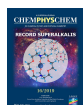


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Supporting Information

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Record Low Ionization Potentials of Alkali Metal Complexes with Crown Ethers and Cryptands

Nikolay V. Tkachenko, Zhong-Ming Sun, and Alexander I. Boldyrev*

Supporting Information

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1. Optimized geometries, total energies, ZPE corrections of investigated molecules

Table S1. Cartesian coordinates of optimized geometries, total energies, ZPE corrections of investigated molecules

[Li(9-Crown-3) ₂]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -929.6946909, ZPE correction= 0.375597)			
	8	0.125709000	1.563854000	1.372885000
	8	1.292206000	-0.889042000	1.372132000
	8	-1.415160000	-0.672868000	1.371588000
	6	1.133374000	1.334829000	2.353474000
	6	-1.721764000	0.313890000	2.352282000
	6	2.039481000	0.217279000	1.863164000
	6	0.590233000	-1.648045000	2.352216000
	6	-0.830698000	-1.873544000	1.861822000
	6	-1.206332000	1.657611000	1.863191000
	1	0.677444000	1.085960000	3.318320000
	1	1.722406000	2.249119000	2.498740000
	1	-1.279656000	0.042917000	3.317631000
	1	-2.808252000	0.366986000	2.495995000
	1	2.628971000	0.559216000	1.009973000
	1	2.728276000	-0.089558000	2.660431000
	1	0.602812000	-1.129589000	3.317481000
	1	1.087501000	-2.615442000	2.496507000
	1	-0.829254000	-2.554344000	1.007919000
	1	-1.440880000	-2.317204000	2.658711000
	1	-1.285446000	2.407038000	2.660866000
	1	-1.796697000	1.997696000	1.009708000
	3	0.000000000	0.000000000	0.000000000
	8	-1.292206000	0.889042000	-1.372132000
	6	-0.590233000	1.648045000	-2.352216000
	1	-1.087501000	2.615442000	-2.496507000
	1	-0.602812000	1.129589000	-3.317481000
	1	0.829254000	2.554344000	-1.007919000
	1	1.440880000	2.317204000	-2.658711000
	6	0.830698000	1.873544000	-1.861822000
	8	1.415160000	0.672868000	-1.371588000
	1	2.808252000	-0.366986000	-2.495995000
	6	1.721764000	-0.313890000	-2.352282000

	1	1.279656000	-0.042917000	-3.317631000
	6	1.206332000	-1.657611000	-1.863191000
	1	1.285446000	-2.407038000	-2.660866000
	1	1.796697000	-1.997696000	-1.009708000
	8	-0.125709000	-1.563854000	-1.372885000
	6	-1.133374000	-1.334829000	-2.353474000
	1	-0.677444000	-1.085960000	-3.318320000
	1	-1.722406000	-2.249119000	-2.498740000
	6	-2.039481000	-0.217279000	-1.863164000
	1	-2.628971000	-0.559216000	-1.009973000
	1	-2.728276000	0.089558000	-2.660431000
[Li(9-Crown-3) ₂] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -929.6158829, ZPE correction= 0.377006)			
	8	0.127586000	1.562277000	1.383464000
	8	1.290987000	-0.890797000	1.383993000
	8	-1.413486000	-0.670321000	1.381332000
	6	1.132561000	1.332503000	2.366282000
	6	-1.719923000	0.314523000	2.363573000
	6	2.040306000	0.216231000	1.872929000
	6	0.588371000	-1.646992000	2.365727000
	6	-0.831484000	-1.874051000	1.870139000
	6	-1.206409000	1.658801000	1.871097000
	1	0.672679000	1.078998000	3.327167000
	1	1.719755000	2.245532000	2.516887000
	1	-1.272360000	0.043370000	3.325492000
	1	-2.804592000	0.365749000	2.511943000
	1	2.623661000	0.560556000	1.016602000
	1	2.734744000	-0.090809000	2.664079000
	1	0.597742000	-1.122455000	3.326834000
	1	1.085481000	-2.612010000	2.516162000
	1	-0.823940000	-2.550335000	1.013007000
	1	-1.446503000	-2.322019000	2.659691000
	1	-1.287822000	2.413649000	2.662270000
	1	-1.795109000	1.992424000	1.014235000
	3	0.000000000	0.000000000	0.000000000
	8	-1.290987000	0.890797000	-1.383993000
	6	-0.588371000	1.646992000	-2.365727000
	1	-1.085481000	2.612010000	-2.516162000

	1	-0.597742000	1.122455000	-3.326834000
	1	0.823940000	2.550335000	-1.013007000
	1	1.446503000	2.322019000	-2.659691000
	6	0.831484000	1.874051000	-1.870139000
	8	1.413486000	0.670321000	-1.381332000
	1	2.804592000	-0.365749000	-2.511943000
	6	1.719923000	-0.314523000	-2.363573000
	1	1.272360000	-0.043370000	-3.325492000
	6	1.206409000	-1.658801000	-1.871097000
	1	1.287822000	-2.413649000	-2.662270000
	1	1.795109000	-1.992424000	-1.014235000
	8	-0.127586000	-1.562277000	-1.383464000
	6	-1.132561000	-1.332503000	-2.366282000
	1	-0.672679000	-1.078998000	-3.327167000
	1	-1.719755000	-2.245532000	-2.516887000
	6	-2.040306000	-0.216231000	-1.872929000
	1	-2.623661000	-0.560556000	-1.016602000
	1	-2.734744000	0.090809000	-2.664079000
[Li(9-Crown-3) ₂] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -929.6158102)			
[Li(9-Crown-3) ₂]	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -929.7718875)			
[Li(9-Crown-3) ₂] ⁺	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -929.6929415)			
[Li(9-Crown-3) ₂] ⁺ in the geometry of neutral complex	PBE0/aug-cc-pvtz (E _{elec} = -929.6928270)			
[Li(9-Crown-3) ₂]	TPSSh/6-311++G** (0 imaginary Frequencies, E _{elec} = -930.8061435, ZPE correction= 0.371771)			
	8	0.127758000	1.569417000	1.378842000
	8	1.296539000	-0.893812000	1.378496000
	8	-1.420376000	-0.673648000	1.377126000
	6	1.140568000	1.338337000	2.376814000
	6	-1.728333000	0.318376000	2.375297000
	6	2.054690000	0.221301000	1.878475000
	6	0.589891000	-1.656048000	2.375831000
	6	-0.834419000	-1.888382000	1.876737000
	6	-1.217152000	1.668770000	1.878443000
	1	0.674706000	1.078534000	3.333601000
	1	1.720334000	2.257296000	2.524957000

	1	-1.272134000	0.044067000	3.332713000
	1	-2.814307000	0.360907000	2.521578000
	1	2.638594000	0.561781000	1.022242000
	1	2.738877000	-0.095102000	2.675172000
	1	0.597864000	-1.123474000	3.333024000
	1	1.095614000	-2.617853000	2.523220000
	1	-0.831218000	-2.563656000	1.020009000
	1	-1.451212000	-2.322938000	2.672749000
	1	-1.285113000	2.418820000	2.675784000
	1	-1.803545000	2.005303000	1.022389000
	3	0.000000000	0.000000000	0.000000000
	8	-1.296539000	0.893812000	-1.378496000
	6	-0.589891000	1.656048000	-2.375831000
	1	-1.095614000	2.617853000	-2.523220000
	1	-0.597864000	1.123474000	-3.333024000
	1	0.831218000	2.563656000	-1.020009000
	1	1.451212000	2.322938000	-2.672749000
	6	0.834419000	1.888382000	-1.876737000
	8	1.420376000	0.673648000	-1.377126000
	1	2.814307000	-0.360907000	-2.521578000
	6	1.728333000	-0.318376000	-2.375297000
	1	1.272134000	-0.044067000	-3.332713000
	6	1.217152000	-1.668770000	-1.878443000
	1	1.285113000	-2.418820000	-2.675784000
	1	1.803545000	-2.005303000	-1.022389000
	8	-0.127758000	-1.569417000	-1.378842000
	6	-1.140568000	-1.338337000	-2.376814000
	1	-0.674706000	-1.078534000	-3.333601000
	1	-1.720334000	-2.257296000	-2.524957000
	6	-2.054690000	-0.221301000	-1.878475000
	1	-2.638594000	-0.561781000	-1.022242000
	1	-2.738877000	0.095102000	-2.675172000
[Li(9-Crown-3) ₂] ⁺	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -930.7288225, ZPE correction= 0.373232)			
	8	0.129418000	1.567934000	1.389794000
	8	1.294747000	-0.894928000	1.390265000
	8	-1.419439000	-0.671350000	1.387389000
	6	1.139979000	1.336359000	2.389375000

	6	-1.727063000	0.319201000	2.386558000
	6	2.055442000	0.220390000	1.887753000
	6	0.587992000	-1.655089000	2.388548000
	6	-0.835702000	-1.888777000	1.884953000
	6	-1.217137000	1.670073000	1.886277000
	1	0.670299000	1.072301000	3.342100000
	1	1.717732000	2.254145000	2.542379000
	1	-1.266021000	0.044153000	3.340411000
	1	-2.811162000	0.360354000	2.536713000
	1	2.633273000	0.563340000	1.028721000
	1	2.745764000	-0.096212000	2.677912000
	1	0.593503000	-1.117255000	3.341790000
	1	1.093544000	-2.614620000	2.540992000
	1	-0.826819000	-2.559962000	1.025385000
	1	-1.456707000	-2.328251000	2.673798000
	1	-1.288072000	2.425832000	2.676781000
	1	-1.802143000	1.999958000	1.027021000
	3	0.000000000	0.000000000	0.000000000
	8	-1.294747000	0.894928000	-1.390265000
	6	-0.587992000	1.655089000	-2.388548000
	1	-1.093544000	2.614620000	-2.540992000
	1	-0.593503000	1.117255000	-3.341790000
	1	0.826819000	2.559962000	-1.025385000
	1	1.456707000	2.328251000	-2.673798000
	6	0.835702000	1.888777000	-1.884953000
	8	1.419439000	0.671350000	-1.387389000
	1	2.811162000	-0.360354000	-2.536713000
	6	1.727063000	-0.319201000	-2.386558000
	1	1.266021000	-0.044153000	-3.340411000
	6	1.217137000	-1.670073000	-1.886277000
	1	1.288072000	-2.425832000	-2.676781000
	1	1.802143000	-1.999958000	-1.027021000
	8	-0.129418000	-1.567934000	-1.389794000
	6	-1.139979000	-1.336359000	-2.389375000
	1	-0.670299000	-1.072301000	-3.342100000
	1	-1.717732000	-2.254145000	-2.542379000
	6	-2.055442000	-0.220390000	-1.887753000
	1	-2.633273000	-0.563340000	-1.028721000

