Draft of June 6, 2002
prepared for *Journal of Organic Chemistry*

SUPPORTING INFORMATION FOR

Structures and Aggregation States of Fluoromethyllithium and Chloromethyllithium Carbenoids in the Gas Phase and in Ethereal Solvent

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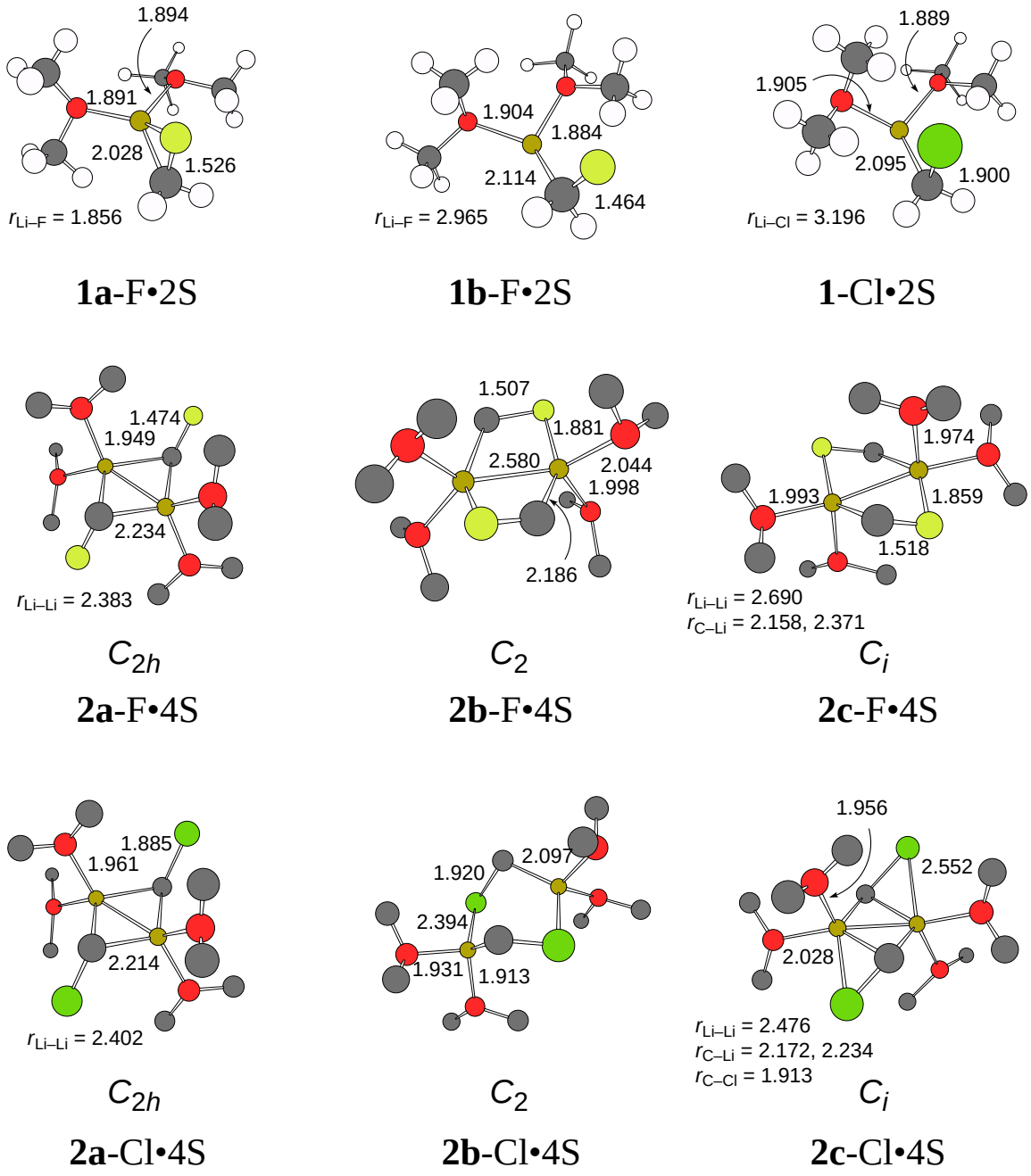
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Cartesian coordinates and electronic energies, all structures: S3



1a-F•2S **1b**-F•2S **1**-Cl•2S

2a-F•4S **2b**-F•4S **2c**-F•4S

2a-Cl•4S **2b**-Cl•4S **2c**-Cl•4S

Figure SI1. Microsolvated monomer and dimer relaxed stereostructures for fluoromethyllithium and chloromethyllithium carbenoids computed at the SM5.42/DFT/MIDI!6D level; molecular point groups and heavy-atom bond lengths (Å) are provided. For clarity, hydrogen atoms are not shown in the dimers. See legend to Figure 1 for other atoms.

