249.1733185
		C_s #2	-247.5782095	-248.3779116	-249.1731927
		C_s #3	-247.5769414	-248.3777248	-249.1720828
		C_s #4	-247.5787726	-248.3794559	-249.1742524
		C_1	-247.5828838	-248.3833670	-249.1767167
3	2	C_s #1	-323.6509532	-324.6658678	-325.6527817
		C_s #2	-323.6490340	-324.6625419	-325.6491789
		C_s #3	-323.6463871	-324.6598902	-325.6466657
		C_s #4	-323.6493843	-324.6630318	-325.6495129
		C_1	N/A	-324.6720067	N/A
3	3	C_{3v} #1	-399.7122058	-400.9387143	-402.1198122

		C_{3v} #2	-399.7143235	-400.9416320	-402.1225552
		C_{3v} #3	-399.7234149	-400.9524779	-402.1299932
		C_{3v} #4	-399.7214128	-400.9497664	-402.1281116
		C_3	-399.7240695	-400.9531904	-402.1321868
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.7354642	-228.5114165	-229.3009533
		T_d #2	-227.7351381	-228.5108835	-229.3002943
		C_3	-227.6987657	-228.5144943	-229.3016392
		C_s	-227.7477007	-228.5279967	-229.3112711
		C_1	-227.7530450	-228.5285667	-229.3112959
4	1	C_{2v} #1	-303.8177238	-304.8057018	-305.7823005
		C_{2v} #2	-303.8167792	-304.8057031	-305.7814852
		C_{2v} #3	-303.8170670	-304.8059541	-305.7816897
		C_{2v} #4	-303.8183665	-304.8070510	-305.7828914
		C_2	N/A	N/A	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.8835099	-381.0851744	-382.2562961
		C_{2h} #2	-379.8839549	-381.0855916	-382.2568754
		C_2	-379.8845535	-381.0861012	-382.2572669
		C_s	-379.8841530	-381.0860033	-382.2568366
		C_1	-379.8860532	-381.0886948	-382.2575163
5	0	C_{3h} #1	-283.9824256	-284.9458022	-285.9157817
		C_{3h} #2	-283.9824256	-284.9458022	-285.9157858
		C_{3v} #1	-283.9816613	-284.9451060	-285.9147079
		C_{3v} #2	-283.9816613	-284.9451060	-285.9147147
		C_3	-283.9825034	-284.9458176	-285.9157808
		C_s	-283.9936468	-284.9573720	-285.9225952
		C_1	-283.9939386	-284.9580394	-285.9228625
5	1	C_s #1	-360.0571748	-361.2343534	-362.3927631
		C_s #2	-360.0570826	-361.2341794	-362.3927492
		C_s #3	-360.0570826	-361.2341794	-362.3926026
		C_s #4	-360.0571748	-361.2343534	-362.3510820
		C_1	-360.0613928	-361.2417293	-362.3998014
6	0	C_s #1	-340.0379579	-341.2189017	-342.3566543
		C_s #2	-340.0379038	-341.3757200	-342.5245665
		C_s #3	-340.0406498	-341.2162385	-342.3556772
		C_1	-340.2249285	-341.3774046	-342.4837762

Detached structure

Table 6A.9: Total energies for all stable geometries of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

			Total Energy (Hartrees)		
n	**m**	**Point Group**	**HF/6-311+G*/ SDD**	**MP2/6-311+G*/ SDD**	**B3LYP/6-311+G*/ SDD**
1	0	C_{3v}	-58.8995228	-59.1096857	-59.3378294
1	1	C_s #1	-135.0060096	-135.4329599	-135.8564243
		C_s #2	-135.0057704	-135.4321588	-135.8553902
		C_1	-135.0064881	-135.4332328	-135.8568714
1	2	C_s	-211.1024878	-211.7447337	-212.3621554
		C_1	-211.1035266	-211.7459482	-212.3629885
1	3	C_{3v} #1	-287.1840787	-288.0400162	-288.8513499
		C_{3v} #2	-287.1822594	-288.0387172	-288.8499488
		C_{3v} #3	-287.1833269	-288.0388882	-288.8505183
		C_{3v} #4	-287.1840598	-288.0400083	-288.8513912
		C_s #1	-287.1842006	-288.0407102	-288.7598005
		C_s #2	N/A	N/A	N/A
		C_3 #1	-287.1846817	-288.0410132	-288.8520871
		C_3 #2	N/A	N/A	N/A
		C_1	-287.1876698	-288.0451116	-288.8542785
1	4	C_s #1	-363.2645778	-364.335718	-365.3378855
		C_s #2	-363.2644898	-364.3355031	-365.3378553
		C_1	-363.2646145	-364.3358146	-365.3378873
1	5	C_s #1	-439.3300376	-440.6138677	-441.8103110
		C_s #2	-439.3302335	-440.6143130	-441.8103372
		C_1	-439.3351353	-440.6230222	-441.8285444
2	0	D_{3h}	-115.1645733	-115.5642671	-115.9777445
		D_{3d}	-115.1645751	-115.5642728	-115.9777462
		D_3	-115.1645751	-115.5642728	-115.9777587
		C_{2v}	-115.1878167	-115.5912742	-116.0039976
		C_2	-115.1883691	-115.5918086	-116.0044296
		C_1	N/A	N/A	-116.0044323
2	1	C_{2v} #1	-191.2657539	-191.8823585	-192.4915225
		C_{2v} #2	-191.2660636	-191.8826752	-192.4917168
		C_{2v} #3	-191.3040380	-191.8822396	-192.4908787
		C_{2v} #4	-191.2660921	-191.8825736	-192.4911679
		C_2	-191.2660937	-191.8827585	-192.4917199
		C_s #1	-191.2825361	-191.9015081	-192.5078610
		C_s #2	-191.2702700	-191.8873069	-192.4939722
		C_1	-191.2827806	-191.9019438	-192.5081055
2	2	C_{2h} #1	-267.3433870	-268.1727133	-268.9746374

		C_{2h} #2	-267.3433887	-268.1720596	-268.9734877
		C_{2v} #1	-267.3433838	-268.1720516	-268.9734896
		C_{2v} #2	-267.3435232	-268.1727664	-268.9748123
		C_{2v} #3	-267.3440433	-268.1731348	-268.9748464
		C_{2v} #4	-267.3432094	-268.1724116	-268.9739831
		C_s #1	-267.3639989	-268.1973592	-268.9959721
		C_1	-267.3648885	- 268.1985657	-268.9968018
2	3	D_{3h} #1	-343.4251478	-344.4685092	-345.4640058
		D_{3h} #2	-343.4246278	-344.4678121	-345.4635266
		D_{3h} #3	-343.4237203	-344.4676372	-345.4631443
		D_{3h} #4	-343.4251828	-344.4687215	-345.4648577
		D_3	-343.4256677	-344.4696951	-345.4651809
		C_{3v}	-343.4251826	-344.4687217	-345.4648547
		C_3	-343.4256539	-344.4696951	-345.4650952
		C_{2v}	-343.4294636	-344.4750507	-345.4690894
		C_2	-343.4325840	-344.4787466	-345.4725298
		C_s	-343.4374210	-344.4872635	-345.4803132
2	4	C_{2h} #1 (trans)	-419.4999219	-420.7577898	-421.9450576
		C_{2h} #2 (trans)	-419.4999443	-420.7578677	-421.9450907
		C_{2v} #1 (cis)	-419.5000937	-420.7585871	-421.9451097
		C_{2v} #2 (cis)	-419.5000899	-420.7582396	-421.9451491
		C_{2v} #3 (cis)	-419.5018243	-420.7617372	-421.9463524
		C_{2v} #4 (cis)	-419.5027786	-420.7629082	-421.9471964
		C_2	-419.5057992	-420.7672577	-421.9514853
3	0	C_{3v} #1	-171.4602393	-172.0561920	-172.6516352
		C_{3v} #2	-171.4616270	-172.0572537	-172.6528931
		C_3	-171.4616271	-172.0575582	-172.6529287
3	1	C_s #1	-247.5351135	-248.3440477	-249.1332130
		C_s #2	-247.5347432	-248.3433666	-249.1327888
		C_s #3	-247.5338274	-248.3430099	-249.1319653
		C_s #4	-247.5357223	-248.3453827	-249.1344487
		C_1	-247.5383570	-248.3481570	-249.1355807
3	2	C_s #1	-323.6068528	-324.6304584	-325.6114237
		C_s #2	-323.6034557	-324.6252941	-325.6058102
		C_s #3	-323.6013415	-324.6228157	-325.6038557
		C_s #4	-323.6038047	-324.6257470	-325.6061142
		C_1	N/A	-324.6347836	-325.6062520