	1	-2.745764000	0.096212000	-2.677912000
[Li(9-Crown-3) ₂] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -930.7287432)			
[Li(9-Crown-3) ₂]	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -930.8826172)			
[Li(9-Crown-3) ₂] ⁺	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -930.8050338)			
[Li(9-Crown-3) ₂] ⁺ in the geometry of neutral complex	TPSSh/aug-cc-pvtz (E _{elec} = -930.8049032)			
[Li(12-Crown-4)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -622.2858350, ZPE correction= 0.248847)			
	8	0.000000000	1.958815000	0.428173000
	8	-1.602221000	0.000000000	-0.274029000
	8	1.602221000	0.000000000	-0.274029000
	8	0.000000000	-1.958815000	0.428173000
	6	1.214666000	2.302412000	-0.222855000
	6	-2.228860000	1.219236000	0.089561000
	6	2.228860000	1.219236000	0.089561000
	6	-2.228860000	-1.219236000	0.089561000
	6	2.228860000	-1.219236000	0.089561000
	6	-1.214666000	-2.302412000	-0.222855000
	6	1.214666000	-2.302412000	-0.222855000
	6	-1.214666000	2.302412000	-0.222855000
	1	1.580009000	3.275513000	0.128328000
	1	1.051520000	2.353124000	-1.306300000
	1	-2.474120000	1.212173000	1.161669000
	1	-3.149120000	1.382122000	-0.490060000
	1	3.149120000	1.382122000	-0.490060000
	1	2.474120000	1.212173000	1.161669000
	1	-3.149120000	-1.382122000	-0.490060000
	1	-2.474120000	-1.212173000	1.161669000
	1	2.474120000	-1.212173000	1.161669000
	1	3.149120000	-1.382122000	-0.490060000
	1	-1.580009000	-3.275513000	0.128328000
	1	-1.051520000	-2.353124000	-1.306300000
	1	1.051520000	-2.353124000	-1.306300000
	1	1.580009000	-3.275513000	0.128328000
	1	-1.580009000	3.275513000	0.128328000
	1	-1.051520000	2.353124000	-1.306300000
	3	0.000000000	0.000000000	0.919405000

[Li(12-Crown-4)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -622.1938051, ZPE correction= 0.251309)			
	8	0.000000000	1.886061000	0.431986000
	8	-1.727653000	0.000000000	-0.352013000
	8	1.727653000	0.000000000	-0.352013000
	8	0.000000000	-1.886061000	0.431986000
	6	1.225849000	2.294105000	-0.184276000
	6	-2.267601000	1.232520000	0.122652000
	6	2.267601000	1.232520000	0.122652000
	6	-2.267601000	-1.232520000	0.122652000
	6	2.267601000	-1.232520000	0.122652000
	6	-1.225849000	-2.294105000	-0.184276000
	6	1.225849000	-2.294105000	-0.184276000
	6	-1.225849000	2.294105000	-0.184276000
	1	1.548380000	3.265737000	0.203514000
	1	1.082433000	2.371508000	-1.268158000
	1	-2.454399000	1.170083000	1.203309000
	1	-3.209275000	1.473154000	-0.382375000
	1	3.209275000	1.473154000	-0.382375000
	1	2.454399000	1.170083000	1.203309000
	1	-3.209275000	-1.473154000	-0.382375000
	1	-2.454399000	-1.170083000	1.203309000
	1	2.454399000	-1.170083000	1.203309000
	1	3.209275000	-1.473154000	-0.382375000
	1	-1.548380000	-3.265737000	0.203514000
	1	-1.082433000	-2.371508000	-1.268158000
	1	1.082433000	-2.371508000	-1.268158000
	1	1.548380000	-3.265737000	0.203514000
	1	-1.548380000	3.265737000	0.203514000
	1	-1.082433000	2.371508000	-1.268158000
	3	0.000000000	0.000000000	0.391414000
[Li(12-Crown-4)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -622.1879969)			
[Li(12-Crown-4)]	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -622.3406275)			
[Li(12-Crown-4)] ⁺	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -622.2482496)			
[Li(12-Crown-4)] ⁺ in the geometry of neutral complex	PBE0/aug-cc-pvtz (E _{elec} = -622.242103256)			
[Li(12-Crown-4)]	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -			

	623.0350335, ZPE correction= 0.246245)			
	8	0.000000000	1.960761000	0.437018000
	8	-1.608470000	0.000000000	-0.271613000
	8	1.608470000	0.000000000	-0.271613000
	8	0.000000000	-1.960761000	0.437018000
	6	1.225947000	2.317239000	-0.224219000
	6	-2.248878000	1.232586000	0.088775000
	6	2.248878000	1.232586000	0.088775000
	6	-2.248878000	-1.232586000	0.088775000
	6	2.248878000	-1.232586000	0.088775000
	6	-1.225947000	-2.317239000	-0.224219000
	6	1.225947000	-2.317239000	-0.224219000
	6	-1.225947000	2.317239000	-0.224219000
	1	1.580072000	3.290897000	0.134982000
	1	1.054664000	2.368322000	-1.305244000
	1	-2.501039000	1.223393000	1.157754000
	1	-3.161281000	1.385472000	-0.505255000
	1	3.161281000	1.385472000	-0.505255000
	1	2.501039000	1.223393000	1.157754000
	1	-3.161281000	-1.385472000	-0.505255000
	1	-2.501039000	-1.223393000	1.157754000
	1	2.501039000	-1.223393000	1.157754000
	1	3.161281000	-1.385472000	-0.505255000
	1	-1.580072000	-3.290897000	0.134982000
	1	-1.054664000	-2.368322000	-1.305244000
	1	1.054664000	-2.368322000	-1.305244000
	1	1.580072000	-3.290897000	0.134982000
	1	-1.580072000	3.290897000	0.134982000
	1	-1.054664000	2.368322000	-1.305244000
	3	0.000000000	0.000000000	0.891747000
[Li(12-Crown-4)] ⁺	TPSSh/6-311++G** (0 imaginary Frequencies, E _{elec} = -622.9456623, ZPE correction= 0.248878)			
	8	0.000000000	1.883714000	0.432995000
	8	-1.745862000	0.000000000	-0.359420000
	8	1.745862000	0.000000000	-0.359420000
	8	0.000000000	-1.883714000	0.432995000
	6	1.238168000	2.307387000	-0.187070000
	6	-2.286600000	1.245490000	0.131806000

	6	2.286600000	1.245490000	0.131806000
	6	-2.286600000	-1.245490000	0.131806000
	6	2.286600000	-1.245490000	0.131806000
	6	-1.238168000	-2.307387000	-0.187070000
	6	1.238168000	-2.307387000	-0.187070000
	6	-1.238168000	2.307387000	-0.187070000
	1	1.546592000	3.279524000	0.208653000
	1	1.092996000	2.382160000	-1.269942000
	1	-2.459342000	1.174797000	1.212891000
	1	-3.230332000	1.483143000	-0.368942000
	1	3.230332000	1.483143000	-0.368942000
	1	2.459342000	1.174797000	1.212891000
	1	-3.230332000	-1.483143000	-0.368942000
	1	-2.459342000	-1.174797000	1.212891000
	1	2.459342000	-1.174797000	1.212891000
	1	3.230332000	-1.483143000	-0.368942000
	1	-1.546592000	-3.279524000	0.208653000
	1	-1.092996000	-2.382160000	-1.269942000
	1	1.092996000	-2.382160000	-1.269942000
	1	1.546592000	-3.279524000	0.208653000
	1	-1.546592000	3.279524000	0.208653000
	1	-1.092996000	2.382160000	-1.269942000
	3	0.000000000	0.000000000	0.339502000
[Li(12-Crown-4)] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -622.9404031)			
[Li(12-Crown-4)]	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -623.0891744)			
[Li(12-Crown-4)] ⁺	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -622.9994885)			
[Li(12-Crown-4)] ⁺ in the geometry of neutral complex	TPSSh/aug-cc-pvtz (E _{elec} = -622.993898831)			
[Na(15-Crown-5)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -930.6833716, ZPE correction= 0.309192)			
	8	-2.305637000	0.625427000	0.234279000
	8	-1.219108000	-1.840632000	-0.234921000
	8	-0.117008000	2.119215000	-0.052403000
	8	1.473184000	-1.771191000	0.146251000
	8	2.154868000	0.847310000	-0.356112000
	6	-0.535914000	-3.013692000	0.159730000
	6	-1.358378000	2.789481000	-0.009060000

	6	0.867230000	-2.926529000	-0.387286000
	6	-3.102873000	-0.429592000	-0.260226000
	6	-2.542720000	-1.733650000	0.250057000
	6	1.034955000	2.927533000	-0.171783000
	6	2.722844000	-1.441166000	-0.420037000
	6	2.227015000	2.108833000	0.273364000
	6	3.122847000	-0.079200000	0.088732000
	6	-2.417056000	1.826938000	-0.495627000
	1	-3.411892000	2.278291000	-0.364291000
	1	-1.033621000	-3.909191000	-0.241813000
	1	-0.510515000	-3.087178000	1.257525000
	1	-1.356633000	3.669505000	-0.666749000
	1	-1.565931000	3.117896000	1.018559000
	1	1.427672000	-3.829652000	-0.103854000
	1	0.838499000	-2.863158000	-1.484926000
	1	-3.082758000	-0.429446000	-1.359445000
	1	-4.145781000	-0.318068000	0.069706000
	1	-2.547610000	-1.750017000	1.350631000
	1	-3.162151000	-2.566464000	-0.115822000
	1	0.963833000	3.816536000	0.470703000
	1	1.145459000	3.254216000	-1.214975000
	1	2.645850000	-1.424960000	-1.516949000
	1	3.486421000	-2.179203000	-0.133676000
	1	3.156459000	2.636398000	0.007418000
	1	2.200272000	1.979563000	1.367074000
	1	3.160892000	-0.091200000	1.188636000
	1	4.122074000	0.180459000	-0.293139000
	1	-2.266428000	1.621808000	-1.565839000
	11	-0.005655000	-0.010990000	0.933389000
[Na(15-Crown-5)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -930.5973944, ZPE correction= 0.311426)			
	8	-0.026307000	-2.138488000	0.343794000
	8	2.225836000	-0.760326000	-0.335535000
	8	-2.206677000	-0.736398000	-0.545387000
	8	1.345605000	1.743734000	0.219869000
	8	-1.341792000	1.860744000	-0.167710000
	6	3.138640000	0.215417000	0.145872000
	6	-2.367946000	-1.810634000	0.370107000

