Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Anti-electrostatic Cation···π-Hole and Cation···lp-Hole Interactions Are Stabilized via Collective Interactions

Ricardo Pino-Rios[1,2*], Rodrigo Báez-Grez[3], Cina Foroutan-Nejad[4*]

1. Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat. Casilla 121, Iquique 1100000, Chile. rpinorios@unap.cl.

2. Instituto de Estudios de la Salud, Universidad Arturo Prat. Iquique, 1100000. Chile.

3. Departamento de Química, Facultad de Ciencias Exactas, Universidad Andres Bello, Av. República 275, Santiago, Chile, 8370146

4. Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224, Warsaw, Poland

Corresponding authors' e-mails:

RPR: rpinorios@unap.cl

CFN: cina.foroutan-nejad@icho.edu.pl

Computational Methods

All structures were optimized at the closed-shell and broken symmetry M06-2X[1]/def2TZVPP[2] computational levels. Single-point calculations were carried out at the same DFT level to obtain electrostatic potential maps using the Gaussian 16 software package.[3] The electrostatic potential cubes were produced using the Gaussian cubegen utility. The electron density cube files with the same grid were produced using the MultiWFN program.[4] The electrostatic potential values were plotted at different electron density isosurfaces for a qualitative study of the collective bonds. The reason for plotting ESPs at different isodensity values and color codes is that our molecules have diverse molecular charges from –1 to +1. It is needless to say that one cannot use the same isodensity values and color codes for cations and anions. Nevertheless, we found the M and A atoms in MAX_3 species are always the most positive parts of the molecules but the negative potential was found to be rather dispersed. The nature of bonding in the target systems was further analyzed within the context of the independent gradient model (IGM)[5,6] via MultiWFN. IGM has an interpretation analogous to the well-known non-covalent interaction index (NCI)[7] but with the advantage that the surfaces are smoother than NCI and allow separation into fragments.[8,9] In this case, the fragments for the MAX_3 systems were M and AX_3 since the intention is to evaluate the existence of collective bonds. The isodensity, minimum, and maximum values for IGM plots are listed in Table S8. In a complementary way, quantification was carried out using the recently proposed intrinsic bond strength index (IBSI)[10], which through a scale allows to evaluate the interaction between two atoms within a molecule. The figures were obtained using the Chemcraft program.[11]

References

1 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.
2 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
3 T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007–1023.
4 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.
5 C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García and E. Hénon, *Phys. Chem. Chem. Phys.*, 2017, **19**, 17928–17936.
6 C. Lefebvre, H. Khartabil, J.-C. Boisson, J. Contreras-García, J.-P. Piquemal and E. Hénon, *ChemPhysChem*, 2018, **19**, 724–735.
7 E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen and W. Yang, *J. Am. Chem. Soc.*, 2010, **132**, 6498–6506.
8 R. Báez-Grez and R. Pino-Rios, *ACS Omega*, 2023, **8**, 23168–23173.
9 M. Ponce-Vargas, C. Lefebvre, J.-C. Boisson and E. Hénon, *J. Chem. Inf. Model.*, 2020, **60**, 268–278.
10 J. Klein, H. Khartabil, J.-C. Boisson, J. Contreras-García, J.-P. Piquemal and E. Hénon, *J. Phys. Chem. A*, 2020, **124**, 1850–1860.
11 G. A. Andrienko, Chemcraft - graphical software for visualization of quantum chemistry computations. Version 1.8, build 654. https://www.chemcraftprog.com (version 1.8)

Chemcraft - graphical software for visualization of quantum chemistry computations. Version 1.8, build 654. https://www.chemcraftprog.com.

