

Coordinates of $\text{Li}(\text{NH}_3)_n$ and $\text{Li}(\text{H}_2\text{O})_n$ optimized at the UMP2/6-311++G(2d,2p) level.

LiA1a 1+0 C3v

Li,0.,0.,-1.6577248406
N,0.,0.,0.3826067716
H,0.9386931125,0.0000000001,0.7649757067
H,-0.4693465563,0.8129320817,0.7649757067
H,-0.4693465561,-0.8129320818,0.7649757067

LiA2a 2+0 C2v

Li,0.,0.,0.8908976027
N,0.,1.8073906068,-0.0339584645
N,0.,-1.8073906068,-0.0339584645
H,-0.815062822,1.9844560033,-0.6127775638
H,0.815062822,-1.9844560033,-0.6127775638
H,0.,2.5220887429,0.6861507541
H,0.,-2.5220887429,0.6861507541
H,0.815062822,1.9844560033,-0.6127775638
H,-0.815062822,-1.9844560033,-0.6127775638

LiA3a 3+0 C3h

Li,-0.0000000001,-0.0000000003,0.
N,0.,2.0393090781,0.
H,0.9331485967,2.4401299412,0.
H,-0.4735785879,2.4245801642,0.8119974754
H,-0.4735785879,2.4245801642,-0.8119974754
N,1.7660934679,-1.0196545396,0.
H,1.6466402193,-2.0281953614,0.
H,2.3365373097,-0.8021589948,0.8119974754
H,2.3365373097,-0.8021589948,-0.8119974754
N,-1.7660934682,-1.0196545394,0.
H,-2.5797888164,-0.4119345807,0.
H,-1.8629587222,-1.6224211702,0.8119974754

H,-1.8629587222,-1.6224211702,-0.8119974754

LiA4a 4+0 T

Li,0.,0.,0.

N,1.2052984711,1.2052984711,1.2052984711

N,-1.2052984711,-1.2052984711,1.2052984711

H,1.8132214285,0.6659159904,1.8131798563

H,1.8131798563,1.8132214285,0.6659159904

H,0.6659159904,1.8131798563,1.8132214285

H,-1.8132214285,-0.6659159904,1.8131798563

H,-1.8131798563,-1.8132214285,0.6659159904

H,-0.6659159904,-1.8131798563,1.8132214285

N,-1.2052984711,1.2052984711,-1.2052984711

N,1.2052984711,-1.2052984711,-1.2052984711

H,-0.6659159904,1.8131798563,-1.8132214285

H,-1.8132214285,0.6659159904,-1.8131798563

H,-1.8131798563,1.8132214285,-0.6659159904

H,0.6659159904,-1.8131798563,-1.8132214285

H,1.8132214285,-0.6659159904,-1.8131798563

H,1.8131798563,-1.8132214285,-0.6659159904

LiA5a 4+1 C1

Li,-0.7682631594,0.1029168018,0.0219180377

N,-2.7226562027,0.8169736833,-0.2701049622

H,-3.3450741494,0.0176166439,-0.3219219622

H,-2.8473992307,1.3259276755,-1.1378269641

H,-3.0865882391,1.4107336572,0.4662280376

N,0.6482497532,1.6020128873,0.2637640376

H,1.5724587794,1.1722179475,0.1936360377

H,0.6129887232,2.0718928842,1.1597130402

H,0.6137607081,2.3315338879,-0.4372529623

N,-0.3077940822,-1.1172751713,-1.6152879643

N,-0.8090260766,-1.2128592016,1.6503470392

H,0.4741699551,-1.7302451193,-1.3994569597
H,0.0901839515,-1.666728143,1.784485037
H,-0.066776111,-0.6508241527,-2.4845899603
H,-1.0718590983,-0.8360872148,2.5554440367
H,-1.0815320449,-1.7379172151,-1.8365949635
H,-1.4647940304,-1.9649852396,1.4583430374
N,3.3361738491,0.0059800536,-0.0137019623
H,3.1594979044,-0.8929289592,0.4174690379
H,4.1897468252,0.360502106,0.3979730377
H,3.5413748584,-0.1832849336,-0.9865149645