	6	2.659802000	1.581188000	-0.284868000
	6	1.131157000	-2.857241000	-0.049657000
	6	2.336405000	-2.021759000	0.306912000
	6	-3.134187000	0.336305000	-0.426766000
	6	0.732953000	2.997092000	-0.030076000
	6	-2.578427000	1.472059000	0.407600000
	6	-0.675957000	2.917389000	0.506526000
	6	-1.258728000	-2.800684000	0.111414000
	1	-1.367690000	-3.663483000	0.780886000
	1	4.146877000	0.033357000	-0.247125000
	1	3.177137000	0.171670000	1.242095000
	1	-3.337812000	-2.300438000	0.217964000
	1	-2.315929000	-1.451450000	1.406868000
	1	3.335330000	2.344895000	0.121526000
	1	2.660496000	1.671235000	-1.380963000
	1	1.100038000	-3.058136000	-1.130099000
	1	1.193479000	-3.818563000	0.476493000
	1	2.375610000	-1.876347000	1.394552000
	1	3.249786000	-2.542003000	-0.008758000
	1	-4.082934000	-0.010471000	-0.002058000
	1	-3.325588000	0.688713000	-1.443638000
	1	0.722476000	3.208759000	-1.108749000
	1	1.275160000	3.805789000	0.476384000
	1	-3.292198000	2.306792000	0.403136000
	1	-2.421292000	1.164668000	1.452128000
	1	-0.651353000	2.715386000	1.585936000
	1	-1.193882000	3.870343000	0.340413000
	1	-1.308110000	-3.155028000	-0.927385000
	11	0.016802000	-0.003147000	-0.555658000
[Na(15-Crown-5)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -930.5857026)			
[Na(15-Crown-5)]	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -930.7618925)			
[Na(15-Crown-5)] ⁺	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -930.6738326)			
[Na(15-Crown-5)] ⁺ in the geometry of neutral complex	PBE0/aug-cc-pvtz (E _{elec} = -930.5857026)			
[Na(15-Crown-5)]	TPSSh/6-311++G** (0 imaginary Frequencies, E _{elec} = -931.6958752, ZPE correction= 0.305904)			
	8	-2.353278000	0.419167000	0.243746000

	8	-1.048110000	-1.951510000	-0.234045000
	8	-0.312907000	2.116777000	-0.058011000
	8	1.639552000	-1.650385000	0.161132000
	8	2.058676000	1.031433000	-0.340511000
	6	-0.260577000	-3.078167000	0.160921000
	6	-1.622259000	2.682139000	0.002803000
	6	1.135070000	-2.864631000	-0.390205000
	6	-3.066116000	-0.711304000	-0.259123000
	6	-2.391583000	-1.966497000	0.256211000
	6	0.774037000	3.035101000	-0.182106000
	6	2.863836000	-1.198914000	-0.417510000
	6	2.036519000	2.320680000	0.274582000
	6	3.133006000	0.199425000	0.099933000
	6	-2.595497000	1.622457000	-0.483344000
	1	-3.627456000	1.968982000	-0.327135000
	1	-0.684548000	-4.005605000	-0.251420000
	1	-0.233161000	-3.151311000	1.257356000
	1	-1.699726000	3.559839000	-0.652468000
	1	-1.843284000	2.982740000	1.034813000
	1	1.776383000	-3.711940000	-0.108284000
	1	1.103302000	-2.790304000	-1.485849000
	1	-3.043956000	-0.702877000	-1.357203000
	1	-4.112338000	-0.685043000	0.076531000
	1	-2.390937000	-1.985007000	1.355480000
	1	-2.927170000	-2.851852000	-0.117325000
	1	0.617505000	3.915220000	0.456305000
	1	0.854223000	3.358664000	-1.227756000
	1	2.775566000	-1.188936000	-1.512435000
	1	3.690526000	-1.864646000	-0.131562000
	1	2.920785000	2.908628000	-0.015689000
	1	2.028308000	2.203559000	1.368670000
	1	3.177571000	0.193227000	1.198514000
	1	4.092554000	0.564662000	-0.295751000
	1	-2.441579000	1.435661000	-1.555271000
	11	0.005213000	-0.010841000	0.885365000
[Na(15-Crown-5)] ⁺	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -931.6126681, ZPE correction= 0.308277)			
	8	-0.022917000	-2.151794000	0.342407000

	8	2.236777000	-0.759413000	-0.337531000
	8	-2.209180000	-0.742013000	-0.542376000
	8	1.346338000	1.754782000	0.214941000
	8	-1.351944000	1.868073000	-0.170910000
	6	3.156861000	0.226225000	0.157435000
	6	-2.378788000	-1.834132000	0.374973000
	6	2.678566000	1.595152000	-0.288886000
	6	1.148674000	-2.876467000	-0.056422000
	6	2.353227000	-2.033391000	0.314749000
	6	-3.155561000	0.336033000	-0.425707000
	6	0.728640000	3.022776000	-0.040636000
	6	-2.602227000	1.478988000	0.414202000
	6	-0.682470000	2.939777000	0.509986000
	6	-1.265395000	-2.826241000	0.099891000
	1	-1.364928000	-3.693306000	0.764024000
	1	4.165202000	0.037496000	-0.230045000
	1	3.179849000	0.181397000	1.253047000
	1	-3.350174000	-2.315546000	0.211709000
	1	-2.324296000	-1.479777000	1.412086000
	1	3.343580000	2.364170000	0.122624000
	1	2.679613000	1.679126000	-1.384239000
	1	1.117938000	-3.067418000	-1.137505000
	1	1.205490000	-3.837591000	0.469072000
	1	2.383472000	-1.881844000	1.400807000
	1	3.271634000	-2.543327000	-0.000547000
	1	-4.098949000	-0.022123000	-0.000408000
	1	-3.340170000	0.681662000	-1.445015000
	1	0.714036000	3.225395000	-1.119773000
	1	1.277110000	3.827176000	0.464212000
	1	-3.310993000	2.316940000	0.401732000
	1	-2.440002000	1.175045000	1.457754000
	1	-0.654513000	2.732864000	1.587269000
	1	-1.208609000	3.886729000	0.340412000
	1	-1.309562000	-3.166186000	-0.942715000
	11	0.016593000	-0.002754000	-0.548570000
[Na(15-Crown-5)] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -931.6025919)			
[Na(15-Crown-5)]	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -931.7745839)			

[Na(15-Crown-5)] ⁺	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -931.6894124)			
[Na(15-Crown-5)] ⁺ in the geometry of neutral complex	TPSSh/aug-cc-pvtz (E _{elec} = -931.6802419)			
[K(18-Crown-6)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1521.965148, ZPE correction= 0.370941)			
	1	-4.625528000	0.029006000	0.043330000
	8	-2.684395000	0.729415000	-0.079565000
	8	-1.983543000	-1.969569000	0.261574000
	8	-0.713856000	2.702464000	0.261830000
	8	0.710744000	-2.689488000	-0.079975000
	8	1.973975000	1.960074000	-0.080244000
	8	2.697312000	-0.732903000	0.262275000
	6	-2.991272000	2.030431000	0.367596000
	6	-1.595716000	-3.237785000	-0.223830000
	6	0.262211000	3.600336000	-0.223440000
	6	-0.262780000	-3.605820000	0.366571000
	6	1.598275000	3.243051000	0.366476000
	6	-3.249160000	-1.573078000	-0.223429000
	6	-2.006328000	3.001076000	-0.222707000
	6	2.009301000	-3.005376000	0.367925000
	6	3.254260000	1.575459000	0.366649000
	6	2.987112000	-2.027375000	-0.222085000
	6	3.602082000	0.236750000	-0.223006000
	6	-3.607622000	-0.237524000	0.367086000
	1	-2.955369000	2.074376000	1.466292000
	1	-4.004178000	2.315807000	0.044131000
	1	-1.528152000	-3.222157000	-1.321889000
	1	-2.336141000	-4.000197000	0.065028000
	1	0.009442000	4.632498000	0.065970000
	1	0.312151000	3.553055000	-1.321485000
	1	-0.318944000	-3.597173000	1.465263000
	1	-0.003572000	-4.625570000	0.042628000
	1	2.337878000	3.991360000	0.042364000
	1	1.545865000	3.264018000	1.465203000
	1	-4.016600000	-2.308204000	0.065781000
	1	-3.233341000	-1.505820000	-1.321485000
	1	-2.027021000	2.935225000	-1.320739000
	1	-2.296157000	4.023404000	0.066835000

	1	2.287830000	-4.020237000	0.044680000
	1	2.052854000	-2.969720000	1.466664000
	1	3.274747000	1.523128000	1.465374000
	1	4.007794000	2.309667000	0.042419000
	1	4.007143000	-2.324479000	0.068167000
	1	2.921815000	-2.047724000	-1.320201000
	1	4.632399000	-0.023295000	0.066526000
	1	3.555337000	0.286790000	-1.321100000
	1	-3.599257000	-0.293743000	1.465794000
	19	-0.000267000	-0.000043000	-0.582924000
[K(18-Crown-6)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1521.885938, ZPE correction= 0.372499)			
	1	3.268988000	3.283213000	0.013933000
	8	1.394467000	2.414485000	0.164044000
	8	2.788239000	0.000401000	-0.164044000
	8	-1.394467000	2.414485000	-0.164044000
	8	1.393772000	-2.414886000	0.164044000
	8	-2.788239000	0.000401000	0.164044000
	8	-1.393772000	-2.414886000	-0.164044000
	6	0.691231000	3.552555000	-0.295950000
	6	3.422218000	-1.177654000	0.295950000
	6	-2.731743000	2.375628000	0.295424000
	6	2.730987000	-2.374901000	-0.295950000
	6	-3.423225000	1.177945000	-0.295424000
	6	3.423225000	1.177945000	0.295424000
	6	-0.691231000	3.552555000	0.295950000
	6	0.691482000	-3.553573000	-0.295424000
	6	-3.422218000	-1.177654000	-0.295950000
	6	-0.691482000	-3.553573000	0.295424000
	6	-2.730987000	-2.374901000	0.295950000
	6	2.731743000	2.375628000	-0.295424000
	1	0.632505000	3.544657000	-1.393838000
	1	1.208584000	4.471992000	0.012194000
	1	3.386016000	-1.224563000	1.393838000
	1	4.477150000	-1.189332000	-0.012194000
	1	-3.268988000	3.283213000	-0.013933000
	1	-2.755067000	2.322293000	1.393400000
	1	2.753511000	-2.320094000	-1.393838000

	1	3.268567000	-3.282660000	0.012194000
	1	-4.477840000	1.189420000	0.013933000
	1	-3.388698000	1.224812000	-1.393400000
	1	4.477840000	1.189420000	-0.013933000
	1	3.388698000	1.224812000	1.393400000
	1	-0.632505000	3.544657000	1.393838000
	1	-1.208584000	4.471992000	-0.012194000
	1	1.208852000	-4.472633000	0.013933000
	1	0.633631000	-3.547104000	-1.393400000
	1	-3.386016000	-1.224563000	-1.393838000
	1	-4.477150000	-1.189332000	0.012194000
	1	-1.208852000	-4.472633000	-0.013933000
	1	-0.633631000	-3.547104000	1.393400000
	1	-3.268567000	-3.282660000	-0.012194000
	1	-2.753511000	-2.320094000	1.393838000
	1	2.755067000	2.322293000	-1.393400000
	19	0.000000000	0.000000000	0.000000000
[K(18-Crown-6)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -1521.881597)			
[K(18-Crown-6)]	PBE0/def2qzvp//PBE0/6-311++G** (E _{elec} = -1522.132682)			
[K(18-Crown-6)] ⁺	PBE0/def2qzvp //PBE0/6-311++G** (E _{elec} = -1522.053118)			
[K(18-Crown-6)] ⁺ in the geometry of neutral complex	PBE0/def2qzvp (E _{elec} = -1522.049368)			
[K(18-Crown-6)]	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1523.2348871, ZPE correction= 0.366939)			
	1	4.563304000	0.887937000	0.034650000
	8	2.790063000	-0.185572000	-0.097755000
	8	1.559154000	2.327569000	0.240452000
	8	1.236000000	-2.512218000	0.241806000
	8	-1.234687000	2.508411000	-0.095797000
	8	-1.555735000	-2.322907000	-0.100666000
	8	-2.795157000	0.185654000	0.241503000
	6	3.354491000	-1.410617000	0.365069000
	6	0.928005000	3.515886000	-0.239046000
	6	0.455441000	-3.607747000	-0.238837000
	6	-0.454600000	3.610679000	0.362462000
	6	-0.929542000	-3.519103000	0.358196000
	6	2.897074000	2.197539000	-0.242719000