3	3	C_{3v} #1	-399.6685124	-400.9023942	-402.0779321
		C_{3v} #2	-399.6705833	-400.9059518	-402.0809207
		C_{3v} #3	-399.6772845	-400.9151831	-402.0864666
		C_{3v} #4	-399.6760054	-400.9127704	-402.0849498
		C_3	-399.6783464	-400.9163560	-402.0894376
		C_s	N/A	N/A	N/A
		C_1	N/A	N/A	N/A
4	0	T_d #1	-227.6965071	-228.4795384	-229.2641831
		T_d #2	-227.6962370	-228.4791023	-229.2636113
		C_3	-227.6987657	-228.4817965	-229.2643149
		C_s	-227.7050023	-228.4936330	-229.2704952
		C_1	-227.7089645	-228.4941490	-229.2704989
4	1	C_{2v} #1	-303.7728310	-304.7695226	-305.7396779
		C_{2v} #2	-303.7721696	-304.7698500	-305.7390968
		C_{2v} #3	-303.7722960	-304.7698360	-305.7391730
		C_{2v} #4	-303.7734821	-304.7709469	-305.7402474
		C_2	N/A	-304.7709618	N/A
		C_s	N/A	N/A	N/A
4	2	C_{2h} #1	-379.8401550	-381.0488665	-382.2141481
		C_{2h} #2	-379.8405563	-381.0492235	-382.2146860
		C_2	-379.8409097	-381.0499348	-382.2149909
		C_s	-379.8405780	-381.0497958	-382.2147219
		C_1	-379.8413218	-381.0518605	-382.2146839
5	0	C_{3h} #1	-283.9413896	-284.9125841	-285.8767354
		C_{3h} #2	-283.9413896	-284.9125841	-285.8767398
		C_{3v} #1	-283.9406826	-284.9118373	-285.8757992
		C_{3v} #2	-283.9406826	-284.9118373	-285.8758092
		C_3	-283.9413896	-284.9125840	-285.8767199
		C_s	-283.9490835	-284.9224177	-285.8807915
		C_1	-283.9493251	-284.9230104	-285.8810368
5	1	C_s #1	-360.0128891	-361.1986505	-362.3510495
		C_s #2	-360.0128320	-361.1983923	-362.3510425
		C_s #3	-360.0128320	-361.1983923	-362.3510425
		C_s #4	-360.0128891	-361.1986504	-362.3510816
		C_1	-360.0159838	-361.2059505	-362.3572752
6	0	C_s #1	-339.9551362	-341.1527485	-342.2834798
		C_s #2	Dissociation	-341.3406180	-342.4836598
		C_s #3	-339.9632788	-341.1533714	-342.2866190
		C_1	-340.1809605	-341.3417583	-342.4837045

Detached structure

Table 6A.10: Pb-N and Pb-O bond lengths, in Angstroms, for stable minimum energy structures of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n).

		Optimized Bond Lengths (Å)						
n	**m**	**Point Group Symmetry**	**HF SDD/6-311+G***		**MP2 SDD/6-311+G***		**B3LYP/ SDD/6-311+G***	
			Pb-N	**Pb-O**	**Pb-N**	**Pb-O**	**Pb-N**	**Pb-O**
1	0	C_{3v}	2.457	N/A	2.451	N/A	2.452	N/A
1	1	C_1	2.487	2.437	2.478	2.413	2.485	2.409
1	2	C_1	2.505	2.488 2.489	2.490	2.463 2.464	2.507	2.463 2.467
1	3	C_1	2.509	2.631 2.630 2.472	2.491	2.597 2.597 2.440	2.515	2.609 2.612 2.443
		C_3	N/A	N/A	N/A	N/A	2.425	2.496
1	4	C_1	2.481	2.648 2.684 2.693 2.669	2.459	2.586 2.638 2.676 2.625	2.487	2.632 2.650 2.650 2.647
2	0	C_2	2.501	N/A	2.489	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A	2.496 2.496	N/A
2	1	C_1	2.522 2.525	2.512	2.508 2.505	2.483	2.520 2.523	2.486
2	2	C_1	2.521 2.521	2.654 2.654	2.501 2.501	2.612 2.612	2.513 2.514	2.637 2.638
2	4	C_2	2.558	2.723 2.983	2.514	2.671 2.967	N/A	N/A
3	0	C_3	2.540	N/A	2.522	N/A	2.536	N/A
3	1	C_1	2.531 2.533 2.643	2.771	2.735 2.509 2.608	2.509	2.509 2.541 2.622	2.807
3	2	C_s #4	2.510 2.575	2.542 2.403	N/A	N/A	N/A	N/A
		C_1	N/A	N/A	N/A	N/A	2.723 2.724 2.637	2.532 2.748
3	3	C_3	2.584	2.973	2.536	2.949	N/A	N/A
4	0	C_1	2.549 2.546 2.753 2.753	N/A	2.523 2.527 2.708 2.708	N/A	2.543 2.543 2.747 2.747	N/A

4	1	C_{2v} #4	2.758 2.761	2.565	N/A	N/A	2.741 2.743	2.547
		C_2	N/A	N/A	2.702 2.713	2.543	N/A	N/A
4	2	C_2	N/A	N/A	N/A	N/A	2.805 2.804	2.742 2.683
		C_1	2.946 2.800 2.800 2.659	2.925 2.671	2.759 2.865 2.533 2.628	2.963 2.608	N/A	N/A
5	0	C_1	2.531 2.796 2.796 2.809 2.784	N/A	2.440 2.667 2.686 2.686 2.667	N/A	2.537 2.787 2.770 2.786 2.772	N/A
5	1	C_1	--	--	--	--	--	--
6	0	C_1	2.979 2.979 2.723 2.723 2.723 2.979	N/A	2.950 2.911 2.633 2.655 2.654 2.914	N/A	2.826 2.835 2.824 2.833 2.826 2.832	N/A

Table 6A.11: Pb-N and Pb-O vibrational stretching frequencies of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n) calculated at HF/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	H_2O/NH_3	Mixing
1	0	C_{3v}	336.9	a_1	NH_3	-
1	1	C_1	227.3 313.3	a a	H_2O/NH_3 H_2O/NH_3	- -
1	2	C_1	94.1 243.3 256.2 297.2	a a a a	H_2O/NH_3 H_2O H_2O/NH_3 H_2O/NH_3	- - - -
1	3	C_1	186.8 212.8 250.0 283.9	a a a a	H_2O H_2O/NH_3 H_2O/NH_3 H_2O/NH_3	- - H_2O twisting H_2O rocking
1	4	C_1	169.7 177.0 194.9 209.9 283.3	a a a a a	H_2O H_2O H_2O H_2O/NH_3 NH_3	- - - H_2O twisting H_2O wagging
1	5	C_1	N/A	N/A	N/A	N/A
2	0	C_2	296.5 310.2	b a	NH_3 NH_3	- -
2	1	C_1	238.7 277.6 292.4	a a a	H_2O NH_3 H_2O/NH_3	- H_2O rocking -
2	2	C_1	180.5 208.2 269.8 282.9	a a a a	H_2O H_2O/NH_3 NH_3 NH_3	- - H_2O wagging H_2O rocking
2	4	C_2	174.2 180.1 193.2 219.7 265.8 278.7 333.7	b a b a b a a	H_2O H_2O H_2O H_2O/ NH_3 NH_3 NH_3 NH_3	- - H_2O twisting H_2O twisting H_2O rock/twist H_2O rock/twist H_2O rocking
3	0	C_3	268.1 286.8	e a	NH_3 NH_3	- -
3	1	C_1	165.1 232.3	a a	H_2O/NH_3 H_2O/NH_3	- -