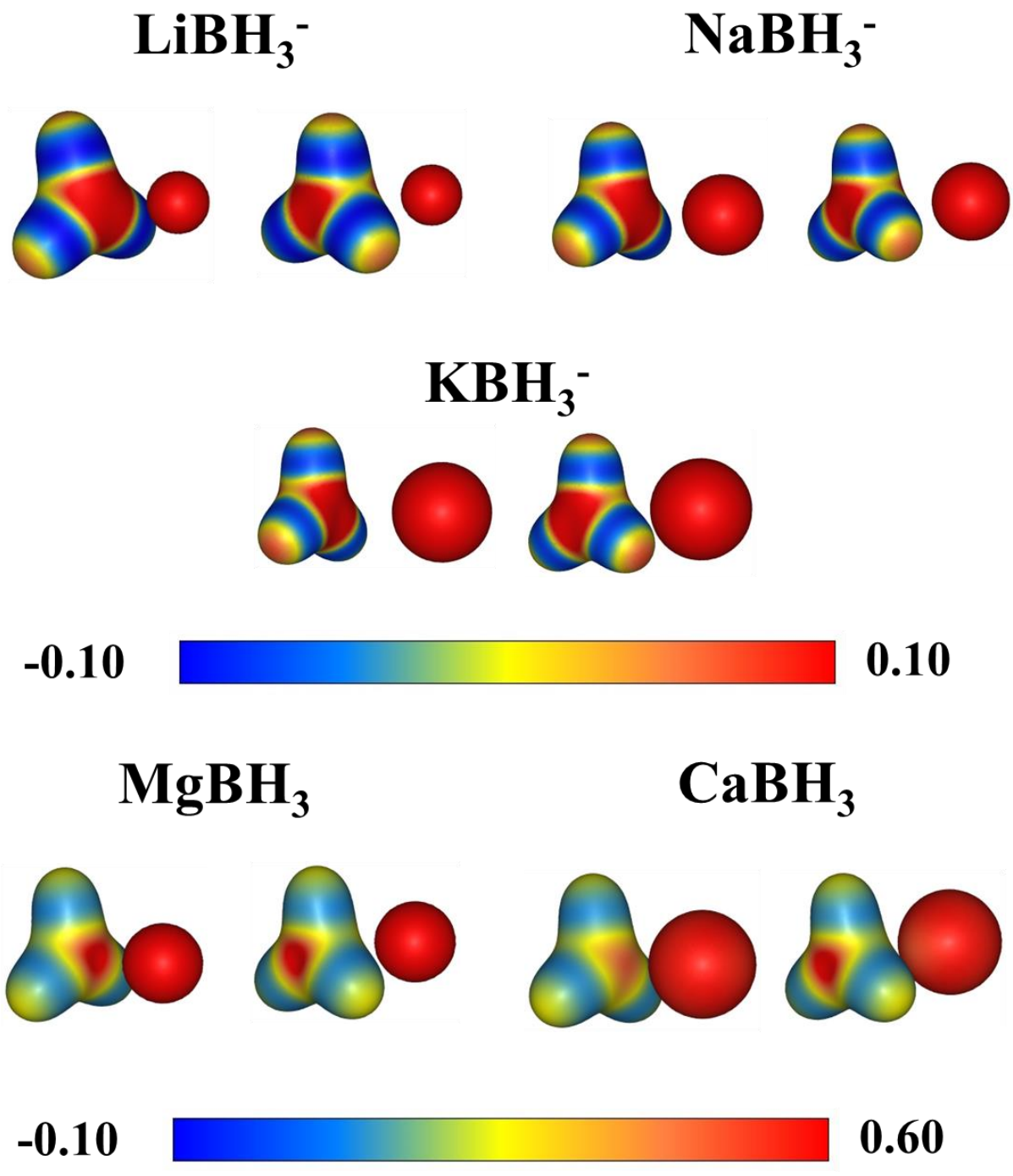

Figure S1. The electrostatic potential maps (in a.u) of $(M^{n+}BH_3)^{n-2}$ (M = Li, Na, K, Mg and Ca).

Density isovalue: 0.05 a.u.