Cartesian Coordinates

(note that all *structures are minima as characterized by positive definite Hessian matrices)*

Gas-phase optimizations

1-F (DFT/MG3S: -146.645 55)

Li	-1.452955	-.245069	.000000
F	.000000	.757482	.000000
C	.383616	-.743191	.000000
H	1.028584	-.811495	.878972
H	1.028584	-.811495	-.878972

1-Cl (DFT/MG3S: -507.049 51)

Li	-1.510727	-.902327	.000000
Cl	.000000	.713821	.000000
C	.406188	-1.155567	.000000
H	1.047525	-1.247288	.877636
H	1.047525	-1.247288	-.877636

2-F (DFT/MG3S: -293.363 55)

Li	.053822	1.152324	.000000
F	1.821328	1.381611	.000000
Li	-.053822	-1.152324	.000000
F	-1.821328	-1.381611	.000000
C	-1.821328	.126367	.000000
C	1.821328	-.126367	.000000
H	-2.445361	.349364	.870819
H	-2.445361	.349364	-.870819
H	2.445361	-.349364	.870819
H	2.445361	-.349364	-.870819

2-Cl (DFT/MG3S: -1014.161 52)

Li	-.157198	1.114157	.000000
Cl	1.820440	2.107011	.000000
Li	.157198	-1.114157	.000000
Cl	-1.820440	-2.107011	.000000
C	-1.820440	-.238103	.000000
C	1.820440	.238103	.000000
H	-2.440229	-.014961	.871362
H	-2.440229	-.014961	-.871362
H	2.440229	.014961	.871362
H	2.440229	.014961	-.871362

1a-F•2S
(DFT/MG3S//DFT/MIDIX6D: -456.760 42)

Li	.097193	.479330	-.166430
F	.974929	1.865550	-.834757
C	.698264	2.194794	.646378
H	1.713887	2.389155	1.052282
H	.215511	3.191873	.590204
O	1.254205	-1.029164	-.260315
O	-1.659247	-.284545	-.026530
C	-2.546663	-.792658	-1.026409
C	-2.360013	.474260	.980259
C	1.008833	-2.051002	.712059
C	2.613343	-.552582	-.213924
H	-3.291589	-1.473263	-.584386
H	-1.930035	-1.345637	-1.743324
H	-3.072532	.023650	-1.547567
H	-3.010092	1.233472	.517119
H	-1.569054	.981436	1.547900
H	-2.965656	-.190563	1.615548
H	2.926083	-.362218	.824489
H	2.592307	.395574	-.754677
H	3.299614	-1.275092	-.680087
H	1.551051	-2.977204	.465102
H	-.070604	-2.228436	.693067
H	1.302911	-1.717888	1.721012

1b-F•2S
(DFT/MG3S//DFT/MIDIX6D: -456.756 17)

Li	.014158	-.456920	-.443885
F	2.362618	-1.791947	.421101
C	1.238946	-2.108867	-.472325
H	1.720410	-2.408673	-1.431725
H	.837205	-3.067792	-.072848
O	.682507	1.249159	-.005506
O	-1.843192	-.038686	-.138625
C	-1.969601	.111460	1.289257
C	-2.832372	-.951025	-.642937
C	.253626	2.511152	-.520919
C	2.115898	1.176358	.172667
H	-2.926602	.589957	1.546639
H	-1.132330	.747275	1.590911
H	-1.897906	-.861586	1.800665
H	-2.709814	-1.953612	-.204548
H	-2.685384	-1.008593	-1.726335
H	-3.847018	-.579519	-.431216
H	2.633161	1.499485	-.745189
H	2.333645	.115886	.367260
H	2.430126	1.817940	1.010361
H	.474989	3.326105	.186424
H	-.828891	2.427397	-.664964
H	.738874	2.735760	-1.485094

1-Cl•2S

(DFT/MG3S//DFT/MIDIX6D: -817.163 30)

Li	-.166596	.221238	.860501
Cl	1.386315	-1.729976	-.529598
C	.819745	-1.490367	1.302749
H	1.789284	-1.526563	1.832429
H	.335912	-2.463027	1.507498
O	.779732	1.775504	.266123
O	-1.874172	.202041	-.001776
C	-3.117647	.677157	.526236
C	-2.024023	-1.102076	-.606835
C	2.179425	1.593814	.577686
C	.606948	1.782230	-1.167996
H	.988676	.843760	-1.598623
H	1.124507	2.643657	-1.616343
H	-.469551	1.852733	-1.346940
H	2.536508	.633582	.178451
H	2.261794	1.593065	1.668990
H	2.771679	2.424986	.164817
H	-1.011974	-1.430967	-.870132
H	-2.660235	-1.034161	-1.502387
H	-2.464372	-1.816118	.105509
H	-2.926941	1.669564	.949418
H	-3.501029	.008140	1.313620
H	-3.872989	.762318	-.270456