			263.3 276.1	a a	NH_3 NH_3	H_2O twisting H_2O rocking
3	2	C_s #4	154.6 161.8 197.5 216.8 239.4	a' a'' a' a' a'	H_2O/NH_3 NH_3 H_2O/NH_3 H_2O/NH_3 H_2O/NH_3	H_2O wagging H_2O rock/twist - - -
3	3	C_3	143.4 149.6 232.1 253.5	e a e a	H_2O H_2O NH_3 NH_3	- - H_2O twisting H_2O rocking
4	0	C_1	218.6 254.6 269.8	a a a	NH_3 NH_3 NH_3	- - -
4	1	C_{2v} #4	153.8 154.4 190.6 207.2 234.8	b_2 b_1 a_1 a_1 a_1	NH_3 NH_3 H_2O/NH_3 H_2O/NH_3 H_2O/NH_3	H_2O rocking H_2O wagging - - -
4	2	C_1	125.2 138.6 148.3 177.1 202.7 227.8	a a a a a a	H_2O/NH_3 NH_3 H_2O/NH_3 H_2O/NH_3 H_2O/NH_3 H_2O/NH_3	H_2O rocking H_2O twisting - - - -
5	0	C_1	154.5 157.3 204.5 224.9 273.0	a a a a a	NH_3 NH_3 NH_3 NH_3 NH_3	- NH_3 twisting - - NH_3 wagging
5	1	C_1	--	--	--	--
6	0	C_1	120.3 136.8 192.5 218.6	a a a a	NH_3 NH_3 NH_3 NH_3	- - - -

Table 6A.12: Pb-N and Pb-O vibrational stretching frequencies of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n=1 – 6, m=0 – (6-n) calculated at MP2/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	H_2O/NH_3	Mixing
1	0	C_{3v}	341.8	a_1	NH_3	-
1	1	C_1	297.2 322.7	a a	H_2O/NH_3 H_2O/NH_3	- -
1	2	C_1	262.2 276.1 310.9	a a a	H_2O H_2O/NH_3 H_2O/NH_3	- - -
1	3	C_1	206.2 228.8 273.9 300.9	a a a a	H_2O H_2O H_2O/NH_3 $H_2O/NH3$	- - H_2O twisting H_2O twisting
1	4	C_1	188.9 193.7 213.5 229.9 303.2	a a a a a	H_2O H_2O H_2O H_2O/NH_3 NH_3	H_2O rocking H_2O twisting - - H_2O twisting
2	0	C_2	310.2 320.3	b a	NH_3 NH_3	- -
2	1	C_1	259.1 295.1 306.1	a a a	H_2O/NH_3 NH_3 H_2O/NH_3	- - -
2	2	C_1	199.7 225.6 290.4 298.1	a a a a	H_2O H_2O NH_3 NH_3	- - H_2O twisting H_2O rocking
2	4	C_2	177.7 185.4 203.3 273.7 286.5	b a a b a	H_2O H_2O/NH_3 H_2O NH_3 NH_3	H_2O twisting H_2O twisting - H_2O twisting H_2O twisting
3	0	C_3	109.9 286.6 301.4	a e a	NH_3 NH_3 NH_3	- - -
3	1	C_1	180.2 252.3 284.6 294.1	a a a a	H_2O/NH_3 H_2O/NH_3 NH_3 NH_3	- - H_2O twisting H_2O rocking
3	3	C_3	166.5	e	H_2O	-

			166.5 168.6 263.1 279.9	e a e a	H_2O H_2O NH_3 NH_3	- - H_2O twisting H_2O rocking
4	0	C_1	248.4 284.8 324.1 226.3	a a a a	NH_3 NH_3 NH_3 NH_3	- - - -
4	1	C_2	176.7 179.1 195.3 227.9 251.5	b b a a a	NH_3 NH_3 H_2O NH_3 H_2O/NH_3	H_2O wagging H_2O wagging - H_2O twisting -
4	2	C_1	147.1 187.6 228.3 249.1	a a a a	H_2O/NH_3 H_2O/NH_3 NH_3 H_2O/NH_3	- - H_2O twisting H_2O twisting
5	0	C_1	170.6 173.6 217.8 229.4 274.3	a a a a a	NH_3 NH_3 NH_3 NH_3 NH_3	- NH_3 twisting - - NH_3 wagging
5	1	C_1	--	--	--	--
6	0	C_1	131.5 136.1 143.1 159.5 215.6 217.9 234.8	a a a a a a a	NH_3 NH_3 NH_3 NH_3 NH_3 NH_3 NH_3	NH_3 twisting NH_3 twisting NH_3 twisting NH_3 twisting NH_3 wagging - -

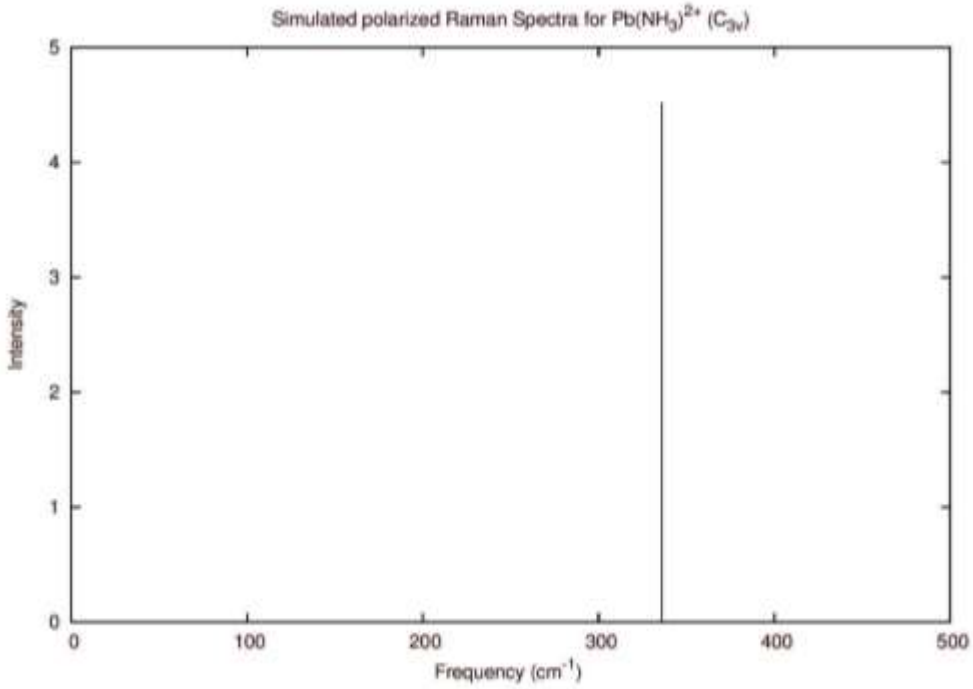
Table 6A.13: Pb-N and Pb-O vibrational stretching frequencies of $[Pb(NH_3)_n(H_2O)_m]^{2+}$, where n =1 – 6, m =0 – (6-n) calculated at B3LYP/SDD/6-311+G*.