LiA5b 5+0 C3v

Li,0.,0.,0.0341988838
N,0.,0.,2.2878914386
H,0.9360633682,0.,2.6760136814
H,-0.4680316841,0.8106546564,2.6760136814
H,-0.4680316841,-0.8106546564,2.6760136814
N,0.,0.,-2.3428757166
H,0.9341104739,0.,-2.7428719661
H,-0.467055237,-0.8089634004,-2.7428719661
H,-0.467055237,0.8089634004,-2.7428719661
N,-2.1524449318,0.,-0.0985839468
H,-2.7074708325,0.,0.7494565118
H,-2.4532754436,0.8091429708,-0.632255143
H,-2.4532754437,-0.8091429707,-0.632255143
N,1.0762224659,1.8640719911,-0.0985839468
H,1.3537354163,2.3447385209,0.7494565118
H,1.9273760898,1.7200273713,-0.632255143
H,0.5258993539,2.529170342,-0.632255143
N,1.0762224659,-1.8640719912,-0.0985839468
H,1.3537354162,-2.344738521,0.7494565118
H,0.5258993539,-2.529170342,-0.632255143
H,1.9273760897,-1.7200273713,-0.632255143

LiA6a 4+2 C2v

Li,0.,0.,0.6651802965
N,1.6951290309,0.,-0.5876981273
N,-1.6951290309,0.,-0.5876981273
H,1.3779342378,0.,-1.5558719527
H,-1.3779342378,0.,-1.5558719527
H,2.3019997141,0.8097766351,-0.5058501244
H,-2.3019997141,-0.8097766351,-0.5058501244
H,2.3019997141,-0.8097766351,-0.5058501244
H,-2.3019997141,0.8097766351,-0.5058501244
N,0.,-1.8242411523,1.6721011332
N,0.,1.8242411523,1.6721011332
H,0.,-2.4741314977,0.8832194253
H,0.,2.4741314977,0.8832194253
H,0.8092219145,-2.045385366,2.2371861849
H,-0.8092219145,2.045385366,2.2371861849
H,-0.8092219145,-2.045385366,2.2371861849
H,0.8092219145,2.045385366,2.2371861849
N,0.,-3.4042237997,-1.0279428459
N,0.,3.4042237997,-1.0279428459
H,0.,-2.6736423174,-1.7324431944
H,0.,2.6736423174,-1.7324431944
H,0.8100636873,-3.9795868063,-1.2252839649
H,-0.8100636873,3.9795868063,-1.2252839649
H,-0.8100636873,-3.9795868063,-1.2252839649
H,0.8100636873,3.9795868063,-1.2252839649

LiA6b 4+2 C1

Li,1.2404981227,0.1116102769,-0.0340523224
N,3.2178256303,-0.5358812245,-0.3085303985
H,3.1695470764,-1.5497042555,-0.2896290698
H,3.6914539089,-0.2905759675,-1.1698105706

H,3.8406753138,-0.2741217589,0.4469566383
N,-2.2738604277,1.6773646155,0.0073069916
H,-2.3760856678,0.6679109428,-0.0422339671
H,-2.8249475388,2.0647835112,-0.7472734085
H,-2.7221568912,1.9710655028,0.8653801305
N,0.6151411269,-0.8964624698,1.6894176544
H,1.2170929089,-0.8006668005,2.5024047483
H,-0.3175921024,-0.6506343732,2.01017289
H,0.5802956382,-1.8968239628,1.5003270249
N,0.8216022917,2.1378473381,0.1673317188
H,-0.1984107854,2.1422400574,0.1054282957
H,1.0650641731,2.5337249252,1.0657793698
H,1.1658710095,2.7839269793,-0.5303014115
N,0.0464244511,-0.5858479769,-1.6025485021
H,-0.8680621814,-0.7685171071,-1.1963172784
H,-0.1013252292,0.0271555898,-2.3951897994
H,0.3647581459,-1.4704702024,-1.9810209813
N,-2.5870429281,-1.6416072985,-0.0042604616
H,-3.3388123865,-1.9236777704,-0.6238690181
H,-1.9608514359,-2.4396223863,0.0520755055
H,-3.000127026,-1.5649334083,0.9192424998

LiAa8 4+4 C2

Li,0.,0.,1.3253586882
N,0.,1.6689774584,0.0655274496
N,0.,-1.6689774584,0.0655274496
H,-0.7042048295,1.548559782,-0.6604815415
H,0.7042048295,-1.548559782,-0.6604815415
H,-0.1858985547,2.5719898787,0.4860759819
H,0.1858985547,-2.5719898787,0.4860759819
H,0.8777762927,1.7736392061,-0.4320187584
H,-0.8777762927,-1.7736392061,-0.4320187584
N,-1.778190654,0.0589932329,2.4267763501

