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Understanding Microsolvation of Li+: Structural and Energetical Analysis

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Cartesian coordinates of the structural motifs for the (H2O)_nLi⁺ clusters.
n = 3, 4, 5. Optimized geometries at the B3LYP/6-311++G** level.

w3s1

H	1.389652000	2.156853000	0.434712000
O	0.601398000	1.809190000	0.000401000
H	0.185109000	2.560587000	-0.438322000
H	-2.564918000	0.084307000	0.480242000
O	-1.871970000	-0.384897000	0.000169000
H	-2.316242000	-1.089180000	-0.487244000
H	1.201072000	-2.259412000	0.476302000
O	1.269659000	-1.423696000	-0.001085000
H	2.116574000	-1.451273000	-0.463110000
Li	-0.001313000	-0.002221000	0.000514000

w3s2

H	0.575826000	1.193358000	-0.007261000
O	-0.293595000	1.635098000	-0.002207000
H	-0.149358000	2.587297000	0.003141000
H	-0.111599000	-1.324540000	-0.000274000
O	-1.084608000	-1.264658000	0.001916000
H	-1.443408000	-2.158164000	-0.019316000
H	2.182652000	-0.586468000	0.773700000
O	1.622322000	-0.436623000	0.000151000
H	2.193159000	-0.593851000	-0.764178000
Li	-1.733407000	0.470611000	0.005103000

w3s3

H	3.516113000	-0.558913000	0.770941000
O	2.964067000	-0.375789000	0.000037000
H	3.515409000	-0.560273000	-0.771060000
H	-3.244518000	-0.787679000	0.772977000
O	-2.705899000	-0.582889000	0.000036000
H	-3.244624000	-0.788074000	-0.772724000
H	-0.765877000	1.854566000	-0.000317000
O	-0.506365000	0.926694000	-0.000045000
H	-1.345025000	0.398956000	-0.000061000
Li	1.184698000	0.232431000	0.000008000

w3s4

H	-0.798073000	0.194247000	-0.000198000
O	-0.000123000	0.772129000	0.000656000
H	0.797497000	0.193810000	0.000851000
H	2.714255000	-1.038519000	-0.771609000
O	2.307746000	-0.627576000	-0.000160000
H	2.717303000	-1.035753000	0.771144000
H	-2.715610000	-1.035663000	0.771984000
O	-2.307618000	-0.627613000	-0.000214000
H	-2.716190000	-1.038219000	-0.770747000
Li	0.000259000	2.541528000	-0.001228000

w4s1

H	2.166856000	-0.117665000	-1.694123000
O	1.801115000	-0.376188000	-0.840626000
H	2.461153000	-0.946657000	-0.430872000
H	-2.303041000	-0.703335000	-0.984224000
O	-1.537183000	-0.178919000	-1.244410000
H	-1.694142000	0.088168000	-2.157016000