n	m	Point Group Symmetry	Frequency (cm^{-1})	Irreducible Representation Symmetry	H_2O/NH_3	Mixing
1	0	C_{3v}	333.5	a_1	NH_3	-
1	1	C_1	293.3 311.8	a a	H_2O/NH_3 H_2O/NH_3	- -
1	2	C_1	256.0 268.8 296.6	a a a	H_2O H_2O/NH_3 H_2O/NH_3	- - -
1	3	C_3	213.2 213.1 235.5 289.7	e e a a	H_2O H_2O H_2O/NH_3 NH_3	H_2O twisting H_2O twisting H_2O twisting H_2O wagging
1	3	C_1	210.5 236.7 279.6 296.6	a a a a	H_2O H_2O H_2O/NH_3 H_2O/NH_3	H2O rocking - H_2O rocking H_2O/NH_3 twist
1	4	C_1	176.6 185.6 203.9 220.9 284.1	a a a a a	H_2O H_2O H_2O H_2O/NH_3 NH_3	H_2O twisting H_2O rocking - H_2O twisting H_2O wagg/twist
2	0	C_1	298.1 308.5	a a	NH_3 NH_3	- -
2	1	C_1	252.5 280.9 292.4	a a a	H_2O/NH_3 NH_3 H_2O/NH_3	- H_2O wagging -
2	2	C_1	188.1 214.1 274.9 287.1	a a a a	H_2O H_2O NH_3 NH_3	- - H_2O twisting H_2O twisting
3	0	C_3	325.1 334.3	e a	NH_3 NH_3	- -
3	1	C_1	169.9 242.0 268.6 285.6	a a a a	H_2O/NH_3 NH_3 NH_3 H_2O/NH_3	- H_2O twisting H_2O twisting -
3	2	C_1	160.1 174.1 204.3	a a a	H_2O/NH_3 NH_3 H_2O/NH_3	H_2O wagging H_2O twisting H_2O rocking

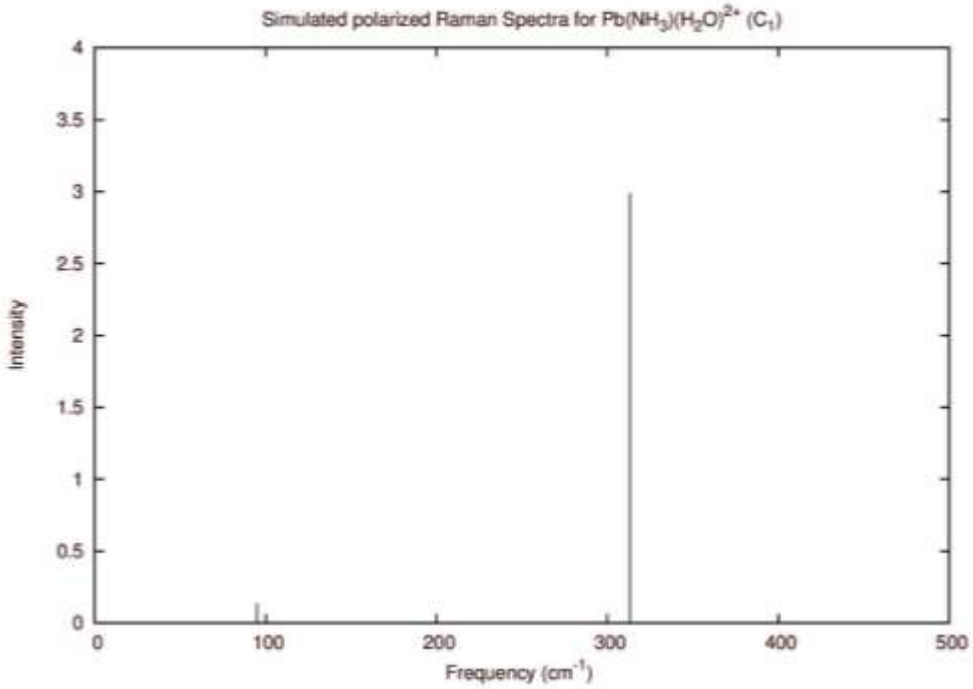
			224.2 243.3	a a	H_2O/NH_3 H_2O/NH_3	- -
4	0	C_1	221.8 261.4 272.5	a a a	NH_3 NH_3 NH_3	- - -
4	1	C_{2v} #4	164.0 165.2 197.4 212.2 237.6	b_2 b_1 a_1 a_1 a_1	NH_3 NH_3 H_2O/NH_3 H_2O/NH_3 H_2O/NH_3	H_2O rocking H_2O wagging - - -
4	2	C_2	146.7 146.9 153.1 184.7 199.7 225.6	b b a a a a	NH_3 NH_3 H_2O H_2O/NH_3 NH_3 H_2O/NH_3	H_2O rock/wagg H_2O rock/wagg - - - -
5	0	C_1	153.6 154.5 203.2 218.1 258.6	a a a a a	NH_3 NH_3 NH_3 NH_3 NH_3	NH_3 twisting - - - NH_3 wagging
5	1	C_1	--	--	--	--
6	0	C_1	133.2 135.4 136.9 190.8 191.1 221.9	a a a a a a	NH_3 NH_3 NH_3 NH_3 NH_3 NH_3	NH_3 wagging NH_3 wagging NH_3 wagging - - -

Figure 6A-1: Simulated polarized Raman spectra for $[Pb(NH_3)_n(H_2O)_m]^{2+}$,, where n = 1 – 6, m = 0 – (6-n).

