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Energies and Cartesian coordinates of computed structures, 6-31 + G* basis, with effective pseudopotentials for heavy atoms as described in the text.

Benzene: E = -230.7110925206 au

C	.6940655265	1.2021567557	0
C	-.6940655265	1.2021567557	0
C	-1.3881310530	.0000000000	0
C	-.6940655265	-1.2021567557	0
C	.6940655265	-1.2021567557	0
C	1.3881310530	.0000000000	0
H	1.2318977763	2.1337095384	0
H	-1.2318977763	2.1337095384	0
H	-2.4637955527	.0000000000	0
H	-1.2318977763	-2.1337095384	0
H	1.2318977763	-2.1337095384	0
H	2.4637955527	.0000000000	0

Phenyl anion E = -230.0505792 au

C	0	.000000	1.541912
C	0	1.173510	.748453
C	0	-1.173510	.748453
C	0	1.191681	-.645549
C	0	-1.191681	-.645549
C	0	.000000	-1.363164
H	0	2.137658	1.243803
H	0	-2.137658	1.243803
H	0	2.134806	-1.176199
H	0	-2.134806	-1.176199
H	0	.000000	-2.442545

Phenyllithium: E = -237.5420788958 au
(E Li^+ = 7.2355)

C	.0000000000	-1.9433607982	0
C	-1.1830037113	-1.1797982349	0
C	1.1830037113	-1.1797982349	0
C	-1.1952036924	.2110547912	0
C	1.1952036924	.2110547912	0
C	.0000000000	.9159434044	0
H	.0000000000	1.9926254300	0
H	-2.1324582733	.7432877714	0
H	2.1324582733	.7432877714	0
H	-2.1422849854	-1.6782390168	0
H	2.1422849854	-1.6782390168	0
Li	.0000000000	-3.9292332808	0

Phenylsodium; E = -391.92734826
(E Na^+ = 161.65929)

C	0.0000000	-1.9524139817	0
C	-1.1818672	-1.1880629890	0
C	1.1818672	-1.1880629890	0
C	-1.1943573	.2036001966	0
C	1.1943573	.2036001966	0
C	0.0000000	.9101054495	0
H	0.0000000	1.9868664794	0
H	-2.1325053	.7351327230	0
H	2.1325053	.7351327230	0
H	-2.1422406	-1.6848930136	0
H	2.1422406	-1.6848930136	0
Na	0.0000000	-4.2775439314	0

Phenylpotassium, all electron Calc:
(E K^+ = -598.99613)
E = -829.2236349121 ,
Units in Angstroms

C	0 .000000	-1.967932347	0
C	-1.1782218	-1.192497415	0
C	1.1782218	-1.192497415	0
C	-1.1932648	.199687847	0
C	1.1932648	.199687847	0
C	0.000000	.908898829	0
H	0.000000	1.986051325	0
H	-2.1325535	.730430197	0
H	2.1325535	.730430197	0
H	-2.1424770	-1.685551557	0
H	2.1424770	-1.685551557	0
K	0.0000000	-4.7426106	0

Phenylcesium ECP from Hay and Wadt: E = -249.6840821450 au
(E Cs^+ = 19.47931)

C	.0000000000	-1.9541363956	0
C	-1.1767860953	-1.1745402372	0
C	1.1767860953	-1.1745402372	0
C	-1.1930141919	.2180184896	0
C	1.1930141919	.2180184896	0
C	.0000000000	.9282573745	0
H	.0000000000	2.0055720052	0
H	-2.1322109337	.7496399082	0
H	2.1322109337	.7496399082	0
H	-2.1418128852	-1.6679312923	0
H	2.1418128852	-1.6679312923	0
CS	.0000000000	-5.1412797164	0

Phenylcesium ECP from Ross *et al*
E = -249.9481351
(E Cs^+ = 19.73221)

C	0	.000000	-3.937757
C	0	1.193934	-3.229159
C	0	-1.193934	-3.229159
C	0	1.177730	-1.836949
C	0	-1.177730	-1.836949
C	0	.000000	-1.061046
H	0	.000000	-5.014678
H	0	2.132623	-3.761025
H	0	-2.132623	-3.761025
H	0	2.142334	-1.342300
H	0	-2.142334	-1.342300
Cs	0	.000000	1.927408

