

Optimized geometries in cartesian coordinates calculated at the M06-
2X/6-31G** level of theory

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C₆H₈

C	-0.05346200	0.73275500	1.25266100
C	-0.05346200	-1.41983800	0.10959200
C	0.31901900	0.69566300	-1.18743900
C	-0.31901900	-0.69566300	-1.18743900
C	0.05346200	1.41983800	0.10959200
C	0.05346200	-0.73275500	1.25266100
H	1.40823500	0.59986500	-1.31484200
H	-1.40823500	-0.59986500	-1.31484200
H	0.00886900	2.50517700	0.10751500
H	0.20084400	-1.24560300	2.19839100
H	-0.20084400	1.24560300	2.19839100
H	-0.00886900	-2.50517700	0.10751500
H	-0.04336500	1.27699700	-2.03995000
H	0.04336500	-1.27699700	-2.03995000

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C₆₀

C	0.23484800	1.91473500	2.96737600
C	-1.14027100	1.79089100	2.83189400
C	-1.77472200	0.49942000	3.02132900
C	2.25503700	2.06788100	1.77970800
C	0.98650200	2.72752200	2.02862500
C	0.32954000	3.38040700	0.99562500
C	-2.85422000	0.38436400	2.05786500
C	-3.11700900	-0.83647700	1.45327000
C	2.81094600	2.09028600	0.50858500
C	-2.88678400	1.60481900	1.27308800
C	-2.28754300	-0.84739500	-2.56446000
C	-2.87474300	0.29687000	-2.04395300
C	-2.24035900	1.58845200	-2.23334300
C	-1.04666500	1.67871300	-2.93482200
C	-0.43262300	0.48178500	-3.47956200
C	-2.25502600	-2.06785700	-1.77959800
C	-2.81104600	-2.09039000	-0.50868000
C	-3.42494300	-0.89319200	0.03606500
C	-3.45599200	0.27350400	-0.71413200
C	-2.42949800	2.36322300	-1.02055200
C	-1.41691200	3.19433700	-0.56330400
C	-0.16835200	3.28896000	-1.29755800
C	0.01258400	2.54801000	-2.45637100
C	1.28121000	1.88846700	-2.70546600
C	1.00605300	0.61137200	-3.33779700
C	2.31311600	1.99860700	-1.78459900
C	2.12375500	2.77341000	-0.57190600

C	0.91102100	3.40417400	-0.33389800
C	-3.18083300	1.55053300	-0.08185600
C	-1.10910600	3.25080800	0.85382300
C	-1.03908100	-0.75286200	-3.29859700
C	-1.82764500	2.47422600	1.75136100
C	1.03895500	0.75285100	3.29854700
C	0.43253500	-0.48169400	3.47954900
C	-1.00600000	-0.61127900	3.33779000
C	2.28762700	0.84748000	2.56451900
C	2.87448600	-0.29681000	2.04372600
C	-1.28120400	-1.88853600	2.70555400
C	-2.31288300	-1.99845400	1.78443100
C	-0.01258500	-2.54799400	2.45649600
C	-0.98641500	-2.72746600	-2.02856900
C	-0.32952700	-3.38073200	-0.99574000
C	1.10917300	-3.25112300	-0.85394200
C	1.82752800	-2.47419000	-1.75132100
C	1.14032300	-1.79100800	-2.83187500
C	-2.12376700	-2.77351200	0.57203200
C	-0.91094000	-3.40406500	0.33398300
C	1.41678900	-3.19426000	0.56340400
C	2.42949400	-2.36331600	1.02070800
C	3.18098600	-1.55060400	0.08178600
C	2.88675900	-1.60478400	-1.27297100
C	2.85411000	-0.38429600	-2.05779800
C	1.77483400	-0.49939900	-3.02133500
C	3.11730300	0.83658300	-1.45343500
C	3.42481100	0.89326000	-0.03597700
C	3.45611000	-0.27342800	0.71424500
C	0.16836900	-3.28880300	1.29741200
C	2.24015100	-1.58836200	2.23312700
C	-0.23489100	-1.91486000	-2.96739500
C	1.04663200	-1.67879900	2.93488200