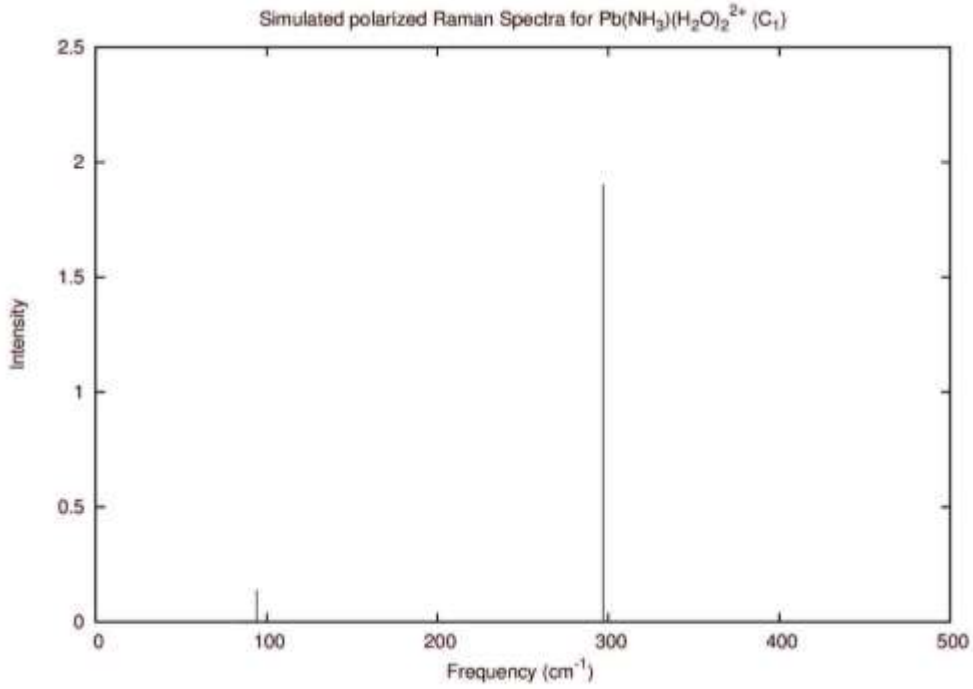
$[Pb(NH_3)]^{2+}$



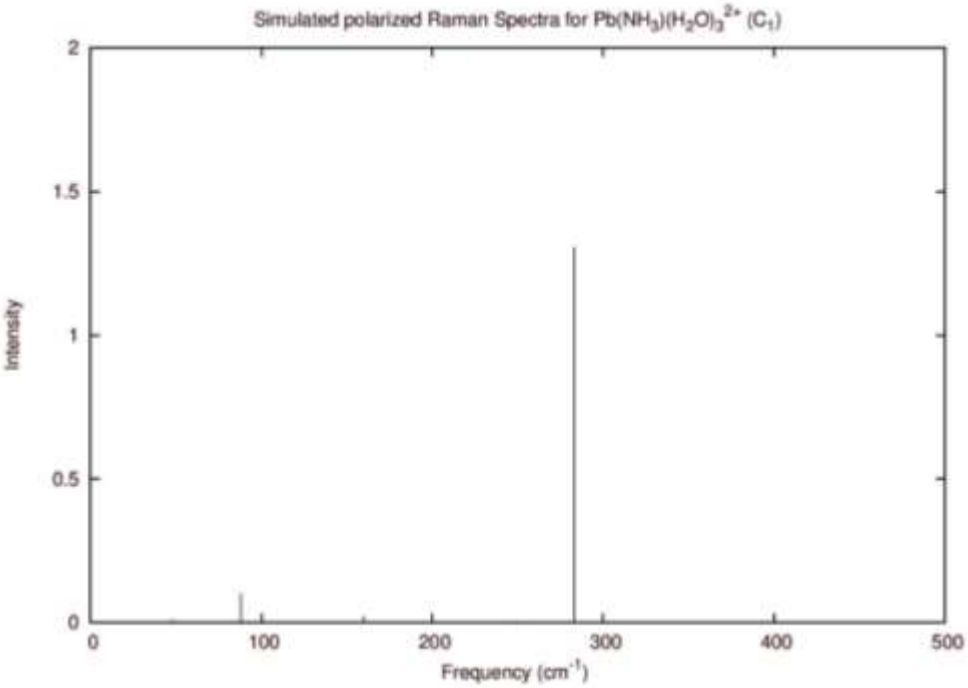
$[Pb(NH_3)(H_2O)]^{2+}$



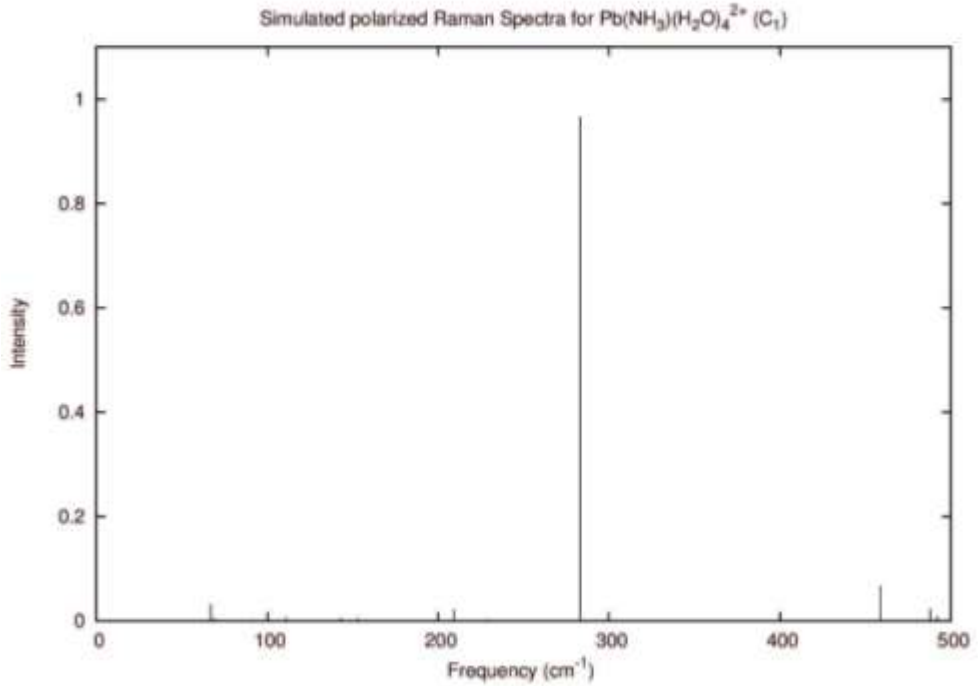
$[Pb(NH_3)(H_2O)_2]^{2+}$



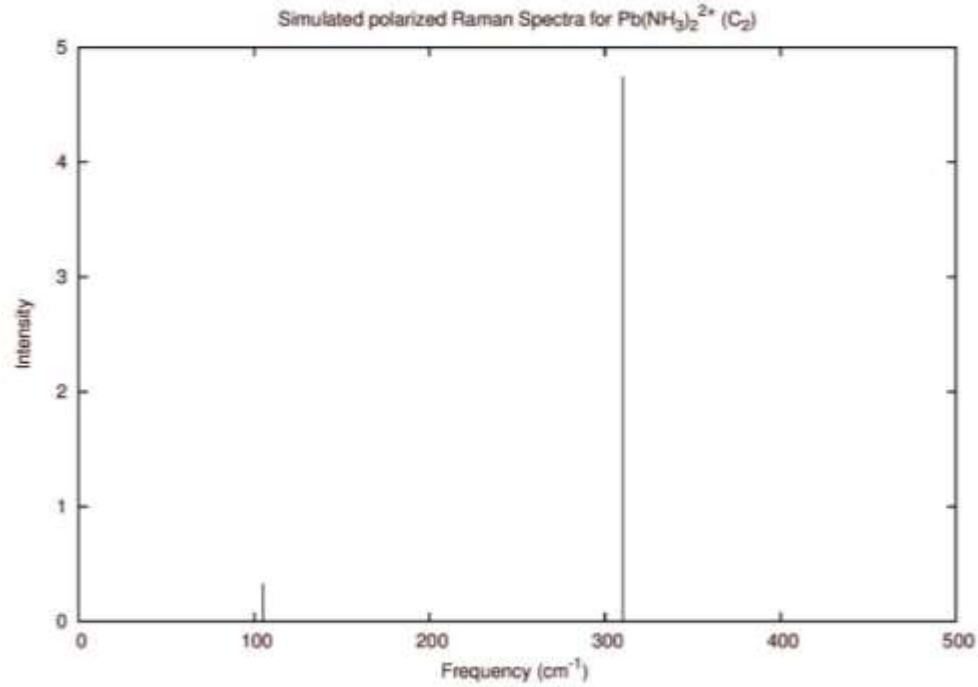
$[Pb(NH_3)(H_2O)_3]^{2+}$