Fluorobenzene (C6H5F)
E = -329.566605 au

C	0	.000000	.924607
C	0	1.209105	.261819
C	0	-1.209105	.261819
C	0	1.200307	-1.125805
C	0	-1.200307	-1.125805
C	0	.000000	-1.822743
F	0	.000000	2.258802
H	0	2.125290	.822506
H	0	-2.125290	.822506
H	0	2.133379	-1.659991
H	0	-2.133379	-1.659991
H	0	.000000	-2.897597

o-fluorophenylanion (o-$C6H4F^-$)
E = -328.9251862369 au

C	-1.28797781	.561811710	0
C	-1.17248008	-.84441466	0
C	.03241512	-1.55152894	0
C	1.23623457	-.86018522	0
C	1.19892624	.53083219	0
C	-.03596083	1.15557875	0
F	.04214497	2.52937214	0
H	2.105175065	1.1152361	0
H	2.180485433	-1.3813921	0
H	.03129440	-2.63237248	0
H	-2.07926659	-1.43709439	0

m-fluorophenylanion (m-$C6H4F^-$)
E = -328.9179697452 au

C	-1.5040085972	-.0273153633	0
C	-.8025308298	-1.2269051501	0
C	.5919341656	-1.2347127774	0
C	1.2060908794	-.0005684245	0
C	.5132666557	1.1933066877	0
C	-.9004848542	1.2578283445	0
H	1.1058265217	2.0977206967	0
F	2.5685755426	.0235234930	0
H	1.1717219473	-2.1414325504	0
H	-1.3323494619	-2.1695725217	0
H	-2.5845958432	-.0956844601	0

p-fluorophenylanion (p-$C6H4F^-$)
E = -328.9137648874 au

C	-2.22194724	.00000000	0
C	.64388610	.00000000	0
C	-.03140396	-1.19898011	0
C	-.03140396	1.198980117	0
C	-1.42932496	-1.171073402	0
C	-1.42932496	1.171073402	0
H	-1.921122869	-2.13593848	0
H	-1.921122869	2.13593848	0
H	.52305833	-2.124673886	0
H	.52305833	2.124673886	0
F	2.00767440	.000000000	0

o-Fluorophenyllithium (o-C6H4FLi)
Fully optimized
E = =-336.4183884

Li	-2.036743	1.875057	0
C	-1.192080	.077092	0
C	-1.010078	-1.316619	0
C	.247866	-1.905173	0
C	1.399471	-1.119824	0
C	1.286734	.261663	0
C	.000000	.751422	0
H	-1.872392	-1.963322	0
H	.340329	-2.977998	0
H	2.372012	-1.579230	0
H	2.142573	.911736	0
F	-.140418	2.165809	0

o-Fluorophenyllithium (o-C6H4FLi)
Idealized 120 LiCC angle
E = -336.41187289 au

C	.154550	.098275	0
C	.921823	-1.291186	0
C	.000000	.840456	0
C	-.345277	-1.858570	0
C	-1.291410	.339518	0
C	-1.463540	-1.034140	0
Li	2.930258	.982428	0
H	1.764721	-1.965991	0
H	-.462635	-2.928969	0
H	-2.130184	1.012484	0
H	-2.454656	-1.453013	0
F	.070567	2.202455	0

m-Fluorophenyllithium (m-C6H4FLi)
E = -336.4019273072 au

C	-1.5157007537	-.0941665534	0
C	-.7851341256	-1.2759219215	0
C	.6032045736	-1.2454923190	0
C	1.2063442073	-.0075027655	0
C	.4907609973	1.1727971774	0
C	-.9153784985	1.1804665855	0
H	1.0619267064	2.0879366235	0
F	2.5488922841	.0484089299	0
H	1.1984247001	-2.1402616829	0
H	-1.2915297415	-2.2267212909	0
H	-2.5922232115	-.1810638612	0
Li	-1.9758333671	2.8643148671	0

p-Fluorophenyllithium (p-C6H4FLi)
E = -336.4001228707 au

C	-2.1923301	.0000000	0
C	.6341244	.0000000	0
C	-.0356198	-1.2026165	0
C	-.0356198	1.2026165	0
C	-1.4272616	-1.1812440	0
C	-1.4272616	1.1812440	0
H	-1.9220387	-2.1413976	0
H	-1.9220387	2.1413976	0
H	.5204665	-2.1235511	0
H	.5204665	2.1235511	0
F	1.9762876	.0000000	0
Li	-4.1771443	.0000000	0

o-Fluorophenylsodium
Idealized NaCC angle
E = -490.7987218

C	0.000000	.718060	0
C	1.404682	.616066	0
C	-.627212	-.499155	0
C	2.090585	-.591684	0
C	-.006817	-1.739233	0
C	1.376624	-1.783667	0
Na	-1.267224	2.660561	0
H	1.998232	1.518408	0
H	3.167669	-.606359	0
H	-.598292	-2.637661	0
H	1.886850	-2.731179	0
F	-1.993574	-.570190	0

m-Fluorophenylsodium
E = -490.7879476651

C	-.00630140	.000807	0
C	1.3834599	.000683	0
C	2.0892986	1.197028	0
C	1.3515968	2.359606	0
C	-.0292229	2.371306	0
C	-.7766524	1.180568	0
H	-.5050514	3.33979	0
F	2.0094375	3.532959	0
H	3.1634014	1.232840	0
H	1.9252323	-.930930	0
H	-.4965088	-.961845	0
Na	-3.1056013	1.16277	0