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H	-0.294289000	-2.198809000	1.453239000	
O	-0.293057000	-1.235967000	1.408382000	
H	-0.432755000	-0.925262000	2.309985000	
H	-0.730898000	2.402343000	0.704973000	
O	0.021808000	1.800508000	0.689526000	
H	0.788966000	2.320772000	0.953546000	
Li	0.032230000	0.001658000	-0.086160000	
w4s2				
H	1.149699000	1.251295000	-0.000560000	
O	0.200649000	1.468712000	-0.008502000	
H	0.116131000	2.424646000	-0.079268000	
H	3.213731000	-0.001628000	-0.769397000	
O	2.629185000	-0.000019000	0.000081000	
H	3.213654000	0.001556000	0.769610000	
H	-3.486523000	0.596553000	0.487290000	
O	-2.906042000	-0.000012000	0.000044000	
H	-3.486647000	-0.596656000	-0.486932000	
H	1.149677000	-1.251195000	0.000477000	
O	0.200653000	-1.468681000	0.008343000	
H	0.116214000	-2.424615000	0.079293000	
Li	-0.993831000	0.000010000	-0.000079000	
w4s3				
H	-1.534664000	-0.683626000	-0.105331000	
O	-0.618190000	-1.009299000	-0.259069000	
H	-0.698033000	-1.920282000	-0.559501000	
H	-3.578647000	-0.090619000	1.006469000	
O	-3.105208000	-0.016783000	0.169980000	
H	-3.777326000	0.102911000	-0.510588000	
H	2.878884000	-1.601218000	0.729800000	
O	2.671853000	-0.856973000	0.152256000	
H	3.487660000	-0.650124000	-0.318680000	
H	0.159268000	2.419326000	-0.398796000	
O	0.885927000	1.883306000	-0.060311000	
H	1.521110000	2.500482000	0.320791000	
Li	0.955566000	-0.026286000	-0.062336000	
w4s4				
H	4.500163000	0.363761000	-0.870020000	
O	3.812072000	0.720364000	-0.296825000	
H	4.159293000	1.540558000	0.071905000	
H	-4.251623000	0.831102000	0.980139000	
O	-3.703135000	0.874958000	0.188695000	
H	-4.144862000	1.478613000	-0.419272000	
H	-2.522235000	-0.254112000	-0.242263000	
O	-1.785550000	-0.872977000	-0.470765000	
H	-2.190870000	-1.644057000	-0.881581000	
H	1.943943000	-1.149380000	1.368236000	
O	1.679272000	-0.635781000	0.597525000	
H	2.483960000	-0.147786000	0.295428000	
Li	0.000321000	-0.570401000	-0.150536000	
w4s5				
H	2.520766000	0.360996000	-0.120277000	
O	1.753067000	0.984384000	-0.098821000	
H	2.120514000	1.871169000	-0.172809000	
H	4.272893000	-1.013803000	-0.961567000	
O	3.830431000	-0.708223000	-0.161124000	
H	4.393103000	-0.957425000	0.580525000	
H	-4.695382000	0.442689000	-0.368332000	
O	-3.984234000	-0.197104000	-0.487384000	
H	-4.362165000	-0.944147000	-0.965075000	
H	-2.482078000	-0.168788000	0.292475000	
O	-1.599094000	-0.148043000	0.736963000	
H	-1.724099000	-0.547718000	1.604396000	
Li	-0.014970000	0.502972000	0.064532000	
w4s6				

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H	-2.141948000	2.711882000	-0.765552000	
O	-1.721476000	2.307972000	0.001662000	
H	-2.123705000	2.716631000	0.776422000	
H	-2.129822000	-2.715650000	-0.773770000	
O	-1.723099000	-2.307087000	-0.001590000	
H	-2.140389000	-2.709629000	0.768106000	
H	3.999949000	0.072714000	-0.767511000	
O	3.419360000	-0.000540000	0.000216000	
H	4.000624000	-0.073888000	0.767075000	
H	-0.848181000	0.793063000	-0.001978000	
O	-0.269843000	-0.000224000	-0.000348000	
H	-0.848662000	-0.793083000	-0.001075000	
Li	1.530863000	-0.001004000	-0.000410000	
w4s7				
H	1.398062000	2.572957000	-0.022196000	
O	0.780367000	1.833950000	-0.010373000	
H	1.312972000	1.011412000	-0.004598000	
H	2.639446000	-0.875497000	-0.746864000	
O	2.081828000	-0.657639000	0.012227000	
H	2.613594000	-0.865786000	0.792378000	
H	-3.126330000	0.199507000	0.029914000	
O	-2.175057000	0.341535000	0.011642000	
H	-1.733077000	-0.543041000	0.003385000	
H	-0.777660000	-2.770961000	-0.032219000	
O	-0.616944000	-1.822193000	-0.013166000	
H	0.341447000	-1.678701000	-0.009662000	
Li	-1.076667000	1.794961000	-0.004259000	
w4s8				
H	-1.613670000	2.441723000	-0.171874000	
O	-1.551203000	1.481948000	-0.153721000	
H	-0.691170000	1.228168000	0.244844000	
H	0.735706000	-0.000176000	1.775094000	
O	0.544509000	-0.000179000	0.829077000	
H	1.421942000	-0.000167000	0.375662000	
H	-1.614457000	-2.441530000	-0.172204000	
O	-1.551734000	-1.481759000	-0.153904000	
H	-0.691829000	-1.228216000	0.245117000	
H	3.489667000	0.771714000	-0.618638000	
O	2.947630000	-0.000087000	-0.420766000	
H	3.489999000	-0.771857000	-0.617881000	
Li	-2.546601000	0.000319000	-0.621873000	
w4s9				
H	-2.228680000	0.046829000	0.378564000	
O	-1.463330000	0.531524000	0.756300000	
H	-1.794239000	1.046769000	1.498782000	
H	-4.273736000	-0.484497000	-0.871973000	
O	-3.586300000	-0.839143000	-0.297857000	
H	-3.910373000	-1.687697000	0.022976000	
H	4.546553000	-0.521470000	0.742910000	
O	3.863940000	-0.766558000	0.105615000	
H	4.197241000	-1.547296000	-0.354199000	
H	-0.145993000	0.915473000	-0.060790000	
O	0.729300000	1.083801000	-0.521604000	
H	0.589788000	1.812431000	-1.134666000	
Li	2.223518000	0.114158000	-0.187078000	
w4s10				
H	-1.956628000	0.093126000	0.374994000	
O	-1.206869000	0.546325000	0.814801000	
H	-1.400350000	0.550299000	1.757584000	
H	-4.146118000	-0.252008000	-0.672093000	
O	-3.320380000	-0.690846000	-0.440483000	
H	-3.495655000	-1.637005000	-0.484843000	
H	3.079999000	-1.918367000	-0.571037000	
O	3.033546000	-1.144514000	0.001320000	
H	3.563343000	-1.351785000	0.779274000	