2a-F•4S

(DFT/MG3S//DFT/MIDIX6D: -913.554 30)

Li	1.169497	.000000	.000000
F	-.004375	1.428227	-2.509444
Li	-1.169497	.000000	.000000
F	.004375	-1.428227	2.509444
C	.001409	-.088523	1.875907
C	-.001409	.088523	-1.875907
H	-.870235	.417080	2.354399
H	.868055	.422367	2.357792
H	.870235	-.417080	-2.354399
H	-.868055	-.422367	-2.357792
O	2.544980	-1.385859	.098933
C	3.414203	-1.576368	-1.021546
C	2.073152	-2.632311	.639264
H	3.678506	-.572402	-1.366123
H	4.322854	-2.126139	-.727246
H	2.909436	-2.124909	-1.833726
H	1.350202	-2.350307	1.412282
H	1.581420	-3.237930	-.141024
H	2.906314	-3.211835	1.068374
O	-2.544980	1.385859	-.098933
C	-3.414203	1.576368	1.021546
C	-2.073152	2.632311	-.639264
H	-3.678506	.572402	1.366123
H	-4.322854	2.126139	.727246
H	-2.909436	2.124909	1.833726
H	-1.350202	2.350307	-1.412282
H	-1.581420	3.237930	.141024
H	-2.906314	3.211835	-1.068374
O	2.543549	1.387183	-.105903
C	2.067849	2.633466	-.643255
C	3.413772	1.577883	1.013802
H	1.343622	2.351214	-1.414973
H	2.898789	3.215449	-1.073335
H	1.576622	3.236781	.139140
H	3.678715	.573953	1.357985
H	4.321995	2.127973	.718776
H	2.909557	2.126148	1.826510
O	-2.543549	-1.387183	.105903
C	-2.067849	-2.633466	.643255
C	-3.413772	-1.577883	-1.013802
H	-1.343622	-2.351214	1.414973
H	-2.898789	-3.215449	1.073335
H	-1.576622	-3.236781	-.139140
H	-3.678715	-.573953	-1.357985
H	-4.321995	-2.127973	-.718776
H	-2.909557	-2.126148	-1.826510

2b-F•4S

(DFT/MG3S//DFT/MIDIX6D: -913.555 99)

Li	-.112324	1.279807	-.193811
F	1.709004	1.523834	-.499091
Li	.112324	-1.279807	-.193811
F	-1.709004	-1.523834	-.499091
C	-1.841492	-.017056	-.414671
C	1.841492	.017056	-.414671
H	-2.353499	.229018	-1.370278
H	-2.633465	.111397	.356227
H	2.353499	-.229018	-1.370278
H	2.633465	-.111397	.356227
O	-.550009	2.801087	-1.481121
C	.203523	3.969514	-1.123959
C	-.112324	2.303085	-2.754181
H	1.283766	3.767327	-1.163528
H	-.041152	4.813848	-1.788860
H	-.077775	4.204527	-.094319
H	.945960	2.011321	-2.701202
H	-.724542	1.419658	-2.962813
H	-.261769	3.052004	-3.548912
O	.550009	-2.801087	-1.481121
C	-.203523	-3.969514	-1.123959
C	.112324	-2.303085	-2.754181
H	-1.283766	-3.767327	-1.163528
H	.041152	-4.813848	-1.788860
H	.077775	-4.204527	-.094319
H	-.945960	-2.011321	-2.701202
H	.724542	-1.419658	-2.962813

H	.261769	-3.052004	-3.548912
O	-.193944	2.318758	1.554996
C	1.031747	2.234535	2.295486
C	-1.333835	2.236540	2.413047
H	1.059818	1.322474	2.914851
H	1.165258	3.114862	2.944757
H	1.809894	2.179860	1.533319
H	-1.350384	1.283951	2.967508
H	-1.347033	3.072258	3.132131
H	-2.216218	2.288859	1.769034
O	.193944	-2.318758	1.554996
C	-1.031747	-2.234535	2.295486
C	1.333835	-2.236540	2.413047
H	-1.059818	-1.322474	2.914851
H	-1.165258	-3.114862	2.944757
H	-1.809894	-2.179860	1.533319
H	1.350384	-1.283951	2.967508
H	1.347033	-3.072258	3.132131
H	2.216218	-2.288859	1.769034

2c-F•4S
(DFT/MG3S//DFT/MIDIX6D: -913.557 93)