p-Fluorophenylsodium
E = -490.7856322117

C	-.0083881	0.0000000000	0
C	2.8217324	0.0000000000	0
C	2.1508052	-1.2015812688	0
C	2.1508052	1.2015812688	0
C	.7580302	-1.1795913361	0
C	.7580302	1.1795913361	0
H	.2654817	-2.1411681720	0
H	.2654817	2.1411681720	0
H	2.7055894	-2.1236341575	0
H	2.7055894	2.1236341575	0
F	4.1659296	0.0000000000	0
Na	-2.3337009	0.0000000000	0

o-Fluorophenylpotassium
Idealised KCC angle
Full electron calc
E = -928.0973944 au

C	0.0000	.381934	0
C	-1.210452	1.106458	0
C	-.203496	-.971435	0
C	-2.470872	.521832	0
C	-1.426222	-1.626389	0
C	-2.581672	-.863624	0
K	2.583676	1.365408	0
H	-1.174961	2.187373	0
H	-3.357175	1.135029	0
H	-1.463528	-2.701805	0
H	-3.546434	-1.341025	0
F	.867616	-1.834996	0

o-Fluorophenylpotassium
Idealised KCC angle
ECP from Hay and Wadt
E = -356.8065327

C	0.000000	.383226	0
C	-1.212024	1.105224	0
C	-.201588	-.970157	0
C	-2.471692	.518705	0
C	-1.423337	-1.627492	0
C	-2.580193	-.866931	0
K	2.580905	1.366926	0
H	-1.178470	2.186259	0
H	-3.358960	1.130508	0
H	-1.458789	-2.702959	0
H	-3.544066	-1.346107	0
F	.870677	-1.832749	0

m-Fluorophenylpotassium
All electron calculation
E = -928.0855188228

C	.00769119	.00287948	0
C	1.39759275	.00052330	0
C	2.10553307	1.19661918	0
C	1.36484610	2.35739340	0
C	-.01618180	2.36715024	00
C	-.77362816	1.17935455	0
H	-.48940968	3.33849729	0
F	2.02409974	3.53325282	0
H	3.17975497	1.23312901	0
H	1.93980853	-.93150779	0
H	-.47968607	-.96307184	0
K	-3.55378319	1.15938001	0

p-Fluorophenylpotassium
All electron calculation
E = -928.0825261298

C	-.01536967	0.00000000	0
C	2.82768168	0.00000000	0
C	2.15522790	-1.20059634	0
C	2.15522790	1.20059634	0
C	.76129518	-1.17596968	0
C	.76129518	1.17596968	0
H	.27084537	-2.14040977	0
H	.27084537	2.14040977	0
H	2.70966072	-2.12343751	0
H	2.70966072	2.12343751	0
F	4.17498982	0.0000000	0
K	-2.79225410	0.0000000	0

o-Fluorophenylcesium (o-C6H4FCs)
Idealized CsCC angle
ECP from Hay and Wadt
E = -348.5587789

C	.000000	1.110048	0
C	-.891292	2.204355	0
C	1.308001	1.513131	0
C	-.498167	3.537782	0
C	1.778707	2.818256	0
C	.855987	3.851008	0
Cs	-.674007	-1.993806	0
H	-1.956377	2.012368	0
H	-1.234898	4.324834	0
H	2.837371	3.012257	0
H	1.187443	4.875293	0
F	2.324162	.580787	0

o-Fluorophenylcesium (o-C6H4FCs)
Idealized CsCC angle
ECP from Ross et al
E = -348.8217866 au

C	.000000	1.012763	0
C	-.899974	2.098473	0
C	1.307144	1.422849	0
C	-.514778	3.434252	0
C	1.768802	2.730086	0
C	.837290	3.755313	0
Cs	-.666096	-1.908460	0
H	-1.963672	1.898536	0
H	-1.255859	4.216846	0
H	2.825845	2.931693	0
H	1.161336	4.781815	0
F	2.319634	.490446	0

m-Fluorophenylcesium (m-C6H4FCs)
ECP from Hay and Wadt
E = -348.5466283556 au

C	.0076911914	.0028794832	0
C	1.3975927245	.0005233056	0
C	2.1055330741	1.1966191820	0
C	1.3648461095	2.3573934062	0
C	-.0161818043	2.3671502454	0
C	-.7736281687	1.1793545583	0
H	-.4894096865	3.3384972936	0
F	2.0240997418	3.5332528282	0
H	3.1797549752	1.2331290198	0
H	1.9398085313	-.9315077918	0
H	-.4796860782	-.9630718452	0
Cs	-3.5537831922	1.1593800111	0