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Li⁺@C₆₀

C	3.22213400	-0.62855100	-1.32594400
C	3.24274600	0.76220600	-1.20129000
C	3.26158000	1.37577100	0.12165500
C	1.83100000	-2.48210400	-1.74199100
C	2.36105100	-1.25821700	-2.31757200
C	1.55898100	-0.47094600	-3.13495600
C	2.43176500	2.57198400	0.07128000
C	1.63695600	2.90749000	1.16093600
C	0.52279300	-2.86211200	-2.01270200
C	1.90573300	2.69898500	-1.27712700
C	-2.37840900	2.60342500	0.38959500
C	-1.58047800	3.11601400	-0.62253800
C	-1.59835200	2.50547000	-1.93921300

C	-2.41355100	1.41038700	-2.18459700
C	-3.25202800	0.87657700	-1.12653300
C	-1.85198300	2.47495400	1.73693400
C	-0.55087200	2.86611900	2.01547300
C	0.28611400	3.39866000	0.95521900
C	-0.21575000	3.51902600	-0.33301900
C	-0.24487400	2.53120100	-2.46448200
C	0.22936300	1.46527500	-3.21637000
C	-0.62566300	0.32099300	-3.47653700
C	-1.91585200	0.29390800	-2.96860600
C	-2.44717600	-0.92955600	-2.39457500
C	-3.27268900	-0.56915700	-1.25610400
C	-1.66427700	-2.07373800	-2.35048900
C	-0.31080200	-2.04382600	-2.87524000
C	0.19551100	-0.87516400	-3.42666500
C	0.60952400	3.15846800	-1.47212700
C	1.57982100	0.97664000	-3.00501000
C	-3.23483800	1.45987100	0.13173800
C	2.40208200	1.58261100	-2.06259700
C	3.21908200	-1.46762200	-0.13328000
C	3.23728500	-0.88049500	1.13354500
C	3.25891800	0.57203200	1.26396800
C	2.35649000	-2.61196900	-0.39390100
C	1.55015600	-3.11385400	0.62056600
C	2.42586700	0.93025000	2.40394400
C	1.63403900	2.07124100	2.34984800
C	1.89517400	-0.29466000	2.97726300
C	-2.38299900	1.25139900	2.31086100
C	-1.58939000	0.46988600	3.13757900
C	-1.61022900	-0.97564500	3.00805300
C	-2.42361400	-1.57444200	2.05743900
C	-3.25743100	-0.75680200	1.19505100
C	0.28146100	2.04619400	2.87727200
C	-0.22499000	0.87529600	3.42371500
C	-0.25867000	-1.46440100	3.21379200
C	0.21561600	-2.53333600	2.46620700
C	-0.63763000	-3.16250900	1.47418500
C	-1.92628100	-2.69084400	1.27346000
C	-2.45273900	-2.56240300	-0.07398600
C	-3.27556200	-1.36731500	-0.12180400
C	-1.66713700	-2.90884500	-1.16329900
C	-0.31535700	-3.39585300	-0.95380000
C	0.18638400	-3.52165700	0.33401700
C	0.59742500	-0.32039900	3.47176600
C	1.56816000	-2.50251800	1.93930300
C	-3.23763700	0.62457700	1.31886600
C	2.39190100	-1.41241200	2.19382700
Li	1.44429500	-0.01111100	-0.00200100

RC-Li⁺@C₆₀(C₆H₈)