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H	0.321406000	0.634014000	0.217087000	
O	1.203131000	0.858085000	-0.186376000	
H	1.806562000	0.090982000	-0.079435000	
Li	1.517338000	2.412781000	-0.945210000	
w4s11				
H	-2.741609000	0.000038000	1.027042000	
O	-2.318342000	-0.000006000	0.158571000	
H	-3.042503000	-0.000051000	-0.480485000	
H	1.250420000	-0.775813000	-0.087180000	
O	1.859147000	-0.000017000	-0.012915000	
H	1.250444000	0.775824000	-0.087222000	
H	-0.222689000	2.689987000	-0.521402000	
O	-0.087796000	1.836215000	-0.098462000	
H	-0.950829000	1.391188000	-0.052502000	
H	-0.223204000	-2.690284000	-0.520585000	
O	-0.087804000	-1.836112000	-0.098615000	
H	-0.950849000	-1.391130000	-0.052506000	
Li	3.569724000	-0.000131000	0.395402000	
w5s1				
H	3.555475000	0.612567000	-0.464837000	
O	2.971783000	0.000344000	0.001368000	
H	3.556255000	-0.610672000	0.468179000	
H	-1.735884000	2.317079000	-0.752664000	
O	-1.963911000	1.380984000	-0.737698000	
H	-2.773244000	1.290879000	-1.252242000	
H	-1.749617000	-2.312824000	0.765469000	
O	-1.973781000	-1.376189000	0.734838000	
H	-2.789869000	-1.276336000	1.236791000	
H	0.443627000	1.312632000	2.012721000	
O	0.512214000	0.917997000	1.138030000	
H	1.455213000	0.758830000	0.963312000	
H	1.457570000	-0.762199000	-0.962057000	
O	0.514865000	-0.922771000	-1.136856000	
H	0.447549000	-1.327200000	-2.007161000	
Li	-0.785481000	-0.001890000	-0.001658000	
w5s2				
H	-1.676452000	-0.647434000	2.368359000	
O	-1.255607000	-0.983595000	1.569376000	
H	-0.842219000	-1.819188000	1.813424000	
H	-1.395855000	2.581879000	0.251832000	
O	-0.672409000	1.955298000	0.362739000	
H	0.104668000	2.477936000	0.588982000	
H	1.808859000	-0.470033000	-0.497184000	
O	0.889214000	-0.704603000	-0.742210000	
H	0.952576000	-1.315919000	-1.482399000	
H	-2.509248000	-0.010224000	-2.100538000	
O	-2.300420000	-0.287278000	-1.201863000	
H	-3.001675000	-0.891220000	-0.932799000	
H	4.059127000	0.516130000	-0.522141000	
O	3.434178000	0.014437000	0.013126000	
H	3.963857000	-0.483934000	0.645490000	
Li	-0.741098000	0.035978000	-0.047456000	
w5s3				
O		0.00591800	-0.40092800	1.90458300
Li		-0.02162700	0.03108600	-0.06618000
O		0.62396300	-1.59140900	-1.00344200
O		-0.61087500	1.87104900	-0.47317200
H		-0.12900400	0.17512000	2.66539000
H		1.57179300	-1.54798600	-1.17747600
H		-0.26177500	2.76236800	-0.57162100
H		0.17115600	-1.28271700	2.25718300
H		0.28202200	-2.36804900	-1.45746700
H		-1.57021700	1.92496000	-0.55570200
O		2.13509000	0.52985800	-0.16097000
O		-2.14923700	-0.40606700	-0.29864100