m-Fluorophenylcesium (m-C6H4FCs)
ECP from Ross et al
E = -348.8100626 au

C	1.680777	2.568683	0
C	1.340301	1.230259	0
C	.744556	3.578541	0
C	.000000	.797200	0
C	-.592144	3.196360	0
C	-.940296	1.850878	0
F	2.984990	2.909674	0
H	1.051384	4.608721	0
H	2.160894	.525906	0
H	-1.356525	3.956945	0
H	-1.998600	1.622440	0
Cs	-.729477	-2.113320	0

p-Fluorophenylcesium (p-C6H4FCs)
ECP from Hay and Wadt
E = -348.5432965250

C	.0150850859	.0000000000	0
C	2.8631435551	.0000000000	0
C	2.1902923867	-1.2002577629	0
C	2.1902923867	1.2002577629	0
C	.7958249416	-1.1745948107	0
C	.7958249416	1.1745948107	0
H	.3066217328	-2.1406053383	0
H	.3066217328	2.1406053383	0
H	2.7453374904	-2.1230420961	0
H	2.7453374904	2.1230420961	0
F	4.2121344329	.0000000000	0
CS	-3.1768163409	.0000000000	0

p-Fluorophenylcesium (p-C6H4FCs)
ECP from Ross et al
E = -348.8070059 au

C	0	.000000	-3.502501
C	0	1.201020	-2.830455
C	0	-1.201020	-2.830455
C	0	1.175500	-1.436531
C	0	-1.175500	-1.436531
C	0	.000000	-.659135
F	0	.000000	-4.849953
H	0	2.123371	-3.385782
H	0	-2.123371	-3.385782
H	0	2.140836	-.945739
H	0	-2.140836	-.945739
Cs	0	.000000	2.336114

1,2-Difluorobenzene
E = -428.4145607 au

C	0	.689733	-.533675
C	0	-.689733	-.533675
C	0	1.391117	.651970
C	0	-1.391117	.651970
C	0	.693275	1.851940
C	0	-.693275	1.851940
F	0	1.336603	-1.691534
F	0	-1.336603	-1.691534
H	0	2.464878	.622261
H	0	-2.464878	.622261
H	0	1.234467	2.780135
H	0	-1.234467	2.780135

1,3-Difluorobenzene
E = -428.4211506

C	0	0	-1.025563
C	0	1.175837	-.304384
C	0	-1.175837	-.304384
C	0	1.208193	1.074555
C	0	-1.208193	1.074555
C	0	0.00000	1.756342
H	0	0.00000	-2.098433
F	0	2.324209	-.974246
F	0	-2.324209	-.974246
H	0	2.150569	1.588576
H	0	-2.150569	1.588576
H	0	0.00000	2.830995

1,4-Difluorobenzen
E = -428.4196449 au

C	0	0	1.359589
C	0	0	-1.359589
C	0	1.207023	.693640
C	0	-1.207023	.693640
C	0	-1.207023	-.693640
C	0	1.207023	-.693640
F	0	0.00000	2.693735
F	0	0.00000	-2.693735
H	0	2.125030	1.250746
H	0	-2.125030	1.250746
H	0	-2.125030	-1.250746
H	0	2.125030	-1.250746

2,3 Difluorophenyl anion
E = -427.78488

C	.423827	-1.604988	0
C	-.984209	-1.719180	0
C	.837802	-.286081	0
C	-1.865070	-.641101	0
C	0.00000	.810272	0
C	-1.371391	.659403	0
H	-1.424585	-2.707783	0
H	-2.933150	-.802870	0
F	.511182	2.061054	0
H	-2.007688	1.527167	0
F	2.168782	.013782	0

2,4-Difluorophenyl anion
E = -427.78738

C	-1.371402	-1.102436	0
C	-.128123	-1.763116	0
C	-1.194355	.269982	0
C	1.127300	-1.141046	0
C	0.00000	.978171	0
C	1.158767	.232700	0
H	-.117280	-2.845404	0
H	2.047443	-1.702452	0
H	.028092	2.053690	0
F	2.352936	.879924	0
F	-2.298644	1.081036	0

2,5 Difluorophenyl anion
E = -427.789992

C	-1.342834	-.728161	0
C	-.097951	-1.344894	0
C	-1.220657	.675720	0
C	1.139662	-.735887	0
C	0.00000	1.327035	0
C	1.201683	.657872	0
F	-.044279	-2.718639	0
H	2.041028	-1.326813	0
F	.027219	2.687993	0
H	2.135524	1.191674	0
H	-2.102432	1.300845	0

2,6-Difluorophenyl anion
E = 427.79926

C	0	0	-1.152129	
C	0	1.128453	-.357380	
C	0	-1.128453	-.357380	
C	0	1.195527	1.028695	
C	0	-1.195527	1.028695	
C	0	0	1.734889	
F	0	2.356273	-.968192	
F	0	-2.356273	-.968192	
H	0	2.148241	1.531303	
H	0	-2.148241	1.531303	
H	0	0.00000	2.812515	