	6	2.582167000	-2.563033000	-0.233210000
	6	-2.582978000	2.563742000	0.365187000
	6	-2.900467000	-2.199949000	0.357721000
	6	-3.353271000	1.411055000	-0.235162000
	6	-3.509824000	-0.953495000	-0.240127000
	6	3.513514000	0.955789000	0.357605000
	1	3.316142000	-1.452081000	1.462569000
	1	4.405289000	-1.483622000	0.046525000
	1	0.865787000	3.494329000	-1.335942000
	1	1.511348000	4.399087000	0.063577000
	1	0.916360000	-4.559669000	0.066613000
	1	0.400634000	-3.579628000	-1.335973000
	1	-0.396715000	3.601005000	1.459841000
	1	-0.917368000	4.556475000	0.042648000
	1	-1.512351000	-4.395091000	0.035762000
	1	-0.874316000	-3.518099000	1.455755000
	1	3.491754000	3.073791000	0.057990000
	1	2.897842000	2.131398000	-1.339617000
	1	2.598125000	-2.504121000	-1.330369000
	1	3.053767000	-3.508597000	0.075698000
	1	-3.050021000	3.507829000	0.046541000
	1	-2.608431000	2.511690000	1.462607000
	1	-2.921020000	-2.148104000	1.455250000
	1	-3.488015000	-3.072781000	0.035367000
	1	-4.408041000	1.487291000	0.070677000
	1	-3.301532000	1.448342000	-1.332171000
	1	-4.566001000	-0.890233000	0.063815000
	1	-3.461252000	-0.993874000	-1.337176000
	1	3.485713000	1.006299000	1.455038000
	19	0.000096000	-0.000608000	-0.486255000
[K(18-Crown-6)] ⁺	TPSSh/6-311++G** (0 imaginary Frequencies, E _{elec} = -1523.1578964, ZPE correction= 0.368619)			
	1	3.280068000	3.299694000	0.006716000
	8	1.399411000	2.423412000	0.162965000
	8	2.798442000	0.000220000	-0.162965000
	8	-1.399411000	2.423412000	-0.162965000
	8	1.399031000	-2.423632000	0.162965000
	8	-2.798442000	0.000220000	0.162965000

	8	-1.399031000	-2.423632000	-0.162965000
	6	0.692204000	3.576275000	-0.302894000
	6	3.443247000	-1.188672000	0.302894000
	6	-2.751487000	2.387960000	0.302704000
	6	2.751043000	-2.387604000	-0.302894000
	6	-3.443778000	1.188878000	-0.302704000
	6	3.443778000	1.188878000	0.302704000
	6	-0.692204000	3.576275000	0.302894000
	6	0.692290000	-3.576838000	-0.302704000
	6	-3.443247000	-1.188672000	-0.302894000
	6	-0.692290000	-3.576838000	0.302704000
	6	-2.751043000	-2.387604000	0.302894000
	6	2.751487000	2.387960000	-0.302704000
	1	0.630144000	3.561308000	-1.399401000
	1	1.217397000	4.490131000	0.006024000
	1	3.399255000	-1.234933000	1.399401000
	1	4.497266000	-1.190769000	-0.006024000
	1	-3.280068000	3.299694000	-0.006716000
	1	-2.769776000	2.327239000	1.399236000
	1	2.769111000	-2.326375000	-1.399401000
	1	3.279869000	-3.299362000	0.006024000
	1	-4.497652000	1.190775000	0.006716000
	1	-3.400336000	1.235076000	-1.399236000
	1	4.497652000	1.190775000	-0.006716000
	1	3.400336000	1.235076000	1.399236000
	1	-0.630144000	3.561308000	1.399401000
	1	-1.217397000	4.490131000	-0.006024000
	1	1.217585000	-4.490469000	0.006716000
	1	0.630561000	-3.562316000	-1.399236000
	1	-3.399255000	-1.234933000	-1.399401000
	1	-4.497266000	-1.190769000	0.006024000
	1	-1.217585000	-4.490469000	-0.006716000
	1	-0.630561000	-3.562316000	1.399236000
	1	-3.279869000	-3.299362000	-0.006024000
	1	-2.769111000	-2.326375000	1.399401000
	1	2.769776000	2.327239000	-1.399236000
	19	0.000000000	0.000000000	0.000000000
[K(18-Crown-6)] ⁺ in the geometry of		TPSSh/6-311++G** (E _{elec} = -1523.155110)		

neutral complex	
[K(18-Crown-6)]	TPSSh/def2qzvp//PBE0/6-311++G** (E _{elec} = -1523.397867)
[K(18-Crown-6)] ⁺	TPSSh/def2qzvp //PBE0/6-311++G** (E _{elec} = -1523.321586)
[K(18-Crown-6)] ⁺ in the geometry of neutral complex	TPSSh/def2qzvp (E _{elec} = -1523.319236)
[Li([2.2.2]crypt)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1274.7293604, ZPE correction= 0.558052)
	3 -0.481643000 0.251561000 0.077968000 8 0.993943000 0.482537000 1.696369000 8 -1.377581000 -0.676848000 1.815672000 8 -1.617053000 1.981575000 -0.405390000 8 0.822710000 1.527308000 -1.070581000 8 1.941765000 -2.026593000 -1.026728000 8 -0.747442000 -1.201872000 -1.428800000 7 -3.214044000 -0.263248000 -0.228286000 7 3.342310000 0.309992000 -0.054006000 6 3.018247000 -2.134431000 -0.123472000 1 3.554855000 -3.085018000 -0.272552000 1 2.643370000 -2.120067000 0.911140000 6 3.954116000 -0.961609000 -0.347689000 1 4.864330000 -1.126465000 0.252173000 1 4.268943000 -0.971346000 -1.396734000 6 2.077431000 1.405234000 1.760002000 1 2.185501000 1.787518000 2.781999000 1 1.827024000 2.255873000 1.121472000 6 3.384627000 0.778640000 1.305665000 1 4.186951000 1.523551000 1.475242000 1 3.610051000 -0.071949000 1.957408000 6 1.940108000 1.181996000 -1.883383000 1 1.959769000 1.825445000 -2.773945000 1 1.784573000 0.146833000 -2.194936000 6 3.248692000 1.284013000 -1.111373000 1 4.078337000 1.173711000 -1.828000000 1 3.350335000 2.292884000 -0.690725000 6 0.850385000 -2.839244000 -0.692236000 1 0.552208000 -2.668969000 0.353607000 1 1.099220000 -3.908302000 -0.791529000 6 -0.300495000 -2.536828000 -1.610476000

	1	0.010502000	-2.674483000	-2.654908000
	1	-1.110915000	-3.249507000	-1.397203000
	6	0.534214000	0.073544000	2.974982000
	1	0.036662000	0.913765000	3.478529000
	1	1.368748000	-0.262978000	3.607062000
	6	-0.426605000	-1.066678000	2.788301000
	1	0.098849000	-1.976716000	2.463887000
	1	-0.918960000	-1.283050000	3.747133000
	6	0.395455000	2.866757000	-1.207076000
	1	0.056946000	3.041637000	-2.238141000
	1	1.204986000	3.578455000	-0.985743000
	6	-0.746901000	3.083154000	-0.242577000
	1	-0.395393000	3.140345000	0.797408000
	1	-1.254829000	4.027624000	-0.480258000
	6	-2.460234000	-1.585079000	1.697628000
	1	-2.774297000	-1.926716000	2.693261000
	1	-2.144645000	-2.471270000	1.126838000
	6	-3.609753000	-0.862582000	1.030227000
	1	-4.461384000	-1.556571000	0.925192000
	1	-3.935191000	-0.064773000	1.704438000
	6	-1.914128000	-0.904342000	-2.190949000
	1	-1.919210000	-1.496699000	-3.114731000
	1	-1.843194000	0.152023000	-2.465188000
	6	-3.172298000	-1.149736000	-1.374157000
	1	-4.058619000	-1.044642000	-2.022815000
	1	-3.174749000	-2.186668000	-1.021533000
	6	-2.918019000	2.140799000	0.136604000
	1	-3.317695000	3.129799000	-0.126154000
	1	-2.884650000	2.066216000	1.232401000
	6	-3.774197000	1.051846000	-0.477958000
	1	-4.808711000	1.145745000	-0.110081000
	1	-3.807244000	1.221284000	-1.558589000
[Li([2.2.2]crypt)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1274.6557926, ZPE correction= 0.559303)			
	3	-0.424223000	0.265554000	0.021181000
	8	0.972307000	0.515933000	1.705591000
	8	-1.379227000	-0.674803000	1.871321000
	8	-1.582324000	1.998341000	-0.389099000

	8	0.866714000	1.537804000	-1.083778000
	8	1.869872000	-1.979990000	-1.025660000
	8	-0.814739000	-1.203135000	-1.432825000
	7	-3.227486000	-0.228853000	-0.179848000
	7	3.328004000	0.275934000	-0.022698000
	6	2.944355000	-2.159356000	-0.131602000
	1	3.451607000	-3.117882000	-0.321045000
	1	2.570197000	-2.175547000	0.904330000
	6	3.915561000	-1.008690000	-0.318188000
	1	4.808262000	-1.203742000	0.296650000
	1	4.252380000	-1.014269000	-1.359895000
	6	2.084454000	1.405967000	1.774925000
	1	2.186646000	1.797519000	2.794598000
	1	1.858562000	2.248896000	1.118802000
	6	3.379612000	0.741951000	1.336667000
	1	4.201071000	1.462534000	1.514060000
	1	3.577675000	-0.115006000	1.989218000
	6	2.000412000	1.193771000	-1.883543000
	1	2.049406000	1.857822000	-2.756026000
	1	1.838565000	0.169927000	-2.226378000
	6	3.288518000	1.260844000	-1.076192000
	1	4.134365000	1.137652000	-1.770028000
	1	3.401500000	2.263987000	-0.645623000
	6	0.808751000	-2.869349000	-0.821108000
	1	0.472883000	-2.834383000	0.227572000
	1	1.106028000	-3.907745000	-1.036755000
	6	-0.324063000	-2.501252000	-1.738991000
	1	0.022871000	-2.521406000	-2.780147000
	1	-1.122764000	-3.248187000	-1.628582000
	6	0.597834000	-0.011884000	2.963998000
	1	0.122175000	0.771839000	3.569538000
	1	1.471075000	-0.389114000	3.512619000
	6	-0.363362000	-1.146152000	2.730829000
	1	0.152565000	-2.004410000	2.276280000
	1	-0.783132000	-1.472225000	3.692154000
	6	0.413586000	2.864668000	-1.259526000
	1	0.044667000	2.997184000	-2.285675000
	1	1.218221000	3.593364000	-1.087037000