Li	1.268422	-.237408	.128304
F	.712601	-1.711254	1.075544
Li	-1.268422	.237408	-.128304
F	-.712601	1.711254	-1.075544
C	.447689	.840763	-1.556446
C	-.447689	-.840763	1.556446
H	.070087	.476971	-2.537478
H	1.204558	1.610481	-1.825876
H	-.070087	-.476971	2.537478
H	-1.204558	-1.610481	1.825876
O	2.007345	1.246389	1.209781
C	2.823246	.987091	2.354857
C	1.030087	2.266189	1.470215
H	3.502707	.182102	2.059889
H	3.402422	1.880659	2.642193
H	2.215542	.661703	3.215045
H	.356660	2.256181	.608907
H	.456319	2.035335	2.381794
H	1.514527	3.250142	1.581834
O	-2.007345	-1.246389	-1.209781
C	-2.823246	-.987091	-2.354857
C	-1.030087	-2.266189	-1.470215
H	-3.502707	-.182102	-2.059889
H	-3.402422	-1.880659	-2.642193
H	-2.215542	-.661703	-3.215045
H	-.356660	-2.256181	-.608907
H	-.456319	-2.035335	-2.381794
H	-1.514527	-3.250142	-1.581834
O	3.151641	-.885553	-.238546
C	3.218703	-2.233624	-.715454
C	3.801931	.020625	-1.139170
H	2.664088	-2.837884	.007247
H	4.262736	-2.581651	-.776885
H	2.748813	-2.328086	-1.708996
H	3.631388	1.016922	-.723464
H	4.882296	-.191309	-1.197475
H	3.364527	-.033254	-2.148803
O	-3.151641	.885553	.238546
C	-3.218703	2.233624	.715454
C	-3.801931	-.020625	1.139170
H	-2.664088	2.837884	-.007247
H	-4.262736	2.581651	.776885
H	-2.748813	2.328086	1.708996
H	-3.631388	-1.016922	.723464
H	-4.882296	.191309	1.197475
H	-3.364527	.033254	2.148803

2a-Cl•4S
(DFT/MG3S//DFT/MIDIX6D: -1634.357 08)

Li	1.182535	.000000	.000000
Cl	-.004079	1.895659	-2.591200
Li	-1.182535	.000000	.000000
Cl	.004079	-1.895659	2.591200
C	.001056	-.161939	1.843817
C	-.001056	.161939	-1.843817
H	-.870322	.297954	2.349672
H	.870230	.301135	2.350592
H	.870322	-.297954	-2.349672
H	-.870230	-.301135	-2.350592
O	2.581907	-1.376346	-.177225
C	3.464635	-1.296020	-1.302757
C	2.188023	-2.730870	.097593
H	3.677586	-.231974	-1.438075
H	4.398802	-1.846445	-1.107399
H	2.993093	-1.699480	-2.213515
H	1.499592	-2.664949	.945901
H	1.681058	-3.179254	-.773320
H	3.063361	-3.346032	.360487
O	-2.581907	1.376346	.177225
C	-3.464635	1.296020	1.302757
C	-2.188023	2.730870	-.097593
H	-3.677586	.231974	1.438075
H	-4.398802	1.846445	1.107399
H	-2.993093	1.699480	2.213515
H	-1.499592	2.664949	-.945901
H	-1.681058	3.179254	.773320
H	-3.063361	3.346032	-.360487
O	2.578859	1.380791	.172223
C	2.174597	2.733916	-.094480
C	3.461188	1.300728	1.298150
H	1.487445	2.667777	-.943790
H	3.045285	3.357642	-.352585

H	1.663236	3.172733	.778747
H	3.680008	.237335	1.429044
H	4.392304	1.857397	1.105964
H	2.986624	1.697444	2.210302
O	-2.578859	-1.380791	-.172223
C	-2.174597	-2.733916	.094480
C	-3.461188	-1.300728	-1.298150
H	-1.487445	-2.667777	.943790
H	-3.045285	-3.357642	.352585
H	-1.663236	-3.172733	-.778747
H	-3.680008	-.237335	-1.429044
H	-4.392304	-1.857397	-1.105964
H	-2.986624	-1.697444	-2.210302

2b-Cl•4S
(DFT/MG3S//DFT/MIDIX6D: -1634.349 79)