3,4-Difluorophenyl anion
E = -427.77292

C	1.142932	-1.796455	0
C	1.905152	-.602043	0
C	-.247561	-1.547169	0
C	1.370800	.684553	0
C	-.798580	-.277894	0
C	0.00000	.839739	0
H	2.984979	-.670096	0
H	1.994551	1.565007	0
F	-2.139923	-.110500	0
F	-.555892	2.073468	0
H	-.953652	-2.366019	0

3,5-Difluorophenyl anion
E = -427.78422 au

C	0	0	1.901275
C	0	1.185102	1.122579
C	0	-1.185102	1.122579
C	0	1.164195	-.253789
C	0	-1.164195	-.253789
C	0	0.00000	-1.000005
H	0	2.155600	1.597029
H	0	-2.155600	1.597029
F	0	2.334620	-.941859
F	0	-2.334620	-.941859
H	0	0.00000	-2.073689

2,3-Difluorophenyllithium
Fully optimized geometry
E = -435.2692912

Li	-1.329268	2.617793	0
C	-1.365602	.621739	0
C	-1.840806	-.700604	0
C	-.985368	-1.792580	0
C	.399332	-1.621187	0
C	.896699	-.339638	0
C	0.00000	.704824	0
H	-2.902103	-.884688	0
H	-1.384601	-2.792263	0
H	1.077324	-2.454675	0
F	2.208303	-.113458	0
F	.521880	2.007116	0

2,3-Difluorophenyllithium
Idealized LiCC angle
E = 435.2643863

C	1.354918	.554478	0
C	1.729183	-.803723	0
C	0.00000	.766213	0
C	.811569	-1.843041	0
C	-.941086	-.247778	0
C	-.550802	-1.565520	0
Li	2.561265	2.136262	0
H	2.775974	-1.064261	0
H	1.144694	-2.866607	0
F	-2.240379	.055820	0
H	-1.295484	-2.340180	0
F	-.507584	2.021789	0

2,4-Difluorophenyllithium
Fully optimized geometry
E = -435.273941558

Li	1.569094	2.775216	0
C	1.347045	.800016	0
C	1.638386	-.574357	0
C	.657257	-1.557042	0
C	-.672419	-1.173901	0
C	-1.053984	.148831	0
C	0.00000	1.039043	0
H	2.665846	-.898047	0
H	.902245	-2.603788	0
F	-1.621531	-2.115323	0
H	-2.084910	.447613	0
F	-.343821	2.407881	0

2,4-Difluorophenyllithium
Idealized LiCC angle
E = -435.2688808

C	1.031679	-1.149126	0
C	-.284120	-1.649784	0
C	1.084111	.222856	0
C	-1.422641	-.854017	0
C	0.00000	1.087730	0
C	-1.249032	.514044	0
Li	2.698366	-2.224754	0
H	-.441171	-2.717138	0
H	-2.413452	-1.270845	0
H	.125687	2.154065	0
F	-2.323418	1.310539	0
F	2.287181	.853679	0

2,5-Difluorophenyllithium
Fully optimized geometry
E = -435.2755149 au

Li	2.004374	2.380626	0
C	1.215751	.551316	0
C	1.100087	-.846161	0
C	-.139607	-1.450550	0
C	-1.328977	-.742311	0
C	-1.263339	.642598	0
C	0.00000	1.185621	0
H	1.970011	-1.480063	0
F	-.209627	-2.789311	0
H	-2.267609	-1.264001	0
H	-2.147196	1.253651	0
F	.090536	2.601028	0

2,5-Difluorophenyllithium
Idealized LiCC angle
E = -435.269203 au

C	1.189267	.580304	0
C	1.038289	-.818563	0
C	0.00000	1.267010	0
C	-.203391	-1.415181	0
C	-1.261548	.698710	0
C	-1.371251	-.682263	0
Li	2.921812	1.556098	0
H	1.895758	-1.471522	0
F	-.285793	-2.755658	0
H	-2.136005	1.324039	0
H	-2.325502	-1.175541	0
F	.002695	2.630617	0

2,6-Difluorophenyllithium
Fully optimized structure
E = -435.282498 au

Li	-1.319131	2.461403	0
C	0.00000	.978956	0
C	1.197513	.286489	0
C	1.317559	-1.090382	0
C	.161196	-1.864807	0
C	-1.085107	-1.256851	0
C	-1.065493	.120236	0
F	2.345601	.985099	0
H	2.291434	-1.544782	0
H	.235462	-2.937289	0
H	-2.002441	-1.815359	0
F	-2.314608	.778387	0