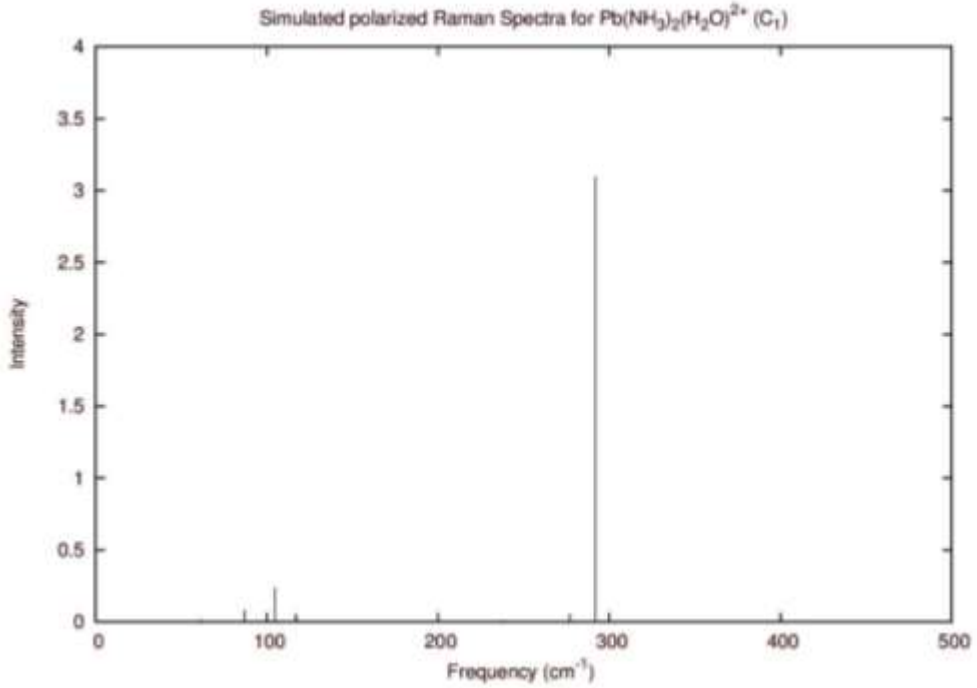
$[Pb(NH_3)(H_2O)_4]^{2+}$



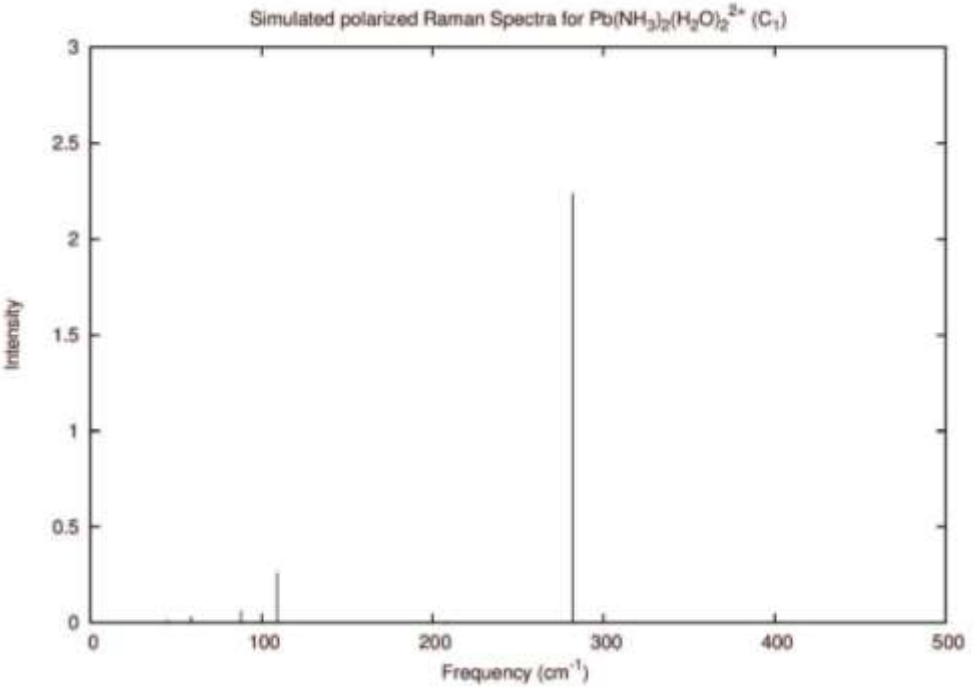
$[Pb(NH_3)_2]^{2+}$



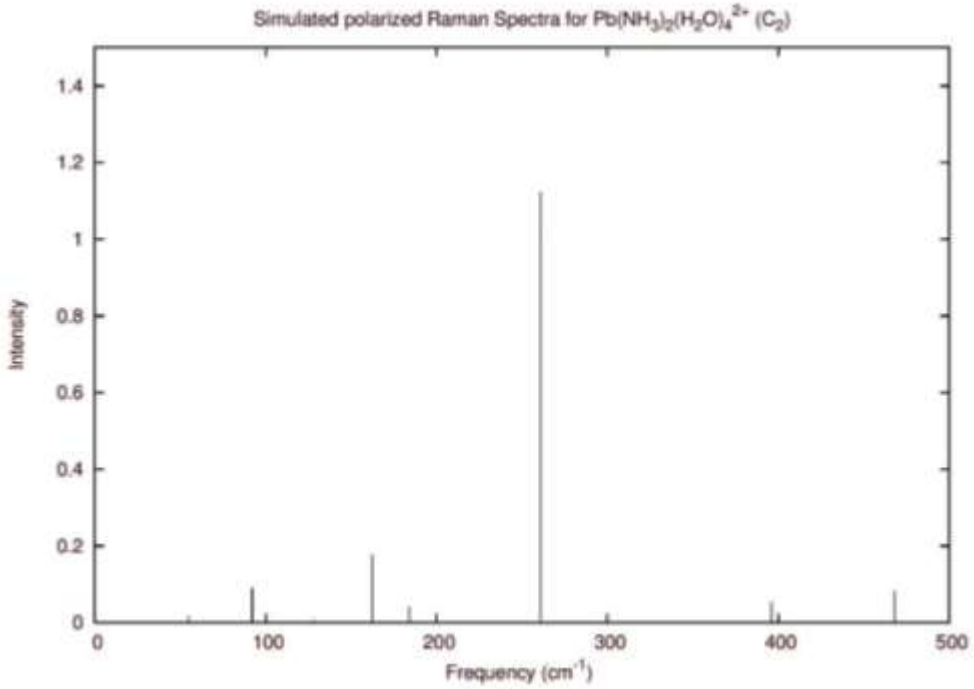
$[Pb(NH_3)_2(H_2O)]^{2+}$



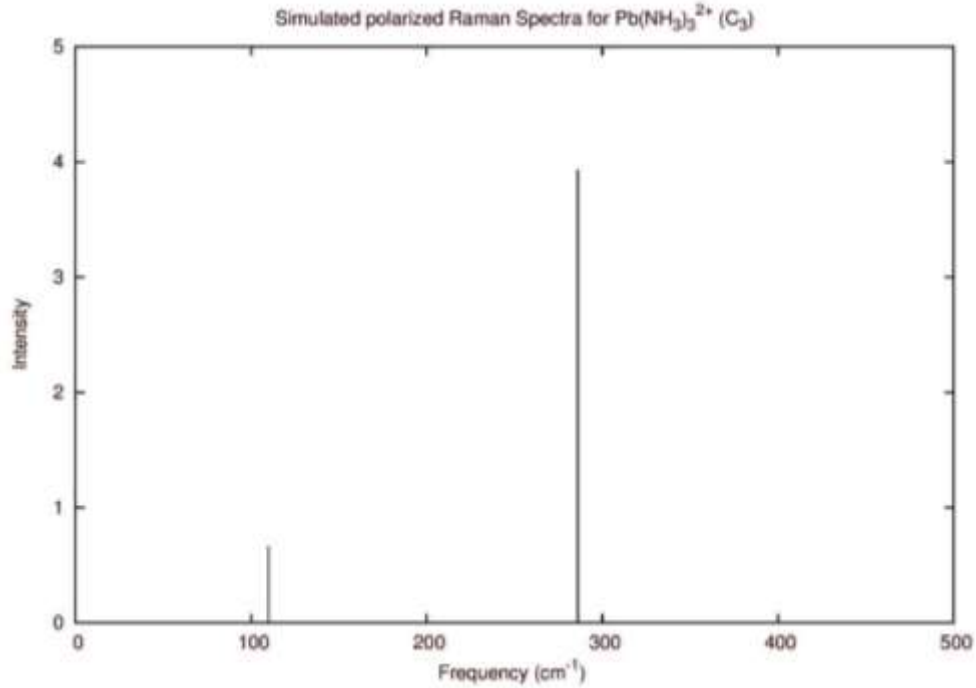
$[Pb(NH_3)_2(H_2O)_2]^{2+}$