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H	2.58920100	1.14868400	-0.74479000	
H	2.64735100	0.52036700	0.65610700	
H	-2.61792800	-0.72547900	-1.07857000	
H	-2.65658900	-0.72055500	0.45861800	
w5s4				
H	-2.606133000	0.421284000	-0.055627000	
O	-1.817062000	0.996216000	-0.175492000	
H	-2.150782000	1.882444000	-0.346257000	
H	-4.448172000	-0.739675000	0.992448000	
O	-3.961408000	-0.637523000	0.166993000	
H	-4.555037000	-0.924984000	-0.535585000	
H	1.741650000	2.433710000	0.191903000	
O	1.549875000	1.497160000	0.084454000	
H	2.394444000	1.014663000	0.111820000	
H	1.682175000	-1.371187000	-0.090849000	
O	0.714846000	-1.301986000	-0.159815000	
H	0.358410000	-2.188917000	-0.266819000	
H	3.972367000	-0.811431000	0.883873000	
O	3.466806000	-0.597788000	0.089013000	
H	4.077647000	-0.718610000	-0.649505000	
Li	-0.030340000	0.451356000	-0.092208000	
w5s5				
H	-3.362803000	-1.467731000	-0.760424000	
O	-2.879234000	-1.134279000	0.006283000	
H	-3.354250000	-1.472627000	0.776188000	
H	-2.424932000	0.726196000	0.006668000	
O	-1.837719000	1.504354000	0.001002000	
H	-2.386265000	2.294374000	0.004942000	
H	2.424438000	0.725846000	0.006613000	
O	1.838344000	1.504813000	0.002221000	
H	2.387679000	2.294251000	0.006209000	
H	0.795964000	-1.367398000	-0.010093000	
O	0.000321000	-0.817334000	-0.015195000	
H	-0.795200000	-1.367439000	-0.008593000	
H	3.363158000	-1.468984000	-0.760247000	
O	2.878240000	-1.135152000	0.005464000	
H	3.351716000	-1.473147000	0.776471000	
Li	0.000293000	1.065814000	-0.011977000	
w5s6				
H	3.776853000	-1.186520000	0.785676000	
O	3.244744000	-0.991948000	0.006366000	
H	3.786974000	-1.221073000	-0.756404000	
H	-1.997529000	-2.753886000	-0.755145000	
O	-1.774447000	-2.204101000	0.006883000	
H	-1.975867000	-2.742561000	0.782918000	
H	1.515879000	-0.657443000	-0.009211000	
O	0.562025000	-0.435609000	-0.016929000	
H	0.060164000	-1.263624000	-0.017475000	
H	-2.343447000	-0.398275000	0.003352000	
O	-2.233602000	0.570718000	-0.001258000	
H	-3.108743000	0.968765000	-0.024526000	
H	1.203036000	3.154372000	-0.102078000	
O	0.272581000	2.925050000	0.003667000	
H	-0.198513000	3.758056000	0.118616000	
Li	-0.429738000	1.143102000	-0.005187000	
w5s7				
H	-4.253016000	-0.771744000	-1.093297000	
O	-3.762829000	-0.000002000	-0.789411000	
H	-4.253008000	0.771740000	-1.093311000	
H	-0.227395000	-1.193086000	0.478860000	
O	-1.584489000	0.000002000	0.842613000	
H	-2.369597000	0.000001000	0.246788000	
H	4.259396000	0.770356000	-0.660242000	
O	3.696774000	-0.000002000	-0.520019000	
H	4.259423000	-0.770363000	-0.660120000	