	6	-0.704790000	3.100717000	-0.272194000
	1	-0.323950000	3.173376000	0.756180000
	1	-1.217603000	4.039914000	-0.515570000
	6	-2.451898000	-1.586991000	1.708370000
	1	-2.759829000	-1.985057000	2.684588000
	1	-2.129056000	-2.434773000	1.086371000
	6	-3.607719000	-0.842135000	1.075446000
	1	-4.466512000	-1.526748000	0.974609000
	1	-3.914505000	-0.052797000	1.767936000
	6	-1.985539000	-0.869471000	-2.178504000
	1	-2.018850000	-1.451657000	-3.106702000
	1	-1.899466000	0.187393000	-2.446850000
	6	-3.230578000	-1.099776000	-1.340422000
	1	-4.128378000	-0.965354000	-1.965881000
	1	-3.244716000	-2.141702000	-1.003580000
	6	-2.863851000	2.166510000	0.196279000
	1	-3.257203000	3.164027000	-0.038622000
	1	-2.793929000	2.072012000	1.288723000
	6	-3.762299000	1.101515000	-0.401002000
	1	-4.782818000	1.217856000	-0.003059000
	1	-3.823702000	1.281955000	-1.478347000
[Li([2.2.2]crypt)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -1274.6551520)			
[Li([2.2.2]crypt)]	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1274.8359424)			
[Li([2.2.2]crypt)] ⁺	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1274.7624020)			
[Li([2.2.2]crypt)] ⁺ in the geometry of neutral complex	PBE0/aug-cc-pvtz (E _{elec} = -1274.7617535)			
[Li([2.2.2]crypt)]	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1276.2649475, ZPE correction= 0.552380)			
	3	-0.538064000	0.256718000	0.077542000
	8	0.975296000	0.524205000	1.722104000
	8	-1.401027000	-0.635990000	1.866251000
	8	-1.650285000	1.975732000	-0.437854000
	8	0.797964000	1.552072000	-1.084648000
	8	2.020352000	-2.064343000	-1.023129000
	8	-0.711540000	-1.271699000	-1.415341000
	7	-3.177970000	-0.302066000	-0.238747000
	7	3.314213000	0.333895000	-0.049821000

	6	3.106112000	-2.131007000	-0.103435000
	1	3.675117000	-3.062111000	-0.249869000
	1	2.721713000	-2.122353000	0.926543000
	6	3.997642000	-0.916911000	-0.339867000
	1	4.914226000	-1.032742000	0.261712000
	1	4.304951000	-0.916054000	-1.390399000
	6	2.067402000	1.462958000	1.765253000
	1	2.174219000	1.859744000	2.781319000
	1	1.806391000	2.293279000	1.105906000
	6	3.377646000	0.821407000	1.314837000
	1	4.185211000	1.564883000	1.466053000
	1	3.599943000	-0.026092000	1.970686000
	6	1.929666000	1.196445000	-1.902979000
	1	1.943210000	1.832938000	-2.797778000
	1	1.776071000	0.156815000	-2.196145000
	6	3.235725000	1.319274000	-1.116118000
	1	4.077291000	1.211023000	-1.818502000
	1	3.316762000	2.327640000	-0.691150000
	6	0.927208000	-2.885532000	-0.654482000
	1	0.637777000	-2.686121000	0.387416000
	1	1.188264000	-3.952980000	-0.731608000
	6	-0.234214000	-2.616029000	-1.581418000
	1	0.076812000	-2.756033000	-2.624393000
	1	-1.035668000	-3.334235000	-1.355415000
	6	0.510003000	0.150566000	3.024783000
	1	0.001810000	1.002490000	3.494868000
	1	1.347662000	-0.158485000	3.665301000
	6	-0.442101000	-1.009848000	2.859311000
	1	0.090111000	-1.918054000	2.545400000
	1	-0.942979000	-1.212428000	3.815726000
	6	0.344406000	2.891658000	-1.280217000
	1	0.002942000	3.013209000	-2.316987000
	1	1.145214000	3.620130000	-1.086176000
	6	-0.805872000	3.122179000	-0.317275000
	1	-0.457452000	3.225956000	0.718570000
	1	-1.346816000	4.035552000	-0.596204000
	6	-2.487620000	-1.565378000	1.759831000
	1	-2.815292000	-1.868625000	2.762707000

	1	-2.154676000	-2.464669000	1.223029000
	6	-3.623389000	-0.856948000	1.040647000
	1	-4.475764000	-1.548028000	0.930398000
	1	-3.956944000	-0.029712000	1.673089000
	6	-1.895617000	-1.017252000	-2.196199000
	1	-1.891418000	-1.649656000	-3.092068000
	1	-1.835660000	0.028280000	-2.508869000
	6	-3.146874000	-1.251679000	-1.353623000
	1	-4.045661000	-1.183617000	-1.989011000
	1	-3.123523000	-2.268891000	-0.949846000
	6	-2.988321000	2.131329000	0.052371000
	1	-3.392481000	3.099862000	-0.269426000
	1	-2.993647000	2.096382000	1.149416000
	6	-3.787127000	0.991139000	-0.563898000
	1	-4.838635000	1.052914000	-0.241161000
	1	-3.772731000	1.118787000	-1.649981000
[Li([2.2.2]crypt)] ⁺	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1276.1928895, ZPE correction= 0.553569)			
	3	-0.483228000	0.271589000	0.041164000
	8	0.953083000	0.558776000	1.727424000
	8	-1.395008000	-0.641421000	1.909526000
	8	-1.626370000	1.991408000	-0.426220000
	8	0.834195000	1.564408000	-1.092937000
	8	1.962625000	-2.022367000	-1.029882000
	8	-0.770672000	-1.273805000	-1.416762000
	7	-3.193888000	-0.274289000	-0.194194000
	7	3.303404000	0.308391000	-0.020301000
	6	3.043998000	-2.151899000	-0.111288000
	1	3.588486000	-3.091106000	-0.289166000
	1	2.654776000	-2.168767000	0.917748000
	6	3.968019000	-0.955248000	-0.308773000
	1	4.866050000	-1.098072000	0.312189000
	1	4.301345000	-0.948944000	-1.350855000
	6	2.071053000	1.469114000	1.776267000
	1	2.169985000	1.876080000	2.789494000
	1	1.831024000	2.290886000	1.099993000
	6	3.372215000	0.795774000	1.343618000
	1	4.194762000	1.519706000	1.501872000

	1	3.570826000	-0.055503000	2.002323000
	6	1.979961000	1.207513000	-1.900508000
	1	2.017995000	1.860619000	-2.781021000
	1	1.819563000	0.176468000	-2.218047000
	6	3.269486000	1.300986000	-1.084693000
	1	4.122981000	1.179559000	-1.768731000
	1	3.361538000	2.305530000	-0.653659000
	6	0.895426000	-2.914165000	-0.774883000
	1	0.573641000	-2.834004000	0.274592000
	1	1.196668000	-3.957515000	-0.955997000
	6	-0.250616000	-2.583332000	-1.702428000
	1	0.092271000	-2.611717000	-2.743585000
	1	-1.039699000	-3.336437000	-1.572078000
	6	0.570343000	0.073069000	3.016495000
	1	0.079872000	0.875504000	3.582813000
	1	1.445510000	-0.272537000	3.581348000
	6	-0.378890000	-1.085569000	2.809005000
	1	0.146841000	-1.951602000	2.384611000
	1	-0.818316000	-1.380786000	3.770651000
	6	0.352744000	2.887478000	-1.330548000
	1	-0.017153000	2.963791000	-2.361068000
	1	1.146201000	3.633248000	-1.185869000
	6	-0.775671000	3.137638000	-0.347441000
	1	-0.400938000	3.256183000	0.677439000
	1	-1.321616000	4.045689000	-0.630117000
	6	-2.473341000	-1.574521000	1.766793000
	1	-2.791203000	-1.928968000	2.755613000
	1	-2.136376000	-2.441275000	1.181701000
	6	-3.618735000	-0.843857000	1.084198000
	1	-4.478453000	-1.525992000	0.981318000
	1	-3.932178000	-0.024713000	1.736952000
	6	-1.958815000	-0.984361000	-2.183417000
	1	-1.979004000	-1.605333000	-3.085674000
	1	-1.886215000	0.063282000	-2.486499000
	6	-3.199264000	-1.208197000	-1.324072000
	1	-4.107495000	-1.114093000	-1.940915000
	1	-3.184514000	-2.231288000	-0.935669000
	6	-2.945979000	2.153512000	0.111416000

	1	-3.349255000	3.130788000	-0.180552000
	1	-2.911847000	2.099151000	1.207150000
	6	-3.785265000	1.033801000	-0.489692000
	1	-4.824696000	1.115224000	-0.135524000
	1	-3.801138000	1.171038000	-1.574281000
[Li([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -1276.19246232)			
[Li([2.2.2]crypt)]	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1276.37091672)			
[Li([2.2.2]crypt)] ⁺	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1276.29884874)			
[Li([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/aug-cc-pvtz (E _{elec} = -1276.29844411)			
[Na([2.2.2]crypt)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1429.4193538, ZPE correction= 0.557567)			
	11	-0.154674000	-0.002350000	0.002137000
	8	-1.394919000	0.435831000	2.286895000
	8	1.420547000	0.365164000	2.313529000
	8	1.414132000	-2.188323000	-0.838692000
	8	-1.400405000	-2.200892000	-0.764891000
	8	-1.395992000	1.765116000	-1.520692000
	8	1.419886000	1.822904000	-1.473251000
	7	3.153617000	-0.002009000	-0.001698000
	7	-3.115792000	0.001555000	0.000352000
	6	-2.731367000	2.121866000	-1.220683000
	1	-3.148254000	2.723988000	-2.041529000
	1	-2.759006000	2.744130000	-0.314309000
	6	-3.559924000	0.869205000	-1.082132000
	1	-4.621700000	1.154367000	-0.965410000
	1	-3.484637000	0.321814000	-2.025012000
	6	-2.730767000	-0.001034000	2.446783000
	1	-3.146632000	0.409485000	3.378762000
	1	-2.759450000	-1.097056000	2.532719000
	6	-3.559256000	0.506036000	1.292877000
	1	-4.621236000	0.263565000	1.481787000
	1	-3.482769000	1.596218000	1.290210000
	6	-2.735303000	-2.116791000	-1.224756000
	1	-3.154120000	-3.127852000	-1.336379000
	1	-2.761124000	-1.642411000	-2.216631000
	6	-3.562605000	-1.368942000	-0.209257000