C	-1.78897300	0.90087400	3.26299400
C	-0.62816300	0.07489400	3.54248200
C	0.55854600	0.83787400	3.19619900
C	0.13088700	2.13333500	2.70220900
C	-1.31991700	2.17239300	2.74328200
C	0.76122400	3.15320500	-0.65878800
C	0.07692400	3.40637000	0.59659100
C	0.81303300	2.73669500	1.65399200
C	1.95289900	2.06965300	1.05336300
C	1.92193100	2.32764300	-0.37847000
C	-1.87815900	-1.89580200	2.76449800
C	-1.48322800	-2.93419400	1.82971500
C	-0.03245000	-2.97205300	1.78830100
C	0.46874400	-1.95545200	2.69636800
C	-0.67260000	-1.29075400	3.30090300
C	1.53758100	1.12040300	-2.48927000
C	2.30360500	1.33539700	-1.27390100
C	2.74184300	0.03790700	-0.77918700
C	2.23505900	-0.98141100	-1.69023500
C	1.49135300	-0.30892900	-2.74616300
C	0.42310200	1.90623700	-2.75239700
C	-0.78364900	1.30250700	-3.29023200
C	-1.92402600	1.97041700	-2.68953200
C	-1.42229600	2.98537100	-1.78106300
C	0.02838500	2.94605100	-1.81981400
C	-2.93981800	0.32325100	2.74712100
C	-3.67779900	0.99147800	1.69071100
C	-4.17878400	-0.02361900	0.78215500
C	-3.75057100	-1.31954200	1.27664400
C	-2.98494600	-1.10551600	2.49164100
C	1.65408100	0.20155400	2.62599700
C	1.60809700	-1.22810700	2.37111800
C	2.30005100	-1.48547500	1.11641200
C	2.77702400	-0.20919200	0.59478700
C	2.36844900	0.83210400	1.53010200
C	-2.02298400	2.80905800	1.73116400
C	-1.30920200	3.43845900	0.63398000
C	-2.07542700	3.22451700	-0.58083100
C	-3.26170300	2.46319800	-0.23427200
C	-3.22933300	2.20660700	1.19404500
C	-3.05552100	1.24022600	-2.35657200
C	-3.10077000	-0.18841300	-2.61240000
C	-3.81400300	-0.81799500	-1.51539000
C	-4.20980700	0.22160200	-0.58272000
C	-3.74098900	1.49324200	-1.10235900
C	-0.13989800	-3.43499200	-0.62761600
C	0.57303600	-2.80655600	-1.72650900

C	1.78782300	-2.20658800	-1.19285300
C	1.82014900	-2.46456300	0.24480100
C	0.62550300	-3.22160100	0.58890700
C	-3.40816000	-2.05748300	-1.04324600
C	-2.26593800	-2.72179800	-1.64493100
C	-1.52764100	-3.38905000	-0.58772100
C	-2.21367400	-3.13708200	0.66706700
C	-3.37578900	-2.31407900	0.38510400
C	0.33346900	-0.88660100	-3.25327700
C	-0.13513000	-2.15961600	-2.73341000
C	-1.58585000	-2.12117200	-2.69525800
C	-2.01371200	-0.82566100	-3.19212700
C	-0.82820000	-0.06226700	-3.53737700
C	5.91061900	-0.80531800	1.15908900
C	5.66283100	-1.45178000	0.00980300
C	5.73760600	-0.74562200	-1.27219700
C	5.79720400	0.59508600	-1.31333200
H	5.88872900	-1.33766900	2.10639100
H	5.42151700	-2.51142000	0.01102200
H	5.72878900	-1.32616500	-2.19016700
H	5.82668700	1.11559900	-2.26681500
Li	0.62304100	-0.55237100	-0.11865100
C	5.79278800	1.41293300	-0.04678800
H	4.75915100	1.73460400	0.16379500
H	6.36067200	2.33606300	-0.19019000
C	6.35405300	0.63569600	1.14998600
H	7.45278600	0.64408700	1.11030700
H	6.07981400	1.13430800	2.08383300

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TS-Li⁺@C₆₀(C₆H₈)