2,6-Difluorophenyllithium
Idealized LiCC angle
E = -435.2806451 au

C	0	0.00000	-.959436
C	0	1.145195	-.188375
C	0	-1.145195	-.188375
C	0	1.202875	1.192099
C	0	-1.202875	1.192099
C	0	0.00000	1.884156
Li	0	0.00000	-2.939174
F	0	2.335041	-.840912
F	0	-2.335041	-.840912
H	0	2.149398	1.700706
H	0	-2.149398	1.700706
H	0	0.00000	2.959514

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3,4-Difluorophenyllithium
E = -435.2521754 au

C	0.00000	.907613	0
C	1.319088	.500582	0
C	-1.019926	-.015797	0
C	1.688765	-.855842	0
C	-.723372	-1.360617	0
C	.609043	-1.758438	0
F	-.303905	2.207500	0
H	2.056485	1.287677	0
F	-2.287686	.398584	0
Li	3.586966	-1.451367	0
H	-1.530407	-2.072033	0
H	.795750	-2.821304	0

3,5-Difluorophenyllithium
E = -435.2608135 au

C	0	0.00000	1.676401
C	0	1.190945	.927228
C	0	-1.190945	.927228
C	0	1.168311	-.451867
C	0	-1.168311	-.451867
C	0	0.00000	-1.184622
Li	0	0.00000	3.670101
H	0	2.159141	1.400892
H	0	-2.159141	1.400892
F	0	2.326978	-1.122747
F	0	-2.326978	-1.122747
H	0	0.00000	-2.257638

Chlorobenzene
E = -689.610160326

C	0	0	.502971
C	0	1.206166	-.176086
C	0	-1.206166	-.176086
C	0	1.199673	-1.563364
C	0	-1.199673	-1.563364
C	0	0.00000	-2.259665
Cl	0	0.00000	2.247156
H	0	2.131094	.369336
H	0	-2.131094	.369336
H	0	2.133651	-2.096035
H	0	-2.133651	-2.096035
H	0	0.00000	-3.334695

o-Chlorophenyl anion
E = -688.971158472

C	0.00000	.461104	0
C	1.345798	.136016	0
C	-1.086146	-.405617	0
C	1.518927	-1.271558	0
C	-.837666	-1.769775	0
C	.486532	-2.201477	0
Cl	-.473407	2.219754	0
H	-2.095552	-.031690	0
H	2.528121	-1.663530	0
H	-1.654916	-2.473030	0
H	.705595	-3.259725	0

m-Chlorophenyl anion
E = -688.9653429

C	0	.443252	0
C	1.246849	-.159288	0
C	-1.180855	-.276834	0
C	1.421239	-1.564784	0
C	-1.061932	-1.663092	0
C	.191845	-2.266003	0
Cl	-.113292	2.225326	0
H	-2.136911	.215075	0
H	2.109845	.489146	0
H	-1.959546	-2.265713	0
H	.209707	-3.348567	0

p-Chlorophenyl anion
E = -688.962976477 au

C	0	0.00000	.451434
C	0	1.198949	-.236231
C	0	-1.198949	-.236231
C	0	1.171572	-1.630738
C	0	-1.171572	-1.630738
C	0	0.00000	-2.424162
Cl	0	0.00000	2.227879
H	0	2.131548	.304624
H	0	-2.131548	.304624
H	0	2.136740	-2.121599
H	0	-2.136740	-2.121599

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o-Chlorophenyllithium
Fully optimized geometry
E = -696.4608615 au

Li	-2.482281	1.012863	0
C	-1.118025	-.436290	0
C	-.790166	-1.805118	0
C	.517198	-2.267649	0
C	1.583579	-1.371520	0
C	1.330062	-.010688	0
C	0.00000	.372453	0
H	-1.584723	-2.533712	0
H	.714190	-3.326307	0
H	2.598533	-1.727803	0
H	2.127516	.709202	0
Cl	-.326151	2.173700	0

o-Chlorophenyllithium
Optimized with constrained LiCC angle
E = -696.455693968 au

C	0.00000	.429174	0
C	-1.326860	.027208	0
C	1.104279	-.400122	0
C	-1.598803	-1.330761	0
C	.763002	-1.768357	0
C	-.544174	-2.234344	0
Cl	.276135	2.199257	0
H	-2.122161	.749590	0
H	-2.618188	-1.674812	0
H	1.550992	-2.506509	0
H	-.743066	-3.292734	0
Li	2.951156	.333433	0

m-Chlorophenyllithium
E = -696.446299128 au

C	0	.601306	0
C	-1.038767	-.315982	0
C	1.322750	.200801	0
C	-.810531	-1.703607	0
C	1.587813	-1.161040	0
C	.545467	-2.079295	0
Cl	-.366294	2.319525	0
H	2.115566	.925533	0
H	-2.042568	.076619	0
H	2.610634	-1.499010	0
H	.812234	-3.125906	0
Li	-2.303085	-3.020751	0

p-Chlorophenyllithium
E = -696.44502928 au

C	0	0.00000	.671583
C	0	1.200199	-.013645
C	0	-1.200199	-.013645
C	0	1.180475	-1.404140
C	0	-1.180475	-1.404140
C	0	0.00000	-2.169159
Cl	0	0.00000	2.424284
H	0	2.129550	.527291
H	0	-2.129550	.527291
H	0	2.141488	-1.897347
H	0	-2.141488	-1.897347
Li	0	0.00000	-4.157948

o-Clorophenylcesium
Optimized with idealized CsCC angle
ECP From Hay and Wadt
E = -708.6037453