N,1.778190654,-0.0589932329,2.4267763501
H,-2.4808077614,0.3500759386,1.7419838785
H,2.4808077614,-0.3500759386,1.7419838785
H,-2.088936211,-0.8256129827,2.806003227
H,2.088936211,0.8256129827,2.806003227
H,-1.820914993,0.7212744458,3.1898236003
H,1.820914993,-0.7212744458,3.1898236003
N,-3.67502786,0.9103961622,0.1257274431
N,3.67502786,-0.9103961622,0.1257274431
H,-3.0735945785,1.0624457661,-0.6800770529
H,3.0735945785,-1.0624457661,-0.6800770529
H,-4.3159137208,0.1715230494,-0.1336776078
H,4.3159137208,-0.1715230494,-0.1336776078
H,-4.2354332389,1.7458956516,0.2321887046
H,4.2354332389,-1.7458956516,0.2321887046
N,-1.8645839134,1.2057181933,-2.5661669238
N,1.8645839134,-1.2057181933,-2.5661669238
H,-1.8677035612,0.2287406933,-2.8494736107
H,1.8677035612,-0.2287406933,-2.8494736107
H,-2.6324117292,1.6396995969,-3.0702990163
H,2.6324117292,-1.6396995969,-3.0702990163
H,-1.0192437652,1.5904342042,-2.9811360487
H,1.0192437652,-1.5904342042,-2.9811360487

LiA8b 4+4 C1

Li,-0.2624804536,1.4432145676,0.2053727334
N,1.9354395263,-1.9048918026,1.0644986719
H,2.3488035404,-1.4615399667,1.8782146329
H,2.3207877593,-2.8420501422,1.0449687246
H,2.3329134139,-1.4156507385,0.2657410348
N,0.1904871984,0.1372509039,-1.3614064271
H,-0.3210445655,-0.7248173423,-1.2094975263
H,-0.0153597802,0.442229892,-2.3039513703

H,1.1815195825,-0.0937680264,-1.3444599645
N,1.2828180427,2.7916004868,0.5548447437
H,1.7187579086,3.1222280659,-0.3024385782
H,1.0461384129,3.6277596807,1.0805674651
H,2.036568997,2.3502413251,1.0782966082
N,3.4084038482,-0.0712033122,-1.2118832899
H,3.3803328306,0.6332108256,-1.943661438
H,3.8046359569,0.4055113532,-0.4055135719
H,4.1091890983,-0.7438376573,-1.5065661164
N,-2.1696128854,2.1998832874,-0.1871556365
H,-2.2615264488,2.7532052209,-1.0283999654
H,-2.6174316461,2.7276375149,0.5497445617
H,-2.7098707273,1.3450193651,-0.3229095209
N,-0.5086636973,0.1149132989,1.8143801819
H,-0.34610643,0.4841759756,2.742289489
H,0.1570771929,-0.6412045839,1.6800534931
H,-1.4291592351,-0.3062141539,1.8210323541
N,-0.9348736842,-2.792064401,-0.1158169615
H,-1.4116870513,-3.4295450983,0.5091923846
H,-0.0552104511,-2.5497095855,0.3365782982
H,-0.6956269671,-3.3366553257,-0.9348045197
N,-3.389446889,-0.6930904679,-0.5941542307
H,-4.1603039444,-1.0118110771,-0.0226140345
H,-2.6299055618,-1.3585816438,-0.467892158
H,-3.6979107423,-0.7822635328,-1.5532378461

LiW1a 1+0 Cs

Li,0.0546311919,1.5539858328,0.
O,0.0546311919,-0.3742930514,0.
H,-0.3004715555,-0.8338065457,0.7685232711
H,-0.3004715555,-0.8338065457,-0.7685232711

LiW2a 2+0 C1

Li,0.0031635967,1.0011839155,0.0063400463
O,-1.5446259845,-0.1810698825,0.0088080063
O,1.5814274176,-0.1023313784,-0.077863834
H,-2.0963532275,0.0903459464,0.7556360916
H,2.4043677909,0.2451685325,0.2794446177
H,-2.1149150548,-0.0714701372,-0.7628835121
H,1.5029982171,-1.0003860062,0.261229284

LiW3a 3+0 C3

Li,-0.0000000002,0.0000000007,0.2992882523
O,0.6528179654,1.7937796748,0.060758602
O,-1.8798677495,-0.331532894,0.060758602
O,1.2270497836,-1.4622467786,0.060758602
H,1.1813072169,1.8410472912,-0.7495859027
H,-2.1850473318,0.1025184152,-0.7495859027
H,1.0037401144,-1.9435657042,-0.7495859027
H,0.,2.4991858054,-0.0357711659
H,-2.1643583959,-1.2495929015,-0.0357711659
H,2.1643583954,-1.2495929017,-0.0357711659