C	-0.13197200	2.75499500	-2.08488800
C	1.31871600	2.79680600	-2.08032600
C	1.80296000	1.69926100	-2.89831500
C	0.65106800	0.97687200	-3.40548800
C	-0.54317600	1.63177700	-2.89715500
C	0.69196600	-0.40466000	-3.52139500
C	2.94270700	1.00335300	-2.52099100
C	1.99715000	3.14820200	-0.92215500
C	-0.84185900	3.06382000	-0.92979200
C	-1.64550800	0.87148200	-2.52184300
C	-0.46056200	-1.19951400	-3.13040000
C	-1.60364700	-0.57299300	-2.64155100
C	-1.99501000	2.27453000	-0.54920700
C	-2.39355300	1.19813300	-1.32540200
C	-0.13090100	3.43582400	0.28021000
C	1.25584800	3.47479700	0.28355100
C	3.19129800	2.42414100	-0.53063400
C	3.65382400	1.37491200	-1.31188300

C	1.88519000	-1.13280300	-3.13174600
C	2.98421700	-0.44358400	-2.63931100
C	3.72045100	-0.96515200	-1.50239400
C	4.13509000	0.15839700	-0.68261700
C	-1.99519900	2.15551600	0.91002800
C	-0.84214100	2.87265500	1.41375200
C	1.99695800	2.95712900	1.42054400
C	3.19111100	2.30599300	0.91704900
C	-2.33186100	-1.13416800	-1.52100600
C	-2.94682400	-0.03842600	-0.73265300
C	0.01715400	-2.41405500	-2.50851700
C	1.46791900	-2.37391300	-2.50324500
C	-1.87287600	-2.30179500	-0.92763600
C	-0.67126300	-2.94736200	-1.42155300
C	-2.94701100	-0.15662000	0.71595000
C	-2.39385300	0.96752800	1.50138500
C	-0.13248100	2.38063800	2.50364000
C	1.31820000	2.42261200	2.50624100
C	3.65344700	1.14402200	1.51803000
C	4.13489700	0.04560100	0.70003700
C	2.17039700	-2.86950500	-1.41356000
C	3.32353700	-2.15270900	-0.90389300
C	3.32334100	-2.27075500	0.54360200
C	3.72016700	-1.19596500	1.32679200
C	2.94208600	0.58142300	2.65078500
C	1.80227900	1.20701700	3.13570000
C	-0.54383100	1.14062700	3.12299100
C	-1.64608700	0.45124900	2.62920200
C	-2.33209100	-1.36564900	1.31637500
C	-1.87302000	-2.42171000	0.54174300
C	0.06596900	-3.46744400	-0.28296000
C	1.45383600	-3.42695600	-0.27950300
C	2.98362300	-0.86556500	2.53304300
C	0.65029500	0.41197200	3.51877400
C	-1.60418700	-0.99351400	2.51321000
C	-0.67147200	-3.13882500	0.92474900
C	2.17009500	-3.06065700	0.93007300
C	-0.46121900	-1.69102500	2.89433900
C	0.01665200	-2.78872700	2.08394100
C	0.69121400	-0.97008500	3.40926700
C	1.88455600	-1.62550000	2.90707400
C	1.46741100	-2.74829600	2.08555500
H	-4.96680900	0.05884500	-2.44934100
C	-5.11737400	-0.00093600	-1.37328000
C	-5.43106300	-1.33659500	0.59609700
C	-5.47459900	1.15828200	0.87234300
C	-5.11675300	-0.22434000	1.35478700
C	-5.47391200	1.28502600	-0.67213100
C	-5.43147100	-1.22175800	-0.80548500

H	-6.47854100	1.36676000	1.25688900
H	-4.96570300	-0.34037800	2.42617500
H	-4.81700900	2.09299800	-1.00518000
H	-5.46212100	-2.11728200	-1.41850000
H	-5.46130800	-2.31995400	1.05520400
H	-4.81917100	1.90205600	1.33329000
H	-6.47713600	1.55512700	-1.01827300
Li	-0.75510600	-0.43878800	-0.03597700

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product-Li⁺@C₆₀(C₆H₈)