Li	.070164	1.754995	-.237233
Cl	-2.066077	.764208	.047170
Li	-.070164	-1.754995	-.237233
Cl	2.066077	-.764208	.047170
C	1.630367	.716277	-1.125128
C	-1.630367	-.716277	-1.125128
H	2.634194	1.176668	-1.220333
H	1.467882	.171490	-2.076023
H	-2.634194	-1.176668	-1.220333
H	-1.467882	-.171490	-2.076023
O	.579055	2.575326	1.438537
C	-.285686	3.497101	2.109762
C	1.231361	1.684258	2.356072
H	-1.058266	2.967898	2.691599
H	.284183	4.157319	2.783713
H	-.762237	4.086581	1.321380
H	.502635	1.242088	3.056128
H	1.672991	.888851	1.747202
H	2.008194	2.211705	2.932203
O	-.579055	-2.575326	1.438537
C	.285686	-3.497101	2.109762
C	-1.231361	-1.684258	2.356072
H	1.058266	-2.967898	2.691599
H	-.284183	-4.157319	2.783713
H	.762237	-4.086581	1.321380
H	-.502635	-1.242088	3.056128
H	-1.672991	-.888851	1.747202
H	-2.008194	-2.211705	2.932203
O	-.389417	3.449932	-1.091645
C	-1.231361	3.246084	-2.237105
C	.819316	4.139373	-1.441065
H	-.683628	2.730442	-3.042444
H	-1.624440	4.202687	-2.615644
H	-2.045971	2.606832	-1.883517
H	1.369721	3.602426	-2.228702
H	.603045	5.166618	-1.775844
H	1.424844	4.157887	-.530270
O	.389417	-3.449932	-1.091645
C	1.231361	-3.246084	-2.237105
C	-.819316	-4.139373	-1.441065
H	.683628	-2.730442	-3.042444
H	1.624440	-4.202687	-2.615644
H	2.045971	-2.606832	-1.883517
H	-1.369721	-3.602426	-2.228702
H	-.603045	-5.166618	-1.775844
H	-1.424844	-4.157887	-.530270

2c-Cl•4S
(DFT/MG3S//DFT/MIDIX6D: -1634.357 36)

Li	1.218941	.000000	.000000
Cl	1.217954	2.356607	-.818601
Li	-1.218941	.000000	.000000
Cl	-1.217954	-2.356607	.818601
C	.046317	-1.065032	1.471339
C	-.046317	1.065032	-1.471339
H	-.429879	-.758352	2.421093
H	.877430	-1.729318	1.772585
H	.429879	.758352	-2.421093
H	-.877430	1.729318	-1.772585
O	2.032694	-1.351808	-1.172999
C	3.032193	-.905245	-2.096916
C	1.087018	-2.234779	-1.796603
H	3.677321	-.227963	-1.530064
H	3.620010	-1.753920	-2.482905
H	2.581888	-.362757	-2.943360
H	.324789	-2.446676	-1.040378
H	.614452	-1.754060	-2.667815
H	1.579650	-3.167332	-2.116083
O	-2.032694	1.351808	1.172999
C	-3.032193	.905245	2.096916
C	-1.087018	2.234779	1.796603
H	-3.677321	.227963	1.530064
H	-3.620010	1.753920	2.482905
H	-2.581888	.362757	2.943360
H	-.324789	2.446676	1.040378
H	-.614452	1.754060	2.667815
H	-1.579650	3.167332	2.116083
O	3.049672	.204956	.909002
C	3.322617	1.350056	1.724857
C	3.600471	-.984817	1.487933
H	2.864346	2.195818	1.206467
H	4.408145	1.512099	1.826210
H	2.880305	1.240764	2.729320
H	3.320871	-1.796406	.811935
H	4.698190	-.911851	1.560237
H	3.186010	-1.174297	2.491199
O	-3.049672	-.204956	-.909002
C	-3.322617	-1.350056	-1.724857
C	-3.600471	.984817	-1.487933

H	-2.864346	-2.195818	-1.206467
H	-4.408145	-1.512099	-1.826210
H	-2.880305	-1.240764	-2.729320
H	-3.320871	1.796406	-.811935
H	-4.698190	.911851	-1.560237
H	-3.186010	1.174297	-2.491199

Relaxed SCRF optimizations

1a-F•2S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -456.782 19)

Li	.145244	.505805	-.124200
F	1.157840	1.900847	-.812994
C	.946739	2.190661	.670526
H	1.983612	2.346501	1.047376
H	.502430	3.210887	.667961
O	1.122826	-1.108469	-.283986
O	-1.726474	.255847	-.232485
C	-2.506843	-.656241	-1.015446
C	-2.280751	.389397	1.090776
C	.714629	-2.165318	.597766
C	2.528926	-.831361	-.123320
H	-2.547175	-1.655623	-.548063
H	-2.029800	-.732665	-1.997410
H	-3.534370	-.280157	-1.138193
H	-3.284765	.838375	1.047359
H	-1.595682	1.044007	1.636614
H	-2.345661	-.593147	1.591202
H	2.782937	-.688688	.939192
H	2.704603	.100899	-.658016
H	3.134566	-1.650954	-.541187
H	1.250834	-3.098530	.366594
H	-.358614	-2.313281	.434617
H	.893781	-1.894520	1.651452

1b-F•2S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -456.782 48)