C	1.360070	1.325414	0
C	2.037535	2.536970	0
C	0.00000	1.120702	0
C	1.284808	3.698833	0
C	-.704853	2.348065	0
C	-.102600	3.598612	0
Cl	2.447318	-.135500	0
H	3.111685	2.574488	0
H	1.771681	4.658765	0
H	-1.786845	2.328966	0
H	-.704570	4.492973	0
Cs	-1.222657	-1.809514	0

o-Clorophenylcesium
Optimized with idealized CsCC angle
ECP from Ross et al
E = -708.8673118 au

C	1.365941	1.210888	0
C	2.068871	2.407295	0
C	0.00000	1.041903	0
C	1.340969	3.585040	0
C	-.679598	2.281616	0
C	-.048098	3.517733	0
Cl	2.407811	-.275672	0
H	3.143570	2.421181	0
H	1.848559	4.534058	0
H	-1.761674	2.285567	0
H	-.628807	4.425765	0
Cs	-1.233145	-1.695400	0

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m-Chlorophenylcesium
ECP from Hay and Wadt
E = -708.5917285 au

C	2.202262	1.790610	0
C	1.408646	.653625	0
C	1.662173	3.062322	0
C	0.000000	.706907	
0			
C	.277125	3.164932	0
C	-.513449	2.021439	0
Cl	3.959436	1.618318	0
H	2.293070	3.931904	0
H	1.921128	-.296991	0
H	-.177197	4.143092	0
H	-1.585248	2.174669	0
Cs	-1.817867	-1.924783	0

m-Chlorophenylcesium
ECP from Ross et al
E = -708.8549564

C	2.281598	1.529112	0
C	1.397967	.460683	0
C	1.843953	2.839831	0
C	0.000000	.631387	0
C	.472253	3.056070	0
C	-.408532	1.980713	0
Cl	4.016914	1.216338	0
H	2.543035	3.655543	0
H	1.830008	-.529328	0
H	.099541	4.067845	0
H	-1.464860	2.218642	0
Cs	-1.905795	-1.692313	0

p-Chlorophenylcesium
ECP from Hay and Wadt
E = -708.5895518

C	0	0.00000	-3.207145
C	0	1.198482	-2.519193
C	0	-1.198482	-2.519193
C	0	1.174410	-1.126687
C	0	-1.174410	-1.126687
C	0	0.00000	-.345688
Cl	0	0.00000	-4.965607
H	0	2.129354	-3.059464
H	0	-2.129354	-3.059464
H	0	2.141217	-.638960
H	0	-2.141217	-.638960
Cs	0	0.00000	2.852359

p-Chlorophenylcesium
ECP from Ross et al
E = -708.8529454 au

C	0	0.00000	-3.108647
C	0	1.199011	-2.421401
C	0	-1.199011	-2.421401
C	0	1.175313	-1.029294
C	0	-1.175313	-1.029294
C	0	0.00000	-.251594
Cl	0	0.00000	-4.865865
H	0	2.129402	-2.962150
H	0	-2.129402	-2.962150
H	0	2.141448	-.540172
H	0	-2.141448	-.540172
Cs	0	0.00000	2.750802

2,3 Dichlorophenyl anion
E= -1147.8747166

C	1.233422	-1.490853	0
C	2.390205	-.682597	0
C	.057830	-.745654	0
C	2.377616	.705548	0
C	0.00000	.643772	0
C	1.168307	1.387552	0
H	3.357412	-1.166923	0
H	3.300189	1.267243	0
Cl	-1.514431	1.551541	0
H	1.122782	2.461296	0
Cl	-1.494079	-1.637908	0

2,4 Dichlorophenyl anion
E = -1147.8804255

C	-1.399007	-1.405463	0
C	-.156330	-2.084619	0
C	-1.206299	-.033701	0
C	1.094068	-1.477449	0
C	0.00000	.658761	0
C	1.155446	-.094104	0
H	-.161295	-3.166238	0
H	2.000771	-2.058838	0
H	.040080	1.731866	0
Cl	2.725528	.720902	0
Cl	-2.655341	1.050431	0