	1	-4.624495000	-1.408515000	-0.514381000
	1	-3.488186000	-1.911884000	0.736284000
	6	-0.650533000	2.881365000	-1.961137000
	1	-0.495323000	3.589582000	-1.134037000
	1	-1.193533000	3.405339000	-2.762488000
	6	0.667313000	2.419816000	-2.505988000
	1	0.508579000	1.707061000	-3.328986000
	1	1.201350000	3.293711000	-2.910825000
	6	-0.649666000	0.262714000	3.474561000
	1	-0.494576000	-0.807065000	3.677650000
	1	-1.192707000	0.697546000	4.327527000
	6	0.668295000	0.964703000	3.344998000
	1	0.509803000	2.033166000	3.135637000
	1	1.202350000	0.881299000	4.304460000
	6	-0.655886000	-3.141461000	-1.510945000
	1	-0.501294000	-2.780490000	-2.538351000
	1	-1.199111000	-4.097399000	-1.562662000
	6	0.662355000	-3.381837000	-0.839367000
	1	0.504452000	-3.738720000	0.189341000
	1	1.196762000	-4.168687000	-1.394336000
	6	2.739142000	0.870455000	2.277631000
	1	3.170339000	0.855000000	3.290031000
	1	2.730803000	1.918453000	1.943497000
	6	3.586326000	-0.003705000	1.385851000
	1	4.643806000	0.306285000	1.485095000
	1	3.522421000	-1.023423000	1.774084000
	6	2.737021000	1.536733000	-1.895878000
	1	3.168842000	2.420404000	-2.389631000
	1	2.725521000	0.723412000	-2.636437000
	6	3.586428000	1.199894000	-0.694926000
	1	4.643083000	1.129263000	-1.015420000
	1	3.525377000	2.045989000	-0.005638000
	6	2.733007000	-2.411642000	-0.384462000
	1	3.162224000	-3.281538000	-0.904212000
	1	2.725439000	-2.646023000	0.690252000
	6	3.582278000	-1.204104000	-0.697120000
	1	4.639575000	-1.447432000	-0.479943000
	1	3.516935000	-1.030579000	-1.774289000

[Na([2.2.2]crypt)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1429.3487342, ZPE correction= 0.558896)			
	11	0.000000000	0.000000000	0.003447000
	8	0.661045000	2.249779000	1.405764000
	8	0.712145000	2.235031000	-1.406552000
	8	1.579521000	-1.734252000	-1.406552000
	8	1.617843000	-1.697371000	1.405764000
	8	-2.278888000	-0.552408000	1.405764000
	8	-2.291667000	-0.500780000	-1.406552000
	7	0.000000000	0.000000000	-3.129514000
	7	0.000000000	0.000000000	3.128533000
	6	-2.442402000	-0.074959000	2.727570000
	1	-3.368204000	-0.482262000	3.158135000
	1	-2.539951000	1.020240000	2.720857000
	6	-1.279489000	-0.536774000	3.570894000
	1	-1.483596000	-0.286353000	4.627531000
	1	-1.244283000	-1.627420000	3.509058000
	6	1.156285000	2.152662000	2.727570000
	1	1.266451000	3.158082000	3.158135000
	1	2.153529000	1.689542000	2.720857000
	6	0.174885000	1.376457000	3.570894000
	1	0.493809000	1.428009000	4.627531000
	1	-0.787245000	1.891291000	3.509058000
	6	1.286118000	-2.077703000	2.727570000
	1	2.101754000	-2.675819000	3.158135000
	1	0.386422000	-2.709782000	2.720857000
	6	1.104604000	-0.839683000	3.570894000
	1	0.989787000	-1.141655000	4.627531000
	1	2.031528000	-0.263871000	3.509058000
	6	-3.467462000	-0.424981000	0.654577000
	1	-3.701896000	0.635681000	0.482138000
	1	-4.310553000	-0.876600000	1.196960000
	6	-3.302940000	-1.137244000	-0.654839000
	1	-3.047542000	-2.193048000	-0.482212000
	1	-4.258995000	-1.102105000	-1.196806000
	6	1.365686000	3.215401000	0.654577000
	1	2.401464000	2.888095000	0.482138000
	1	1.396119000	4.171348000	1.196960000

	6	0.666588000	3.429051000	-0.654839000
	1	-0.375464000	3.735772000	-0.482212000
	1	1.175047000	4.239450000	-1.196806000
	6	2.101776000	-2.790420000	0.654577000
	1	1.300432000	-3.523777000	0.482138000
	1	2.914434000	-3.294748000	1.196960000
	6	2.636352000	-2.291808000	-0.654839000
	1	3.423006000	-1.542725000	-0.482212000
	1	3.083948000	-3.137345000	-1.196806000
	6	0.243980000	2.430968000	-2.727212000
	1	0.712266000	3.327095000	-3.158603000
	1	-0.842067000	2.602599000	-2.717927000
	6	0.623569000	1.239505000	-3.571692000
	1	0.386808000	1.461147000	-4.627942000
	1	1.709249000	1.129003000	-3.511031000
	6	-2.227270000	-1.004191000	-2.727212000
	1	-3.237482000	-1.046707000	-3.158603000
	1	-1.832883000	-2.030550000	-2.717927000
	6	-1.385228000	-0.079726000	-3.571692000
	1	-1.458794000	-0.395588000	-4.627942000
	1	-1.832370000	0.915751000	-3.511031000
	6	1.983290000	-1.426777000	-2.727212000
	1	2.525215000	-2.280388000	-3.158603000
	1	2.674950000	-0.572048000	-2.717927000
	6	0.761658000	-1.159780000	-3.571692000
	1	1.071986000	-1.065559000	-4.627942000
	1	0.123121000	-2.044754000	-3.511031000
[Na([2.2.2]crypt)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -1429.34857017)			
[Na([2.2.2]crypt)]	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1429.53818274)			
[Na([2.2.2]crypt)] ⁺	PBE0/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1429.46741328)			
[Na([2.2.2]crypt)] ⁺ in the geometry of neutral complex	PBE0/aug-cc-pvtz (E _{elec} = -1429.46726784)			
[Na([2.2.2]crypt)]	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1431.0416062, ZPE correction= 0.551781)			
	11	0.152610000	0.001703000	0.002724000
	8	1.400825000	0.706909000	2.232484000
	8	-1.419180000	0.772849000	2.226848000

	8	-1.420941000	1.544806000	-1.779982000
	8	1.399457000	1.582129000	-1.727847000
	8	1.398885000	-2.288581000	-0.504504000
	8	-1.421780000	-2.315361000	-0.445108000
	7	-3.153992000	-0.000545000	-0.000169000
	7	3.115488000	-0.001207000	-0.001591000
	6	2.748553000	-2.463033000	-0.066131000
	1	3.159719000	-3.383430000	-0.504940000
	1	2.773236000	-2.573889000	1.026907000
	6	3.573651000	-1.286292000	-0.548583000
	1	4.636471000	-1.472281000	-0.309478000
	1	3.491477000	-1.248411000	-1.637285000
	6	2.750333000	1.174139000	2.162454000
	1	3.162632000	1.255546000	3.178362000
	1	2.773902000	2.175575000	1.710672000
	6	3.574780000	0.167556000	1.384477000
	1	4.637728000	0.467184000	1.425229000
	1	3.492440000	-0.794057000	1.896307000
	6	2.747819000	1.286473000	-2.100310000
	1	3.159968000	2.125503000	-2.679000000
	1	2.769124000	0.394915000	-2.742439000
	6	3.574553000	1.114453000	-0.841389000
	1	4.636737000	0.998487000	-1.123573000
	1	3.494796000	2.038469000	-0.264115000
	6	0.650311000	-3.497298000	-0.365694000
	1	0.488155000	-3.723263000	0.697258000
	1	1.204447000	-4.331508000	-0.820873000
	6	-0.666368000	-3.343884000	-1.080995000
	1	-0.501150000	-3.097465000	-2.139363000
	1	-1.211070000	-4.298760000	-1.026014000
	6	0.653358000	1.431573000	3.210787000
	1	0.492218000	2.465582000	2.875887000
	1	1.207963000	1.453098000	4.160567000
	6	-0.663883000	0.736523000	3.435727000
	1	-0.499528000	-0.303184000	3.752158000
	1	-1.208432000	1.262354000	4.234769000
	6	0.650694000	2.068337000	-2.843062000
	1	0.488025000	1.261937000	-3.571444000

	1	1.204988000	2.880183000	-3.336879000
	6	-0.665736000	2.610651000	-2.351472000
	1	-0.500358000	3.403200000	-1.608023000
	1	-1.210537000	3.041498000	-3.205331000
	6	-2.749685000	0.297593000	2.436621000
	1	-3.175933000	0.784474000	3.325967000
	1	-2.732113000	-0.785257000	2.623980000
	6	-3.598119000	0.658348000	1.232365000
	1	-4.655585000	0.427521000	1.459940000
	1	-3.530130000	1.739849000	1.092610000
	6	-2.752851000	-2.260722000	-0.960008000
	1	-3.179081000	-3.274444000	-0.980576000
	1	-2.737311000	-1.883566000	-1.992296000
	6	-3.599871000	-1.396866000	-0.045411000
	1	-4.657581000	-1.477156000	-0.358546000
	1	-3.531880000	-1.816515000	0.961150000
	6	-2.752711000	1.962037000	-1.476402000
	1	-3.178486000	2.486425000	-2.344432000
	1	-2.738600000	2.667485000	-0.633645000
	6	-3.599187000	0.737324000	-1.186701000
	1	-4.657108000	1.048223000	-1.100389000
	1	-3.530286000	0.075718000	-2.053537000
[Na([2.2.2]crypt)] ⁺	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1430.9720732, ZPE correction= 0.553143)			
	11	0.003113000	0.002400000	0.000867000
	8	1.408715000	1.401408000	1.895641000
	8	-1.409776000	1.438959000	1.868445000
	8	-1.410331000	0.899874000	-2.178856000
	8	1.407910000	0.943487000	-2.160954000
	8	1.410024000	-2.343382000	0.264515000
	8	-1.408276000	-2.339177000	0.311711000
	7	-3.130287000	-0.001366000	0.000616000
	7	3.129509000	0.000069000	-0.000290000
	6	2.745615000	-2.333093000	0.776233000
	1	3.170956000	-3.343863000	0.710621000
	1	2.734538000	-2.042314000	1.835671000
	6	3.586064000	-1.395017000	-0.068493000
	1	4.643680000	-1.491582000	0.234519000

	1	3.517264000	-1.732379000	-1.105367000
	6	2.744393000	1.839630000	1.631183000
	1	3.169038000	2.288628000	2.539427000
	1	2.733432000	2.611490000	0.849434000
	6	3.585442000	0.639223000	1.241898000
	1	4.642907000	0.950551000	1.174316000
	1	3.516798000	-0.089739000	2.052725000
	6	2.743216000	0.494345000	-2.408730000
	1	3.167976000	1.055976000	-3.251927000
	1	2.731388000	-0.568662000	-2.686128000
	6	3.585000000	0.756739000	-1.174772000
	1	4.642322000	0.542430000	-1.411070000
	1	3.516724000	1.823393000	-0.948403000
	6	0.655818000	-3.431821000	0.797551000
	1	0.477984000	-3.282373000	1.871492000
	1	1.208365000	-4.372035000	0.662707000
	6	-0.653105000	-3.523203000	0.056348000
	1	-0.475246000	-3.636538000	-1.022012000
	1	-1.204734000	-4.403819000	0.413712000
	6	0.653981000	2.407627000	2.570675000
	1	0.475485000	3.261947000	1.903143000
	1	1.206530000	2.762371000	3.451753000
	6	-0.654527000	1.811008000	3.021057000
	1	-0.475925000	0.934096000	3.658575000
	1	-1.206460000	2.560720000	3.604854000
	6	0.652764000	1.025418000	-3.369515000
	1	0.474433000	0.020246000	-3.775852000
	1	1.204802000	1.611624000	-4.117241000
	6	-0.655952000	1.712996000	-3.077192000
	1	-0.477811000	2.703536000	-2.636234000
	1	-1.208289000	1.843738000	-4.018120000
	6	-2.744284000	1.060731000	2.218023000
	1	-3.169912000	1.808641000	2.900908000
	1	-2.730629000	0.096174000	2.743889000
	6	-3.586673000	1.016030000	0.957673000
	1	-4.643655000	0.863818000	1.239309000
	1	-3.519933000	1.996505000	0.480283000
	6	-2.742747000	-2.451897000	-0.190640000