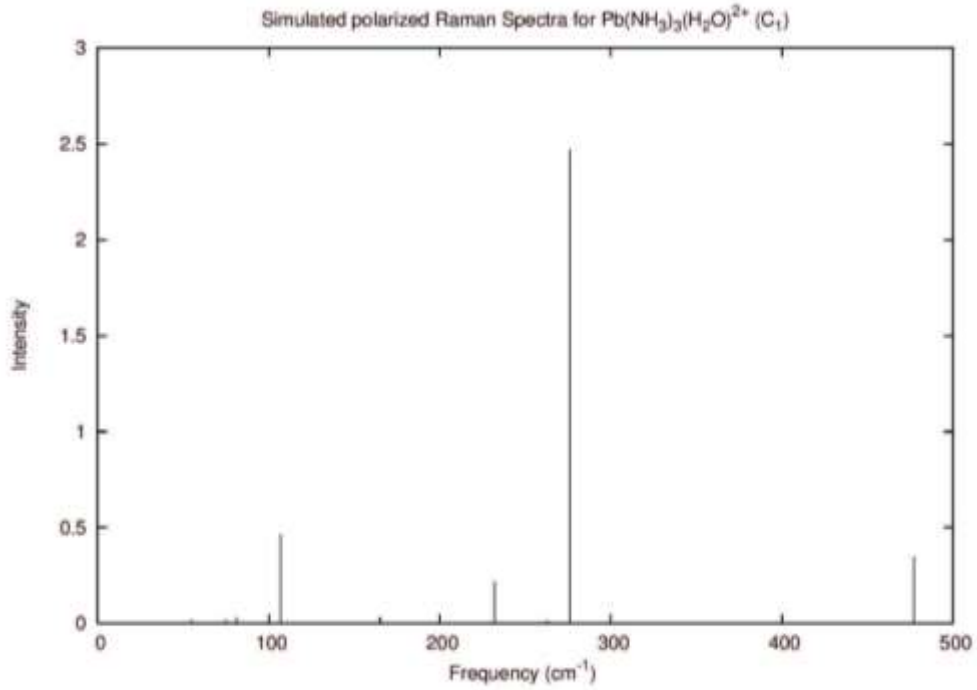
$[Pb(NH_3)_2(H_2O)_4]^{2+}$



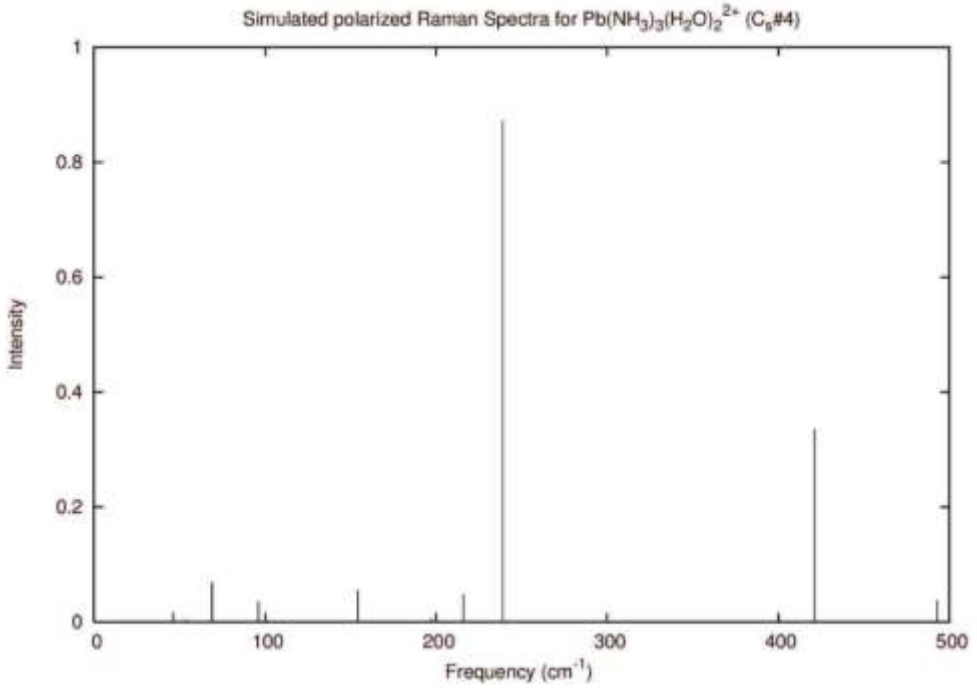
$[Pb(NH_3)_3]^{2+}$



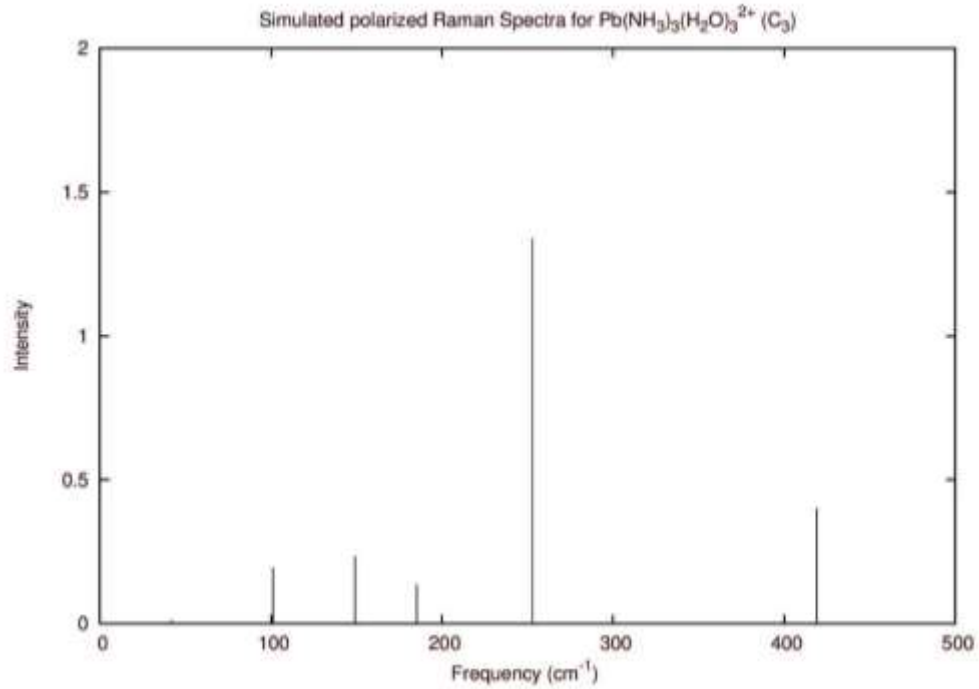
$[Pb(NH_3)_3(H_2O)]^{2+}$



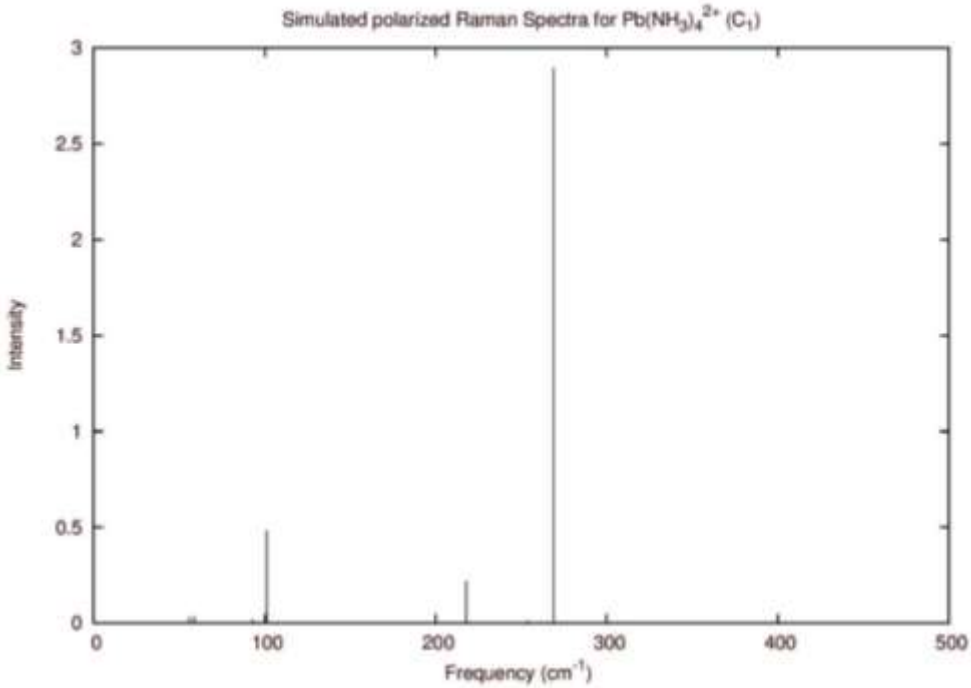
$[Pb(NH_3)_3(H_2O)_2]^{2+}$