Li	.053989	-.490921	-.281130
F	2.707659	-1.664776	.327043
C	1.452624	-2.075299	-.305738
H	1.764651	-2.464784	-1.308755
H	1.167531	-3.011490	.238587
O	.633517	1.281260	-.013733
O	-1.824878	-.232290	-.112208
C	-2.175677	.012986	1.263690
C	-2.788256	-1.106088	-.727510
C	-.009185	2.472938	-.480489
C	2.058846	1.448884	.117147
H	-3.146321	.528478	1.329233
H	-1.386446	.653544	1.668350
H	-2.222377	-.926233	1.836311
H	-2.819077	-2.082640	-.220735
H	-2.477236	-1.245104	-1.767574
H	-3.789960	-.649716	-.702601
H	2.489157	1.853619	-.814271
H	2.456423	.450498	.301191
H	2.295321	2.132698	.948662
H	.093741	3.291548	.249256
H	-1.065496	2.214209	-.606524
H	.409977	2.798833	-1.446201

1-Cl•2S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -817.183 62)

Li	-.118278	-.306440	-.424224
C	1.595371	-1.440010	-.834737
H	1.591543	-2.529027	-.633825
Cl	2.933739	-.827827	.368230
H	2.102945	-1.334544	-1.813235
O	-1.943309	-.712102	-.057743
O	-.172927	1.544941	-.050955
C	-1.207243	2.398560	-.561352
C	1.059867	2.265790	.138275
C	-2.614535	-1.872158	-.579678
C	-2.267111	-.524746	1.333543
H	-1.977439	-1.403038	1.930761
H	-3.345240	-.339498	1.458734
H	-1.697218	.349803	1.659508
H	-2.307743	-2.782813	-.043451
H	-2.332916	-1.959405	-1.633338
H	-3.706272	-1.751718	-.499718
H	1.809686	1.520543	.408110
H	.949200	3.015852	.937829
H	1.363558	2.771167	-.792791
H	-2.083688	1.758147	-.699688
H	-.914143	2.844862	-1.524985
H	-1.439218	3.204726	.152120

2a-F•4S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -913.577 52)

Li	1.191558	.000000	.000000
F	.002258	1.356082	-2.575230
Li	-1.191558	.000000	.000000
F	-.002258	-1.356082	2.575230
C	-.000382	-.051417	1.888376
C	.000382	.051417	-1.888376
H	-.869455	.484909	2.341055
H	.869377	.482546	2.342449
H	.869455	-.484909	-2.341055
H	-.869377	-.482546	-2.342449
O	2.524874	-1.419041	.074862
C	3.441013	-1.623315	-1.008160
C	2.041472	-2.670119	.593734
H	3.732753	-.627376	-1.352214
H	4.330788	-2.177706	-.667536
H	2.967391	-2.175974	-1.835899
H	1.330111	-2.400348	1.375273
H	1.541234	-3.258053	-.195329
H	2.870457	-3.265630	1.010722
O	-2.524874	1.419041	-.074862
C	-3.441013	1.623315	1.008160
C	-2.041472	2.670119	-.593734
H	-3.732753	.627376	1.352214
H	-4.330788	2.177706	.667536
H	-2.967391	2.175974	1.835899
H	-1.330111	2.400348	-1.375273
H	-1.541234	3.258053	.195329
H	-2.870457	3.265630	-1.010722
O	2.527894	1.416363	-.074077
C	2.048540	2.667820	-.595748
C	3.441292	1.620023	1.011385
H	1.337056	2.398395	-1.377262
H	2.879610	3.260171	-1.013055
H	1.549157	3.258556	.191763
H	3.730580	.623891	1.356957
H	4.332859	2.172824	.672872
H	2.966145	2.173976	1.837369
O	-2.527894	-1.416363	.074077
C	-2.048540	-2.667820	.595748
C	-3.441292	-1.620023	-1.011385
H	-1.337056	-2.398395	1.377262
H	-2.879610	-3.260171	1.013055
H	-1.549157	-3.258556	-.191763
H	-3.730580	-.623891	-1.356957
H	-4.332859	-2.172824	-.672872
H	-2.966145	-2.173976	-1.837369

2b-F•4S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -913.578 68)