	1	-3.168372000	-3.417911000	0.113558000
	1	-2.729004000	-2.422326000	-1.288810000
	6	-3.584899000	-1.339362000	0.403307000
	1	-4.642186000	-1.507792000	0.132153000
	1	-3.516369000	-1.416881000	1.490955000
	6	-2.745792000	1.389237000	-2.027052000
	1	-3.171038000	1.606066000	-3.016496000
	1	-2.734384000	2.326772000	-1.454421000
	6	-3.586577000	0.318298000	-1.359126000
	1	-4.644092000	0.636556000	-1.368562000
	1	-3.517925000	-0.585067000	-1.969765000
[Na([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -1430.97189433)			
[Na([2.2.2]crypt)]	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1431.16030968)			
[Na([2.2.2]crypt)] ⁺	TPSSh/aug-cc-pvtz//PBE0/6-311++G** (E _{elec} = -1431.09068131)			
[Na([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/aug-cc-pvtz (E _{elec} = -1431.09053887)			
[K([2.2.2]crypt)]	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1866.9989039, ZPE correction= 0.557304)			
	19	-0.000047000	0.000252000	-0.000039000
	8	-1.410340000	-2.424157000	0.413981000
	8	1.410114000	-2.456370000	0.108411000
	8	1.410559000	1.135038000	-2.181239000
	8	-1.410240000	0.853515000	-2.305902000
	8	-1.410300000	1.570726000	1.891890000
	8	1.410228000	1.322072000	2.073270000
	7	3.062247000	-0.000230000	0.000012000
	7	-3.062052000	-0.000199000	0.000010000
	6	-2.745932000	1.205135000	2.169053000
	1	-3.227293000	1.984379000	2.779768000
	1	-2.765393000	0.276214000	2.758333000
	6	-3.518164000	1.075811000	0.875846000
	1	-4.590879000	0.963275000	1.121144000
	1	-3.419420000	2.025465000	0.344182000
	6	-2.746066000	-2.481320000	-0.040924000
	1	-3.227372000	-3.399847000	0.328618000
	1	-2.765864000	-2.527062000	-1.140016000
	6	-3.518163000	-1.296737000	0.493923000

	1	-4.590924000	-1.452816000	0.273985000
	1	-3.419179000	-1.311147000	1.582159000
	6	-2.746080000	1.275787000	-2.128325000
	1	-3.227285000	1.414660000	-3.108672000
	1	-2.765991000	2.250654000	-1.618680000
	6	-3.518183000	0.220382000	-1.369767000
	1	-4.590915000	0.489033000	-1.394873000
	1	-3.419464000	-0.714815000	-1.926446000
	6	-0.687247000	1.863341000	3.068768000
	1	-0.615184000	0.969251000	3.705972000
	1	-1.199802000	2.650208000	3.644039000
	6	0.687194000	2.353598000	2.710983000
	1	0.615094000	3.233175000	2.053898000
	1	1.199754000	2.661379000	3.635840000
	6	-0.687195000	-3.589474000	0.078443000
	1	-0.615007000	-3.693820000	-1.014504000
	1	-1.199701000	-4.481317000	0.471848000
	6	0.687142000	-3.524886000	0.682081000
	1	0.615003000	-3.396318000	1.772437000
	1	1.199850000	-4.479531000	0.485599000
	6	-0.687129000	1.726903000	-3.147241000
	1	-0.615149000	2.725567000	-2.691046000
	1	-1.199611000	1.832135000	-4.116315000
	6	0.687290000	1.172092000	-3.393295000
	1	0.615210000	0.163446000	-3.826950000
	1	1.199694000	1.819549000	-4.122034000
	6	2.745801000	-2.416355000	0.565188000
	1	3.226900000	-3.392377000	0.398347000
	1	2.765398000	-2.228580000	1.649105000
	6	3.518247000	-1.371994000	-0.208147000
	1	4.590930000	-1.478110000	0.040138000
	1	3.419563000	-1.616593000	-1.268671000
	6	2.745915000	1.697407000	1.809718000
	1	3.227209000	2.041284000	2.738159000
	1	2.765593000	2.541891000	1.104768000
	6	3.518078000	0.505194000	1.292188000
	1	4.590858000	0.772908000	1.260313000
	1	3.418865000	-0.290997000	2.034162000

	6	2.745951000	0.718388000	-2.374871000
	1	3.227420000	1.350133000	-3.137100000
	1	2.764817000	-0.314428000	-2.753560000
	6	3.518575000	0.865843000	-1.083851000
	1	4.591181000	0.703475000	-1.299916000
	1	3.420266000	1.906595000	-0.765355000
[K([2.2.2]crypt)] ⁺	PBE0/6-311++G** (0 imaginary Frequencies, E _{elec} = -1866.9287672, ZPE correction= 0.558785)			
	19	0.000000000	0.000000000	0.000286000
	8	2.412292000	0.519835000	-1.412945000
	8	2.330316000	0.811927000	1.412718000
	8	-1.868307000	1.612150000	1.412718000
	8	-1.656337000	1.829189000	-1.412945000
	8	-0.755956000	-2.349024000	-1.412945000
	8	-0.462009000	-2.424076000	1.412718000
	7	0.000000000	0.000000000	3.059779000
	7	0.000000000	0.000000000	-3.060251000
	6	-0.296684000	-2.464157000	-2.744719000
	1	-0.775867000	-3.325684000	-3.232353000
	1	0.787323000	-2.650452000	-2.751463000
	6	-0.663178000	-1.218569000	-3.519944000
	1	-0.460718000	-1.403823000	-4.590434000
	1	-1.743851000	-1.085546000	-3.426283000
	6	2.282364000	0.975142000	-2.744719000
	1	3.268060000	0.990922000	-3.232353000
	1	1.901697000	2.007068000	-2.751463000
	6	1.386901000	0.034955000	-3.519944000
	1	1.446105000	0.302918000	-4.590434000
	1	1.812037000	-0.967446000	-3.426283000
	6	-1.985680000	1.489014000	-2.744719000
	1	-2.492193000	2.334762000	-3.232353000
	1	-2.689021000	0.643384000	-2.751463000
	6	-0.723723000	1.183614000	-3.519944000
	1	-0.985387000	1.100904000	-4.590434000
	1	-0.068185000	2.052993000	-3.426283000
	6	-0.586595000	-3.547516000	-0.684896000
	1	0.481468000	-3.797188000	-0.601469000
	1	-1.090884000	-4.379374000	-1.198013000

	6	-1.186438000	-3.393876000	0.684852000
	1	-2.243090000	-3.099585000	0.601537000
	1	-1.143834000	-4.365666000	1.198061000
	6	3.365536000	1.265752000	-0.684896000
	1	3.047727000	2.315557000	-0.601469000
	1	4.338091000	1.244954000	-1.198013000
	6	3.532402000	0.669452000	0.684852000
	1	3.805864000	-0.392780000	0.601537000
	1	4.352695000	1.192243000	1.198061000
	6	-2.778941000	2.281764000	-0.684896000
	1	-3.529195000	1.481631000	-0.601469000
	1	-3.247207000	3.134420000	-1.198013000
	6	-2.345964000	2.724424000	0.684852000
	1	-1.562775000	3.492365000	0.601537000
	1	-3.208861000	3.173423000	1.198061000
	6	2.456371000	0.357812000	2.745284000
	1	3.305147000	0.859558000	3.232595000
	1	2.670385000	-0.721037000	2.754023000
	6	1.201486000	0.693678000	3.519434000
	1	1.391137000	0.496855000	4.590215000
	1	1.041577000	1.770590000	3.424623000
	6	-0.918311000	-2.306186000	2.745284000
	1	-0.908175000	-3.292120000	3.232595000
	1	-1.959629000	-1.952102000	2.754023000
	6	0.000000000	-1.387357000	3.519434000
	1	-0.265279000	-1.453187000	4.590215000
	1	1.012588000	-1.787327000	3.424623000
	6	-1.538060000	1.948374000	2.745284000
	1	-2.396972000	2.432562000	3.232595000
	1	-0.710756000	2.673140000	2.754023000
	6	-1.201486000	0.693678000	3.519434000
	1	-1.125858000	0.956332000	4.590215000
	1	-2.054164000	0.016737000	3.424623000
[K([2.2.2]crypt)] ⁺ in the geometry of neutral complex	PBE0/6-311++G** (E _{elec} = -1866.92868687)			
[K([2.2.2]crypt)]	PBE0/def2qzvp//PBE0/6-311++G** (E _{elec} = -1867.21499204)			
[K([2.2.2]crypt)] ⁺	PBE0/def2qzvp//PBE0/6-311++G** (E _{elec} = -1867.14936356)			
[K([2.2.2]crypt)] ⁺ in the geometry of	PBE0/def2qzvp (E _{elec} = -1867.14926753)			

neutral complex				
[K([2.2.2]crypt)]	TPSSH/6-311++G** (0 imaginary Frequencies, E _{elec} = -1868.6968259, ZPE correction= 0.551410)			
	19	0.000015000	0.000349000	-0.000056000
	8	1.415004000	-1.603809000	-1.881997000
	8	-1.415170000	-1.827825000	-1.664663000
	8	-1.415314000	-0.527243000	2.415409000
	8	1.415079000	-0.827855000	2.329427000
	8	1.415231000	2.431661000	-0.447775000
	8	-1.414894000	2.355741000	-0.750892000
	7	-3.064223000	0.000171000	0.000049000
	7	3.064254000	0.000028000	-0.000182000
	6	2.766208000	2.330128000	-0.898113000
	1	3.242214000	3.321396000	-0.861323000
	1	2.784556000	1.992151000	-1.944134000
	6	3.534095000	1.396603000	0.022734000
	1	4.607496000	1.459560000	-0.235112000
	1	3.427967000	1.779123000	1.040460000
	6	2.765780000	-1.943033000	-1.568237000
	1	3.241968000	-2.407914000	-2.444407000
	1	2.783413000	-2.678779000	-0.751515000
	6	3.533891000	-0.678692000	-1.221033000
	1	4.607251000	-0.933653000	-1.146656000
	1	3.427738000	0.011251000	-2.061304000
	6	2.766180000	-0.387572000	2.466825000
	1	3.241990000	-0.915395000	3.306791000
	1	2.784970000	0.687232000	2.697337000
	6	3.534041000	-0.718182000	1.197905000
	1	4.607468000	-0.526461000	1.381310000
	1	3.427906000	-1.790781000	1.020234000
	6	0.689019000	3.422255000	-1.175249000
	1	0.615683000	3.136985000	-2.234212000
	1	1.208671000	4.390430000	-1.110419000
	6	-0.688699000	3.572274000	-0.575966000
	1	-0.615359000	3.819472000	0.492527000
	1	-1.208371000	4.395693000	-1.089297000
	6	0.688651000	-2.729362000	-2.375446000
	1	0.615208000	-3.503120000	-1.598245000