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H	-0.227394000	1.193091000	0.478857000	
O	0.685717000	1.460765000	0.247285000	
H	0.725845000	2.421256000	0.243976000	
H	0.725833000	-2.421253000	0.243950000	
O	0.685715000	-1.460762000	0.247286000	
H	-1.934176000	0.000004000	1.741715000	
Li	1.842331000	0.000000000	-0.049737000	
w5s8				
H	3.102572000	-1.736802000	-0.477266000	
O	2.545327000	-1.271688000	0.160407000	
H	2.911926000	-1.485095000	1.028719000	
H	-3.925518000	-0.920466000	0.407950000	
O	-3.377021000	-0.271672000	-0.047699000	
H	-3.985228000	0.301052000	-0.529536000	
H	0.309912000	1.717642000	0.045836000	
O	-0.656421000	1.615913000	0.213656000	
H	-0.965342000	2.434433000	0.612751000	
H	2.625522000	2.175418000	-0.591994000	
O	1.991448000	1.561315000	-0.209046000	
H	2.415906000	0.692572000	-0.140585000	
H	0.683859000	-1.483449000	-0.020700000	
O	-0.286517000	-1.524994000	-0.120771000	
H	-0.499963000	-2.426796000	-0.381234000	
Li	-1.469395000	-0.046501000	0.024558000	
w5s9				
H	-1.990508000	-0.500364000	-0.252756000	
O	-1.590405000	0.334315000	-0.584744000	
H	-2.158147000	0.637544000	-1.300156000	
H	1.989113000	-0.501983000	0.253384000	
O	1.589387000	0.332907000	0.585216000	
H	2.156541000	0.635201000	1.301522000	
H	-2.746276000	-2.810091000	-0.103628000	
O	-2.734609000	-1.954616000	0.339212000	
H	-3.403224000	-1.996357000	1.031778000	
H	0.762333000	3.647867000	-0.126924000	
O	0.001246000	3.070042000	-0.000128000	
H	-0.758891000	3.649100000	0.126772000	
H	3.403939000	-1.995704000	-1.031303000	
O	2.734349000	-1.955332000	-0.339605000	
H	2.745517000	-2.811616000	0.101689000	
Li	-0.000043000	1.142625000	0.000003000	
w5s10				
H	4.823993000	-0.804743000	-1.009092000	
O	4.313221000	-0.026185000	-0.760516000	
H	4.806036000	0.739214000	-1.076731000	
H	-2.973437000	-2.706563000	-1.038757000	
O	-2.733797000	-2.297475000	-0.200017000	
H	-3.301856000	-2.697119000	0.467724000	
H	-2.913617000	2.727344000	-1.053656000	
O	-2.683563000	2.314630000	-0.214033000	
H	-3.243832000	2.727201000	0.452435000	
H	2.652427000	0.056798000	1.887667000	
O	2.281161000	0.017552000	1.000213000	
H	3.045762000	0.005054000	0.375997000	
H	-1.842166000	-0.789988000	-0.014964000	
O	-1.267006000	-0.005541000	0.106769000	
H	-1.821934000	0.792407000	-0.021181000	
Li	0.496164000	-0.024486000	0.523740000	
w5s11				
H	-5.002805000	-1.706509000	0.392551000	
O	-4.744996000	-0.845734000	0.045647000	
H	-5.507313000	-0.506143000	-0.435288000	
H	-3.302231000	0.056544000	0.512541000	
O	-2.497619000	0.551458000	0.775530000	
H	-2.724463000	1.062902000	1.558365000	