Li	-.035245	1.289427	-.215599
F	1.796949	1.427151	-.616638
Li	.035245	-1.289427	-.215599
F	-1.796949	-1.427151	-.616638
C	-1.823177	.078502	-.553740
C	1.823177	-.078502	-.553740
H	-2.237623	.356417	-1.549018
H	-2.666333	.279695	.147288
H	2.237623	-.356417	-1.549018
H	2.666333	-.279695	.147288
O	-.482907	2.873473	-1.426892
C	.235027	4.039705	-.995872
C	-.070922	2.515810	-2.755226
H	1.321688	3.884141	-1.074153
H	-.053139	4.922075	-1.590981
H	-.028615	4.189412	.054265
H	.995875	2.253886	-2.765158
H	-.661302	1.640216	-3.041830
H	-.264984	3.337422	-3.465137
O	.482907	-2.873473	-1.426892
C	-.235027	-4.039705	-.995872
C	.070922	-2.515810	-2.755226
H	-1.321688	-3.884141	-1.074153
H	.053139	-4.922075	-1.590981
H	.028615	-4.189412	.054265
H	-.995875	-2.253886	-2.765158
H	.661302	-1.640216	-3.041830
H	.264984	-3.337422	-3.465137
O	-.061870	2.180102	1.572553
C	1.175101	2.158417	2.300480
C	-1.175101	2.156282	2.473209
H	1.226267	1.282587	2.969404
H	1.295771	3.075777	2.900387
H	1.953557	2.084583	1.543033
H	-1.170498	1.239827	3.086437
H	-1.156000	3.034909	3.139381
H	-2.081792	2.174243	1.864235
O	.061870	-2.180102	1.572553
C	-1.175101	-2.158417	2.300480
C	1.175101	-2.156282	2.473209
H	-1.226267	-1.282587	2.969404
H	-1.295771	-3.075777	2.900387
H	-1.953557	-2.084583	1.543033
H	1.170498	-1.239827	3.086437
H	1.156000	-3.034909	3.139381
H	2.081792	-2.174243	1.864235

2c-F•4S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -913.581 01)

Li	1.314113	-.241155	.156110
F	.660292	-1.657319	1.167003
Li	-1.314113	.241155	-.156110
F	-.660292	1.657319	-1.167003

C	.513073	.781545	-1.567271
C	-.513073	-.781545	1.567271
H	.162274	.348589	-2.531638
H	1.266502	1.542954	-1.876562
H	-.162274	-.348589	2.531638
H	-1.266502	-1.542954	1.876562
O	1.975972	1.226884	1.297455
C	2.844261	1.115838	2.429563
C	1.051763	2.313402	1.459225
H	3.514279	.275555	2.224429
H	3.436536	2.037163	2.563624
H	2.276487	.916920	3.352795
H	.372648	2.255763	.608617
H	.480230	2.208592	2.396160
H	1.584635	3.279653	1.466101
O	-1.975972	-1.226884	-1.297455
C	-2.844261	-1.115838	-2.429563
C	-1.051763	-2.313402	-1.459225
H	-3.514279	-.275555	-2.224429
H	-3.436536	-2.037163	-2.563624
H	-2.276487	-.916920	-3.352795
H	-.372648	-2.255763	-.608617
H	-.480230	-2.208592	-2.396160
H	-1.584635	-3.279653	-1.466101
O	3.124598	-.953412	-.275257
C	3.141168	-2.222842	-.942153
C	3.884630	.008076	-1.023190
H	2.553528	-2.908902	-.326624
H	4.171683	-2.603523	-1.038361
H	2.687588	-2.147941	-1.944853
H	3.739240	.966437	-.520059
H	4.954051	-.262067	-1.030358
H	3.522675	.084664	-2.060923
O	-3.124598	.953412	.275257
C	-3.141168	2.222842	.942153
C	-3.884630	-.008076	1.023190
H	-2.553528	2.908902	.326624
H	-4.171683	2.603523	1.038361
H	-2.687588	2.147941	1.944853
H	-3.739240	-.966437	.520059
H	-4.954051	.262067	1.030358
H	-3.522675	-.084664	2.060923

2a-Cl•4S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -1634.373 95)

Li	1.200868	.000000	.000000
Cl	-.002639	1.805208	-2.679744
Li	-1.200868	.000000	.000000
Cl	.002639	-1.805208	2.679744
C	.001105	-.109613	1.857099
C	-.001105	.109613	-1.857099
H	-.871417	.378346	2.333359
H	.870942	.380958	2.335612
H	.871417	-.378346	-2.333359
H	-.870942	-.380958	-2.335612
O	2.555935	-1.406853	-.172170
C	3.499056	-1.361343	-1.252047
C	2.160487	-2.759817	.111186
H	3.728067	-.304637	-1.411414
H	4.418226	-1.909295	-.987979
H	3.075980	-1.792398	-2.173597
H	1.471938	-2.694103	.955422
H	1.660444	-3.216776	-.759481
H	3.036232	-3.371358	.383822
O	-2.555935	1.406853	.172170
C	-3.499056	1.361343	1.252047
C	-2.160487	2.759817	-.111186
H	-3.728067	.304637	1.411414
H	-4.418226	1.909295	.987979
H	-3.075980	1.792398	2.173597
H	-1.471938	2.694103	-.955422
H	-1.660444	3.216776	.759481
H	-3.036232	3.371358	-.383822
O	2.557231	1.405674	.166871
C	2.163894	2.758866	-.118302
C	3.501895	1.360172	1.245409
H	1.472954	2.692918	-.960549
H	3.040204	3.367978	-.394538
H	1.667152	3.218687	.752748
H	3.728378	.303246	1.406944
H	4.422156	1.904976	.978639
H	3.081366	1.794590	2.166544
O	-2.557231	-1.405674	-.166871
C	-2.163894	-2.758866	.118302
C	-3.501895	-1.360172	-1.245409
H	-1.472954	-2.692918	.960549
H	-3.040204	-3.367978	.394538
H	-1.667152	-3.218687	-.752748
H	-3.728378	-.303246	-1.406944
H	-4.422156	-1.904976	-.978639
H	-3.081366	-1.794590	-2.166544