2,5 Dichlorophenyl anion
E = -1147.8831157 au

C	-1.352156	-.715401	0
C	-.114727	-1.339797	0
C	-1.221320	.694629	0
C	1.133428	-.734001	0
C	0.00000	1.341016	0
C	1.201281	.650966	0
Cl	-.053852	-3.149000	0
H	2.037718	-1.317248	0
Cl	.056636	3.117129	0
H	2.144295	1.166103	0
H	-2.108380	1.308485	0

2,6 Dichlorophenyl anion
E = -1147.888466

C	0	0.0000000	-.848091
C	0	1.135287	-.051964
C	0	-1.135287	-.051964
C	0	1.195799	1.332766
C	0	-1.195799	1.332766
C	0	0.00000	2.038055
Cl	0	2.752450	-.862491
Cl	0	-2.752450	-.862491
H	0	2.139002	1.849986
H	0	-2.139002	1.849986
H	0	0.00000	3.115319

3,4-Dichlorophenyl anion
E = -1147.8684211

C	2.518059	-.732806	0
C	2.402950	.677449	0
C	1.259078	-1.370102	0
C	1.202838	1.375428	0
C	.040614	-.699338	0
C	0	.684110	0
H	3.303051	1.277841	0
H	1.183876	2.452986	0
Cl	-1.449295	-1.645044	0
Cl	-1.505586	1.592610	0
H	1.204819	-2.447902	0

3,5-Dichlophenyl anion
E = -1147.8772953

C	0	.000000	2.206039
C	0	1.182547	1.430104
C	0	-1.182547	1.430104
C	0	1.169985	.047222
C	0	-1.169985	.047222
C	0	.000000	-.692582
H	0	2.145011	1.917126
H	0	-2.145011	1.917126
Cl	0	2.705638	-.849355
Cl	0	-2.705638	-.849355
H	0	.000000	-1.764838

2,3 Dichlorophenyllithium
Idealized LiCC angle
E = -1155.3508861

C	1.181609	1.327222	0
C	2.350087	.545574	0
C	0.00000	.619408	0
C	2.334053	-.838456	0
C	-.052128	-.775962	0
C	1.120588	-1.507755	0
Li	1.164060	3.320536	0
H	3.311715	1.034913	0
H	3.251975	-1.400843	0
Cl	-1.552609	-1.666690	0
H	1.075988	-2.580550	0
Cl	-1.549574	1.476378	0

2,4 Dichlorophenyllithium
Idealized LiCC angle
E = -1155.3560652

C	1.011125	-1.490852	0
C	-.310555	-1.980071	0
C	1.086202	-.117809	0
C	-1.435316	-1.172267	0
C	0.00000	.752398	0
C	-1.263240	.202433	0
Li	2.694922	-2.556596	0
H	-.476501	-3.045912	0
H	-2.424159	-1.593095	0
H	.134125	1.816787	0
Cl	-2.658999	1.254153	0
Cl	2.667968	.706378	0

2,5 Dichlorophenyllithium
Idealized LiCC angle
E = -1155.3576452

C	1.207728	.628501	0
C	1.098628	-.775688	0
C	0.00000	1.287111	0
C	-.121080	-1.422829	0
C	-1.245296	.669686	0
C	-1.309666	-.710890	0
Li	2.899424	1.684789	0
H	1.986789	-1.384325	0
Cl	-.177905	-3.173430	0
H	-2.148955	1.250516	0
H	-2.255967	-1.218219	0
Cl	-.061037	3.070037	0

2,6 Dichlorophenyllithium
Idealized LiCC angle
E = -1155.3659065

C	0	0.00000	-.687666
C	0	1.154924	.081976
C	0	-1.154924	.081976
C	0	1.201698	1.465027
C	0	-1.201698	1.465027
C	0	0.00000	2.158207
Li	0	0.00000	-2.678230
Cl	0	2.710986	-.781269
Cl	0	-2.710986	-.781269
H	0	2.139581	1.988530
H	0	-2.139581	1.988530
H	0	0.00000	3.233504

3,4 Dichlorophenyllithium
E = -1155.3422096

C	0.00000	.648353	0
C	1.333692	1.043294	0
C	-.322524	-.697418	0
C	2.405496	.140063	0
C	.702423	-1.631693	0
C	2.023197	-1.214052	0
Cl	-1.235368	1.879644	0
H	1.512204	2.105941	0
Cl	-1.970003	-1.259296	0
Li	4.298811	.760857	0
H	.453688	-2.677592	0
H	2.775282	-1.988119	0

3,5 Dichlorophenyllithium
E = -1155.3484843

C	0	0.00000	2.009265
C	0	1.187667	1.257882
C	0	-1.187667	1.257882
C	0	1.179000	-.126774
C	0	-1.179000	-.126774
C	0	0.000000	-.849114
Li	0	0.00000	4.004073
H	0	2.148125	1.745690
H	0	-2.148125	1.745690
Cl	0	2.696264	-1.003422
Cl	0	-2.696264	-1.003422
H	0	0.00000	-1.921438