	1	1.208298000	-3.158016000	-3.245971000
	6	-0.689034000	-2.285494000	-2.805347000
	1	-0.615790000	-1.484347000	-3.554299000
	1	-1.208743000	-3.142088000	-3.261135000
	6	0.688853000	-0.693457000	3.551076000
	1	0.615785000	0.366238000	3.833640000
	1	1.208425000	-1.233996000	4.356955000
	6	-0.688946000	-1.287256000	3.381217000
	1	-0.615764000	-2.336103000	3.060767000
	1	-1.208515000	-1.254613000	4.351059000
	6	-2.766055000	-1.503691000	-1.993457000
	1	-3.242118000	-2.364640000	-2.486073000
	1	-2.784216000	-0.663917000	-2.702760000
	6	-3.533867000	-1.197844000	-0.718356000
	1	-4.607318000	-1.115247000	-0.970415000
	1	-3.427364000	-2.060471000	-0.056616000
	6	-2.765816000	2.478333000	-0.305591000
	1	-3.241798000	3.335699000	-0.804477000
	1	-2.783838000	2.672337000	0.776396000
	6	-3.534004000	1.221244000	-0.678167000
	1	-4.607354000	1.398402000	-0.480270000
	1	-3.428047000	1.079107000	-1.756069000
	6	-2.766088000	-0.974331000	2.298962000
	1	-3.242166000	-0.970853000	3.290884000
	1	-2.784021000	-2.008358000	1.926081000
	6	-3.534224000	-0.023192000	1.396667000
	1	-4.607522000	-0.283435000	1.450848000
	1	-3.428587000	0.981346000	1.812778000
[K([2.2.2]crypt)] ⁺	TPSSh/6-311++G** (0 imaginary Frequencies, E _{elec} = -1868.6276916, ZPE correction= 0.552842)			
	19	-0.000033000	-0.000607000	-0.000233000
	8	1.417598000	2.477270000	0.146212000
	8	-1.418003000	2.476994000	-0.156466000
	8	-1.417611000	-1.373599000	-2.066519000
	8	1.418321000	-1.111809000	-2.218253000
	8	1.418139000	-1.366029000	2.071705000
	8	-1.418130000	-1.103411000	2.222022000
	7	-3.064795000	0.000072000	-0.000097000

	7	3.064666000	0.000249000	0.000255000
	6	2.762521000	-0.944797000	2.310872000
	1	3.245737000	-1.636016000	3.015625000
	1	2.761258000	0.053004000	2.771662000
	6	3.537336000	-0.971813000	1.003502000
	1	4.607647000	-0.820511000	1.230658000
	1	3.438840000	-1.975665000	0.584028000
	6	2.762525000	2.474026000	-0.336720000
	1	3.245397000	3.429895000	-0.089497000
	1	2.762693000	2.374846000	-1.431300000
	6	3.536708000	1.355217000	0.340904000
	1	4.607285000	1.476430000	0.097545000
	1	3.436867000	1.493714000	1.419899000
	6	2.763030000	-1.528660000	-1.973251000
	1	3.246217000	-1.793191000	-2.924306000
	1	2.762501000	-2.426538000	-1.339404000
	6	3.537211000	-0.382296000	-1.343294000
	1	4.607751000	-0.653777000	-1.326225000
	1	3.437652000	0.482763000	-2.002926000
	6	0.685338000	-1.524779000	3.287187000
	1	0.597804000	-0.559762000	3.805566000
	1	1.206306000	-2.230019000	3.950006000
	6	-0.685829000	-2.074156000	2.971019000
	1	-0.598372000	-3.007724000	2.397922000
	1	-1.207143000	-2.291941000	3.913834000
	6	0.685477000	3.609844000	-0.323716000
	1	0.598093000	3.576836000	-1.418663000
	1	1.206813000	4.536109000	-0.043825000
	6	-0.685739000	3.610886000	0.310000000
	1	-0.598310000	3.581082000	1.405041000
	1	-1.206990000	4.536379000	0.027404000
	6	0.685995000	-2.085375000	-2.963519000
	1	0.598499000	-3.016760000	-2.386886000
	1	1.207233000	-2.306772000	-3.905535000
	6	-0.685160000	-1.537099000	-3.281589000
	1	-0.597627000	-0.574111000	-3.803735000
	1	-1.206367000	-2.244848000	-3.941533000
	6	-2.762690000	2.474997000	0.327081000

	1	-3.245938000	3.429916000	0.076954000
	1	-2.762114000	2.379310000	1.421981000
	6	-3.536912000	1.353608000	-0.346277000
	1	-4.607478000	1.475880000	-0.103408000
	1	-3.437118000	1.487854000	-1.425815000
	6	-2.763333000	-1.520467000	1.980092000
	1	-3.245959000	-1.779832000	2.932865000
	1	-2.764196000	-2.421627000	1.350920000
	6	-3.537256000	-0.376724000	1.345113000
	1	-4.607839000	-0.648103000	1.329367000
	1	-3.437509000	0.491244000	2.000914000
	6	-2.762430000	-0.954396000	-2.306935000
	1	-3.245330000	-1.649025000	-3.008542000
	1	-2.762221000	0.041387000	-2.772080000
	6	-3.536865000	-0.976490000	-0.999220000
	1	-4.607364000	-0.827167000	-1.226776000
	1	-3.437264000	-1.978462000	-0.575527000
[K([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/6-311++G** (E _{elec} = -1868.62760283)			
[K([2.2.2]crypt)]	TPSSh/def2qzvp//PBE0/6-311++G** (E _{elec} = -1868.90789084)			
[K([2.2.2]crypt)] ⁺	TPSSh/def2qzvp//PBE0/6-311++G** (E _{elec} = -1868.84356935)			
[K([2.2.2]crypt)] ⁺ in the geometry of neutral complex	TPSSh/def2qzvp (E _{elec} = -1868.84346036)			

2. Natural charges on the selected atoms

Table S2. Natural charges on the selected atoms

Complex	Atoms	Natural charge	
		Neutral molecule	Cation
[Li(9-Crown-3) ₂]	Li	0.10	0.82
	O	-0.65	-0.64
[Li(12-Crown-4)]	Li	0.09	0.85
	O	-(0.65-0.69)	-0.66
[Na(15-Crown-5)]	Na	0.07	0.89
	O	-(0.62-0.64)	-0.64
[K(18-Crown-6)]	K	0.05	0.92
	O	-0.62	-0.63
[Li([2.2.2]crypt)]	Li	0.07	0.82
	O	-(0.60-0.66)	-(0.60-0.66)
	N	-(0.58-0.60)	-(0.58-0.60)
[Na([2.2.2]crypt)]	Na	-0.01	0.85
	O	-0.62	-0.62
	N	-0.58	-0.58
[K([2.2.2]crypt)]	K	0.00	0.86
	O	-0.62	-0.62
	N	-0.59	-0.59

3. Illustration of alpha HOMO of all the investigated neutral complexes

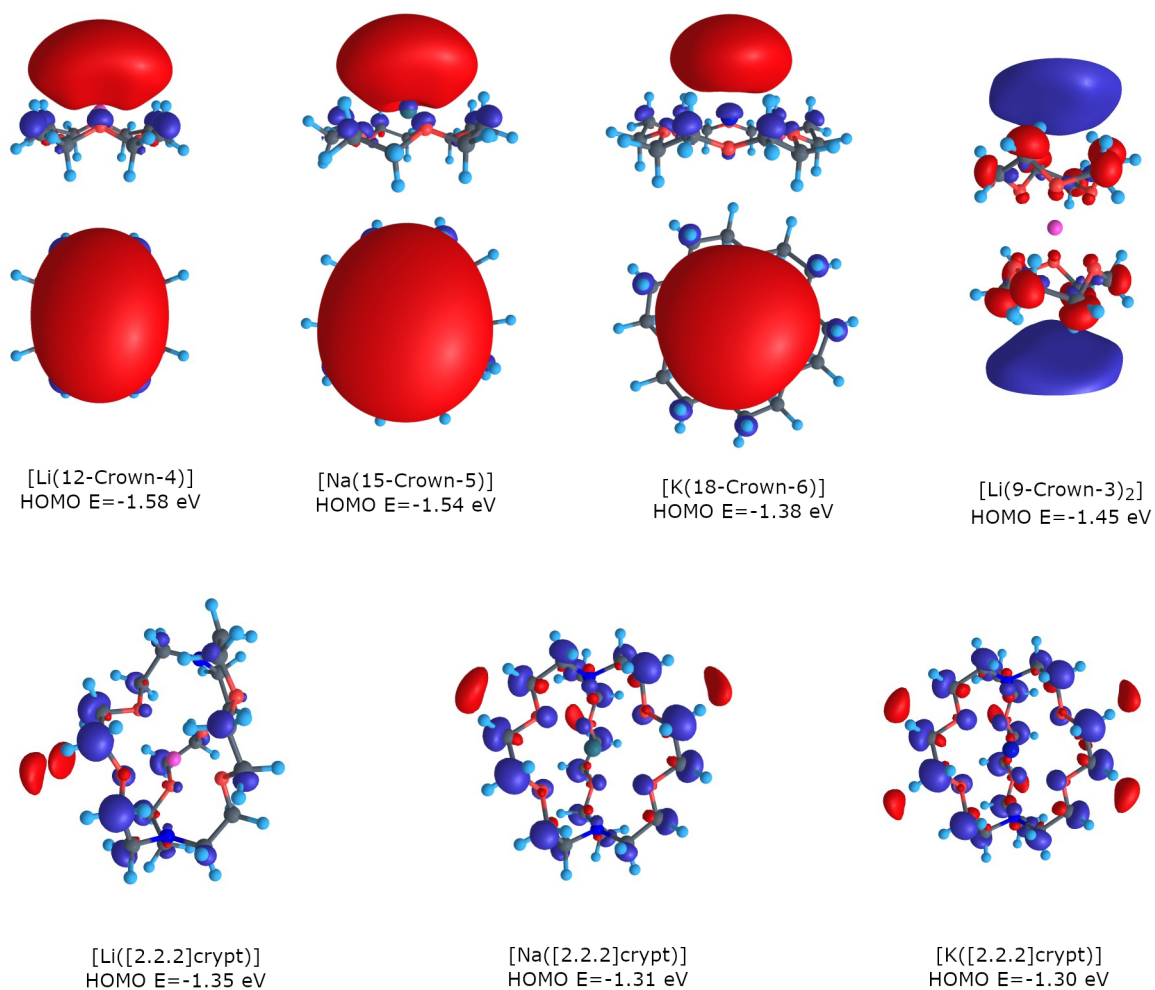


Figure S1. Illustrated HOMO for neutral complexes.