LiW4a 4+0 C1

Li,-0.0277874546,0.0446799521,-0.1578956499
O,1.663769508,0.1840215356,-1.1637406239
O,-1.2868211411,-1.3999817712,-0.5838765682
H,1.9434348841,0.9229907068,-1.7077897279
H,-0.9836828928,-2.2639537726,-0.8840123233
H,2.3122520886,0.1165686393,-0.4548714978
H,-1.7965192834,-1.5850436136,0.2193582232
O,0.9080143515,-0.362136491,1.5555476305
O,-1.1984355613,1.6179282305,-0.0027442534
H,0.69306276,0.2704144409,2.260582882
H,-2.1089745802,1.4030546873,-0.2391507832
H,0.5873553633,-1.2064307727,1.9140375873

H,-1.2557832415,1.8897077867,0.9240430974

LiW5a 4+1 C1

Li,-0.7345822736,0.2755282878,0.087384194
O,-0.0502845389,-1.3522697676,-0.9500537182
O,-2.6709025712,0.1475693022,-0.0636150312
O,0.1873662917,-0.0457355151,1.8151859989
O,0.3915348149,1.7413784151,-0.6072168815
H,-0.3373205612,-1.4344411665,-1.8785019407
H,-0.3988867601,-2.1724636847,-0.540355119
H,-2.8523143715,-0.70053443,-0.496514795
H,-3.2811702229,0.1806409643,0.6796081966
H,1.1123538233,-0.1570356189,1.5510848569
H,-0.0530448107,-0.8783805972,2.232562589
H,1.2823152501,1.3601862587,-0.607334126
H,0.2606694717,2.1081284682,-1.4835516532
O,2.3271850725,-0.212100372,-0.0688778234
H,1.7600494539,-0.8588874022,-0.5250561281
H,3.231903031,-0.5045341756,-0.1974747829

LiW6a 4+2 C1

Li,-0.0222698209,0.5898221494,0.0127618296
O,1.3027643084,1.0009733347,-1.3902511178
O,1.1722017705,0.6611113047,1.5904941177
H,2.0662261266,0.4404222485,-1.1722538098
H,1.9666371827,0.1870734006,1.2913777326
H,1.1084007425,0.8136296961,-2.3112622256
H,0.9123606374,0.2146176923,2.3999088749
O,2.9972001913,-0.7431403973,-0.0129200069
H,2.535081901,-1.5988457141,-0.1152014935
H,3.9343414459,-0.9693291621,0.0038785868
O,-0.5645386815,-1.3856405767,-0.1903479957
O,-1.7444453039,1.4734651334,-0.0077007569

H,-0.2066296872,-1.7754590413,-1.0113296661
H,-2.0403529595,2.2661386341,0.4388670369
H,-0.1376874698,-1.9472586551,0.4876848584
H,-2.4833859022,0.8359942648,0.0188004513
O,-3.3088969019,-0.7438202472,0.0788341571
H,-2.4911213458,-1.2510898154,-0.0504101049
H,-3.9313442973,-1.0889483788,-0.5632129179

LiW8a 4+4 C2

Li,0.,0.,1.354448369
O,0.,1.8315628957,2.1183757732
O,0.,-1.8315628957,2.1183757732
H,0.846372467,2.1983106046,2.3792543318
H,-0.846372467,-2.1983106046,2.3792543318
H,-0.312201343,2.3934232949,1.3888029767
H,0.312201343,-2.3934232949,1.3888029767
O,-1.6293719258,0.0936642087,0.251349064
O,1.6293719258,-0.0936642087,0.251349064
H,-1.7276197071,0.9877845136,-0.1017236855
H,1.7276197071,-0.9877845136,-0.1017236855
H,-1.5770840846,-0.4825904186,-0.5285911895
H,1.5770840846,0.4825904186,-0.5285911895
O,0.9921282382,1.687550991,-1.892974948
O,-0.9921282382,-1.687550991,-1.892974948
H,1.6588387564,2.108735625,-2.4525353419
H,-1.6588387564,-2.108735625,-2.4525353419
H,0.5417317894,1.0553675446,-2.5046688592
H,-0.5417317894,-1.0553675446,-2.5046688592
O,-0.9367605804,2.8368517024,-0.300345378
O,0.9367605804,-2.8368517024,-0.300345378
H,-0.2712508457,2.5851397471,-0.9717793902
H,0.2712508457,-2.5851397471,-0.9717793902
H,-1.3955895527,3.6021653656,-0.6516675024

H,1.3955895527,-3.6021653656,-0.6516675024