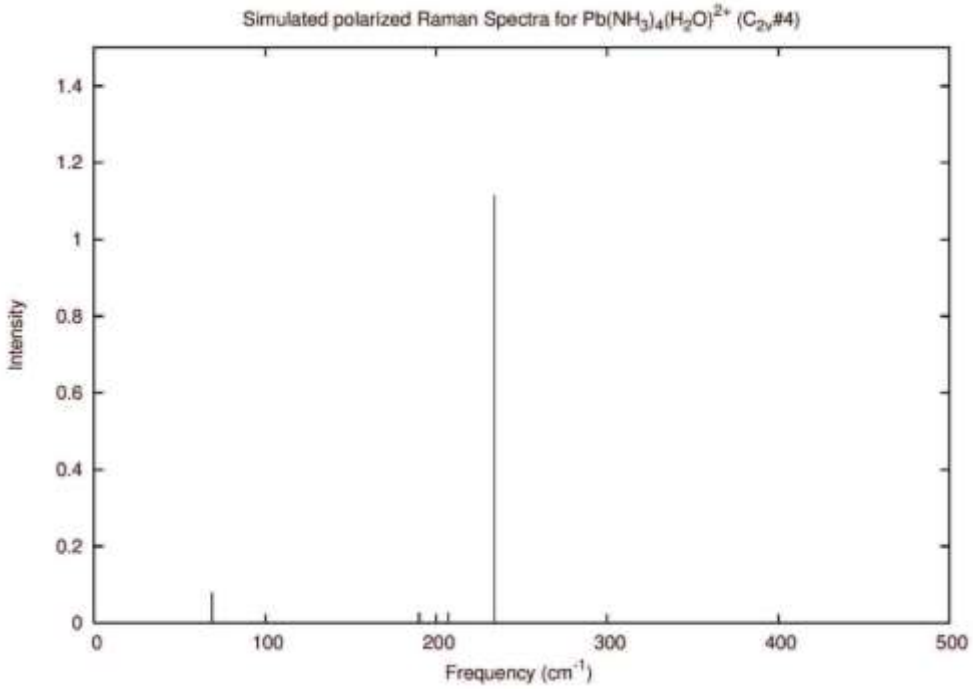
$[Pb(NH_3)_3(H_2O)_3]^{2+}$



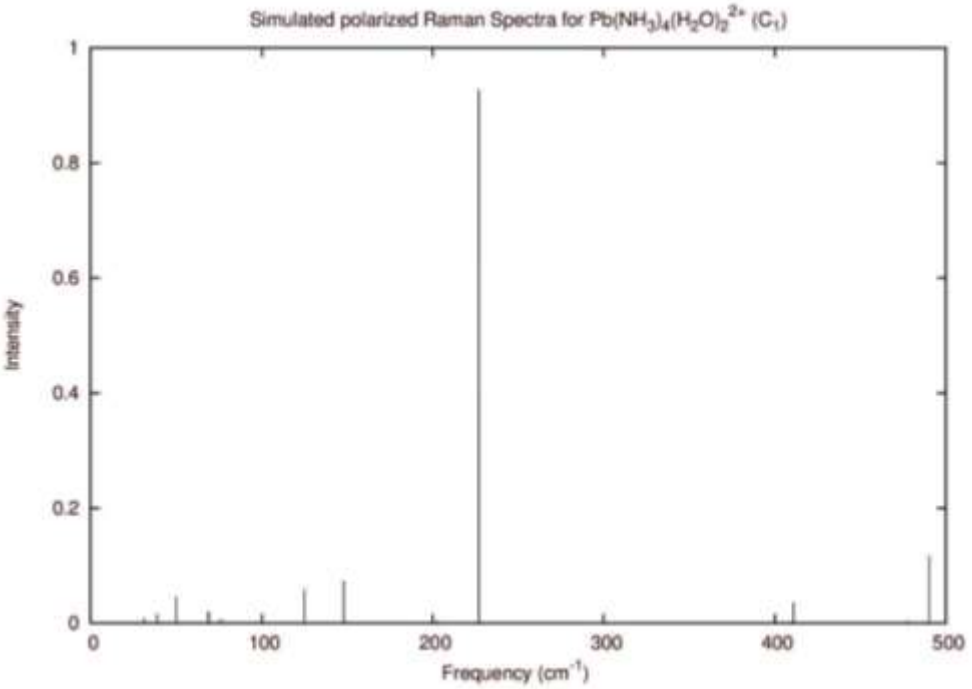
$[Pb(NH_3)_4]^{2+}$



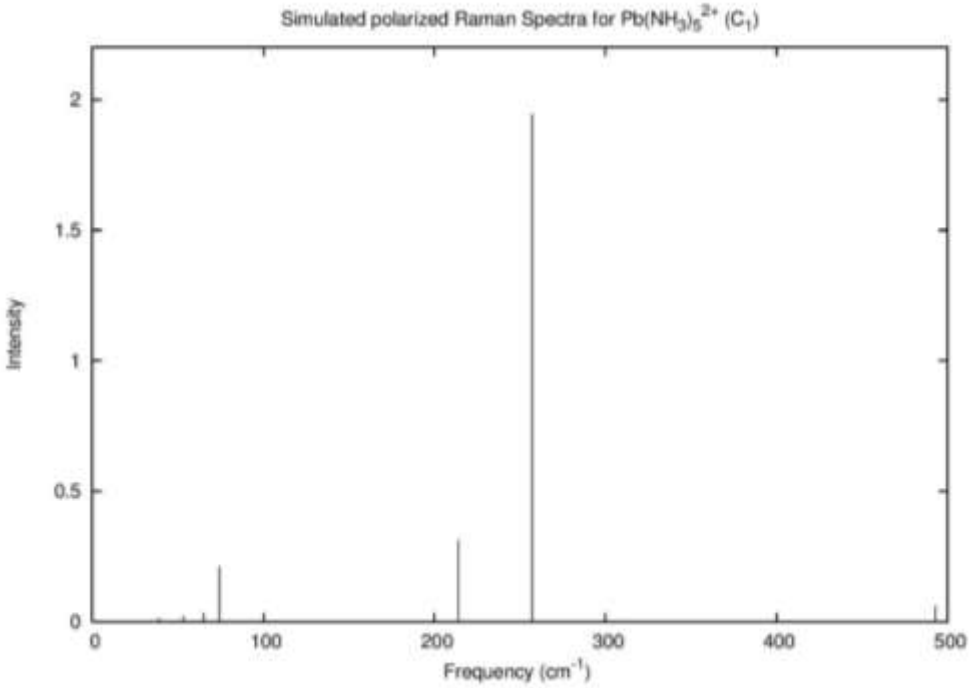
$[Pb(NH_3)_4(H_2O)]^{2+}$



$[Pb(NH_3)_4(H_2O)_2]^{2+}$



$[Pb(NH_3)_5]^{2+}$



$[Pb(NH_3)_6]^{2+}$