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H	5.106582000	-0.356853000	1.588723000	
O	4.835332000	-0.018455000	0.728088000	
H	5.588556000	0.466589000	0.372802000	
H	2.877521000	-1.596629000	-1.130880000	
O	2.666293000	-0.786590000	-0.654964000	
H	3.480485000	-0.531450000	-0.157231000	
H	-1.279991000	0.922566000	-0.212915000	
O	-0.477799000	1.092993000	-0.785807000	
H	-0.709728000	1.807233000	-1.387315000	
Li	1.074569000	0.144121000	-0.656433000	
w5s12				
H	-1.453214000	-0.172492000	1.777587000	
O	-1.288937000	-0.065899000	0.833059000	
H	-1.890033000	-0.703125000	0.383011000	
H	-2.772812000	-2.745807000	-0.623576000	
O	-2.963135000	-1.825697000	-0.410785000	
H	-3.894096000	-1.685922000	-0.615743000	
H	-1.502375000	3.103802000	-0.272500000	
O	-0.843766000	2.405919000	-0.214944000	
H	-1.254263000	1.611452000	0.195088000	
H	2.167470000	-0.198001000	-0.056747000	
O	1.376158000	0.381518000	-0.075199000	
H	0.620222000	-0.101590000	0.301169000	
H	3.920002000	-1.751860000	-0.748003000	
O	3.597880000	-1.185357000	-0.038577000	
H	4.241332000	-1.247597000	0.675715000	
Li	0.930725000	2.069086000	-0.588145000	
w5s13				
H	0.707976000	0.605237000	0.229263000	
O	0.335863000	-0.286365000	0.236090000	
H	-0.622842000	-0.224615000	0.493660000	
H	-4.861652000	0.986475000	-0.854769000	
O	-4.366154000	0.169886000	-0.730010000	
H	-4.877869000	-0.527828000	-1.152805000	
H	-2.533270000	-0.238959000	1.830013000	
O	-2.196556000	-0.176465000	0.931221000	
H	-2.967780000	-0.053346000	0.340694000	
H	3.313512000	-0.127843000	-0.290819000	
O	3.235673000	-1.100996000	-0.353194000	
H	4.107239000	-1.465795000	-0.533854000	
H	3.003163000	2.096883000	0.717517000	
O	2.683023000	1.603058000	-0.048345000	
H	2.738426000	2.217168000	-0.791685000	
Li	1.486102000	-1.646772000	-0.091104000	
w5s14				
H	0.766346000	1.373541000	0.041537000	
O	0.716293000	0.405000000	0.173618000	
H	-0.205036000	0.176463000	0.456021000	
H	-4.512393000	-0.203416000	-0.962316000	
O	-3.894116000	-0.866323000	-0.637066000	
H	-4.313997000	-1.721416000	-0.779078000	
H	-2.009037000	-0.339237000	1.861851000	
O	-1.678200000	-0.433849000	0.963406000	
H	-2.459380000	-0.577284000	0.391663000	
H	4.028147000	-2.360078000	0.459223000	
O	3.428865000	-2.051818000	-0.231658000	
H	3.698098000	-2.504263000	-1.040483000	
H	0.800370000	3.586395000	-1.030647000	
O	1.050448000	3.101358000	-0.236697000	
H	1.173572000	3.761299000	0.454366000	
Li	2.015664000	-0.808982000	-0.034985000	
w5s15				
H	-0.421595000	-0.547924000	1.849119000	
O	-0.528375000	-0.396628000	0.902476000	
H	0.348531000	-0.628474000	0.483704000	

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H	-1.649214000	2.672872000	0.054647000	
O	-1.914222000	1.751909000	-0.023663000	
H	-1.228959000	1.185427000	0.398591000	
H	4.715911000	0.534683000	0.522543000	
O	4.042517000	0.555935000	-0.165994000	
H	4.448589000	0.981309000	-0.928952000	
H	2.025175000	-1.868396000	-0.540555000	
O	1.768077000	-0.992873000	-0.236118000	
H	2.581123000	-0.446393000	-0.214745000	
H	-1.993401000	-1.100350000	0.123090000	
O	-2.848049000	-1.042682000	-0.361438000	
H	-3.192172000	-1.930524000	-0.495319000	
Li	-3.264523000	0.714163000	-0.724738000	
w5s16				
H	2.022857000	0.023848000	1.800457000	
O	1.701150000	-0.001736000	0.892460000	
H	2.316164000	-0.592680000	0.407338000	
H	0.792625000	3.323890000	-0.481494000	
O	0.646311000	2.372926000	-0.488400000	
H	1.405554000	1.952942000	-0.058289000	
O	3.640295000	-2.555164000	-0.362597000	
H	3.453545000	-1.619346000	-0.492795000	
H	4.118954000	-1.293277000	-1.108346000	
H	-4.732858000	-1.363548000	-0.949451000	
O	-4.364011000	-0.941874000	-0.163350000	
H	-5.090516000	-0.873376000	0.468540000	
H	-0.095742000	-0.041561000	0.547588000	
O	-0.934239000	0.340004000	0.209467000	
H	-0.623538000	1.214538000	-0.119591000	
Li	-2.591947000	-0.331801000	0.065595000	
w5s17				
H	-1.823948000	1.089444000	0.300303000	
O	-1.280985000	1.893648000	0.291590000	
H	-1.779304000	2.586910000	0.734982000	
H	1.835077000	0.284542000	-0.144847000	
O	2.108060000	-0.629682000	0.151935000	
H	1.334926000	-1.214494000	-0.028454000	
H	1.460404000	2.256468000	-1.291741000	
O	1.338558000	1.800952000	-0.452761000	
H	0.403919000	1.939998000	-0.184983000	
H	-3.112030000	-1.034219000	0.860703000	
O	-2.629497000	-0.700087000	0.093593000	
H	-3.266225000	-0.702039000	-0.632782000	
H	-0.209185000	-2.817681000	-0.928608000	
O	-0.111048000	-2.104564000	-0.289578000	
H	-0.981723000	-1.678356000	-0.206008000	
Li	3.579129000	-0.930903000	1.054400000	