2b-Cl•4S (SM5.42/DFT/MG3S// DFT/MIDIX6D: -1634.372 11)

Li	-.494021	1.771638	-.286089
Cl	-2.188265	.081266	-.224092
Li	.494021	-1.771638	-.286089
Cl	2.188265	-.081266	-.224092
C	1.288726	1.258416	-1.264020
C	-1.288726	-1.258416	-1.264020
H	2.110809	1.993148	-1.389516
H	1.216228	.743423	-2.242085
H	-2.110809	-1.993148	-1.389516
H	-1.216228	-.743423	-2.242085

O	-.250733	2.491424	1.469962
C	-1.288726	3.124431	2.228618
C	.733504	1.899805	2.331634
H	-1.801597	2.400137	2.882495
H	-.881730	3.942133	2.846266
H	-1.995704	3.526126	1.498327
H	.254359	1.246324	3.081097
H	1.383454	1.301996	1.690702
H	1.314491	2.676999	2.855240
O	.250733	-2.491424	1.469962
C	1.288726	-3.124431	2.228618
C	-.733504	-1.899805	2.331634
H	1.801597	-2.400137	2.882495
H	.881730	-3.942133	2.846266
H	1.995704	-3.526126	1.498327
H	-.254359	-1.246324	3.081097
H	-1.383454	-1.301996	1.690702
H	-1.314491	-2.676999	2.855240
O	-1.450183	3.292681	-.994833
C	-2.300216	3.154191	-2.142135
C	-.621329	4.459253	-1.106494
H	-1.709784	3.095125	-3.070622
H	-3.002284	4.001748	-2.212638
H	-2.850787	2.221590	-1.998633
H	.004104	4.419885	-2.011322
H	-1.236293	5.374365	-1.126914
H	.019872	4.456955	-.221212
O	1.450183	-3.292681	-.994833
C	2.300216	-3.154191	-2.142135
C	.621329	-4.459253	-1.106494
H	1.709784	-3.095125	-3.070622
H	3.002284	-4.001748	-2.212638
H	2.850787	-2.221590	-1.998633
H	-.004104	-4.419885	-2.011322
H	1.236293	-5.374365	-1.126914
H	-.019872	-4.456955	-.221212
H	3.746649	-.264185	-1.521608
H	3.730437	-1.878929	-2.311916
H	2.729414	-.542285	-2.971357
H	.397664	-2.492475	-1.000175
H	.737464	-1.916741	-2.664517
H	1.719360	-3.246630	-1.959705
O	-2.072198	1.348310	1.144655
C	-3.126851	.994299	2.049141
C	-1.183046	2.309338	1.736089
H	-3.746649	.264185	1.521608
H	-3.730437	1.878929	2.311916
H	-2.729414	.542285	2.971357
H	-.397664	2.492475	1.000175
H	-.737464	1.916741	2.664517
H	-1.719360	3.246630	1.959705
O	2.992288	.325405	.964184
C	3.207332	1.480377	1.786731
C	3.655461	-.815616	1.526541
H	2.708276	2.310454	1.283283
H	4.284390	1.697175	1.882209
H	2.779222	1.338441	2.793253
H	3.423609	-1.654305	.867110
H	4.745875	-.652984	1.562350
H	3.292364	-1.030652	2.544460
O	-2.992288	-.325405	-.964184
C	-3.207332	-1.480377	-1.786731
C	-3.655461	.815616	-1.526541
H	-2.708276	-2.310454	-1.283283
H	-4.284390	-1.697175	-1.882209
H	-2.779222	-1.338441	-2.793253
H	-3.423609	1.654305	-.867110
H	-4.745875	.652984	-1.562350
H	-3.292364	1.030652	-2.544460

2c-Cl•4S (SM5.42/DFT/MG3S//
DFT/MIDIX6D: -1634.370 74)

Li	1.237889	.000000	.000000
Cl	1.164296	2.384549	-.905091
Li	-1.237889	.000000	.000000
Cl	-1.164296	-2.384549	.905091
C	.054934	-1.035136	1.499071
C	-.054934	1.035136	-1.499071
H	-.432855	-.688378	2.429005
H	.907888	-1.651548	1.838819
H	.432855	.688378	-2.429005
H	-.907888	1.651548	-1.838819
O	2.072198	-1.348310	-1.144655
C	3.126851	-.994299	-2.049141
C	1.183046	-2.309338	-1.736089