C	1.81778900	3.03411000	1.43000300
C	0.65281700	3.48108800	0.68991100
C	-0.52836700	3.02700600	1.40613300
C	-0.09659200	2.30964300	2.57879100
C	1.35401200	2.30810200	2.59858800
C	-0.80090600	-1.17253700	2.98561600
C	-0.08261000	0.00379900	3.43872000
C	-0.80087700	1.17920000	2.98309800
C	-1.96841000	0.74518400	2.24987800
C	-1.96843200	-0.74006800	2.25146400
C	1.84530000	3.03117400	-1.41277300
C	1.40366900	2.30240200	-2.58832900
C	-0.04707400	2.30411300	-2.59651300
C	-0.50061500	3.02408700	-1.43395400
C	0.66637600	3.47981100	-0.69608600
C	-1.64616900	-2.58262300	0.70806400
C	-2.40151800	-1.43502900	1.14598200
C	-3.16311100	-0.80911900	-0.03529100
C	-2.37568300	-1.43655300	-1.19934700
C	-1.63110000	-2.58354200	-0.74453200
C	-0.52848400	-3.02382000	1.41276800
C	0.65266600	-3.47952100	0.69753500
C	1.81765800	-3.03096700	1.43662500
C	1.35393100	-2.30236400	2.60363100
C	-0.09664200	-2.30386600	2.58382800
C	2.94446200	2.59811800	0.74602900
C	3.66096300	1.42208000	1.20177900
C	4.11920200	0.69366300	0.03301100
C	3.68351100	1.41941900	-1.14576300
C	2.95844800	2.59646800	-0.70635000
C	-1.64604600	2.58427600	0.70235200
C	-1.63100300	2.58196000	-0.75023100
C	-2.37562800	1.43396100	-1.20246700
C	-3.16305200	0.80914900	-0.03705800
C	-2.40136600	1.43769800	1.14280400
C	2.03854800	1.17973500	3.02937200
C	1.30361000	0.00379200	3.46377500
C	2.03848200	-1.17309200	3.03194500

C	3.21838800	-0.72444300	2.32198800
C	3.21840500	0.72948200	2.32038600
C	2.94433000	-2.59655600	0.75172400
C	2.95836900	-2.59811500	-0.70065100
C	3.68345500	-1.42206600	-1.14262100
C	4.11918300	-0.69371700	0.03456000
C	3.66090400	-1.41951900	1.20491500
C	-0.01707900	-0.00379500	-3.45063600
C	-0.74425300	-1.17934900	-3.00911000
C	-1.92680000	-0.74545500	-2.29969000
C	-1.92676000	0.74045100	-2.30127700
C	-0.74422400	1.17277100	-3.01166400
C	3.26207100	-0.72946100	-2.26954300
C	2.09609900	-1.17980300	-3.00108100
C	1.36945700	-0.00381500	-3.44930600
C	2.09616100	1.17315400	-3.00365700
C	3.26209700	0.72436000	-2.27114200
C	-0.50073200	-3.02723500	-1.42732500
C	-0.04714700	-2.30982900	-2.59144600
C	1.40358300	-2.30815900	-2.58327100
C	1.84519200	-3.03436900	-1.40613200
C	0.66626200	-3.48136700	-0.68846100
C	-4.66244500	1.28577600	-0.07922000
C	-5.30511900	0.66594900	-1.29177000
C	-5.30513100	-0.66858600	-1.29037600
C	-4.66246100	-1.28588100	-0.07657300
H	-4.66288700	2.37830500	-0.11515400
H	-5.72848800	1.27457200	-2.08305700
H	-5.72848900	-1.27887700	-2.08038900
H	-4.66283000	-2.37848200	-0.11023600
Li	-0.87198300	-0.00055900	-0.04806100
C	-5.37919400	-0.77166800	1.18843000
H	-4.88658700	-1.16805100	2.08111500
H	-6.39893700	-1.16118500	1.18649300
C	-5.37894900	0.77417800	1.18694100
H	-6.39853300	1.16406600	1.18473800
H	-4.88582500	1.17210300	2.07864900