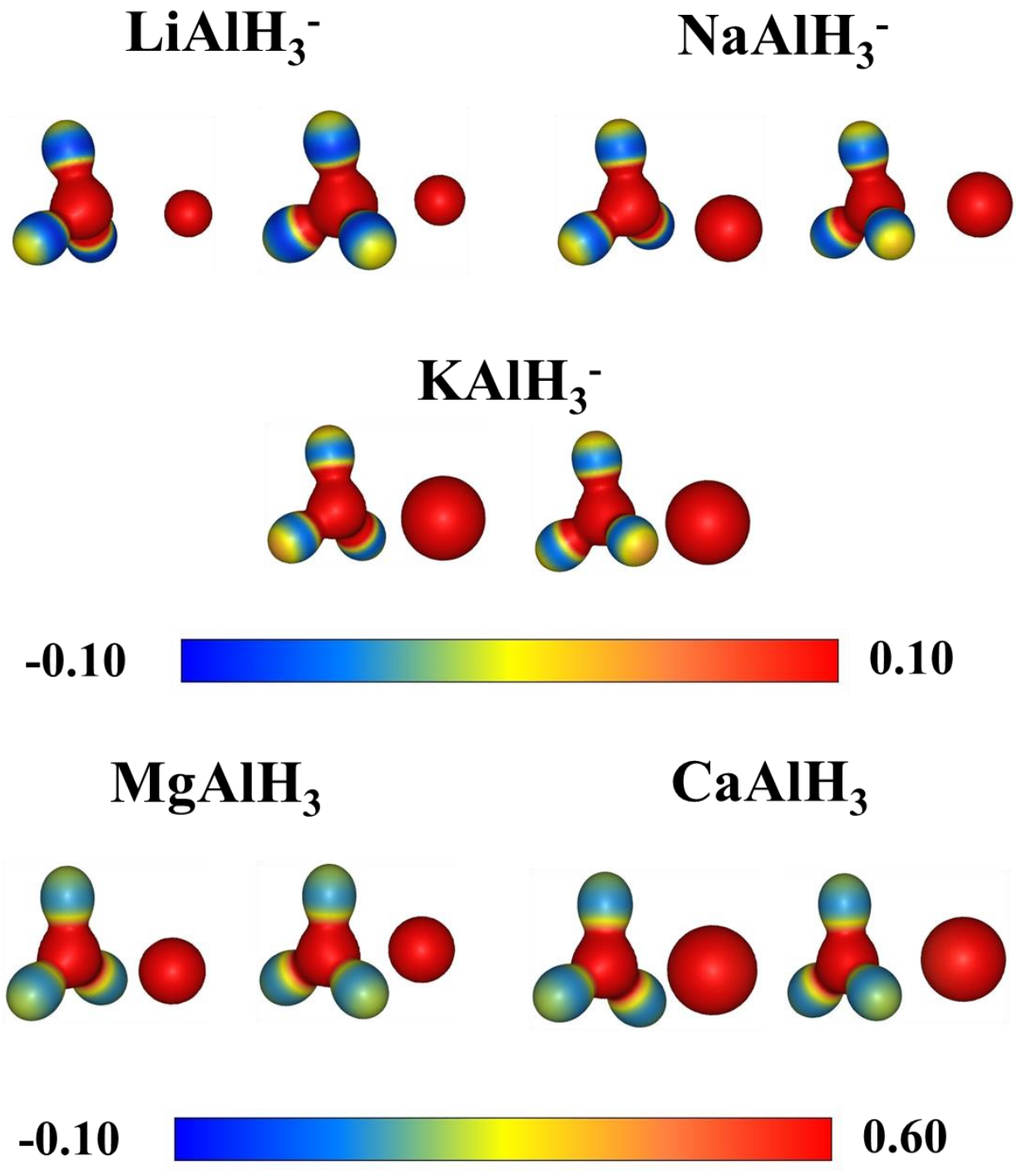

Figure S2. Electrostatic potential maps (in a.u) of $(M^{n+}AlH_3)^{n-2}$ (M = Li, Na, K, Mg and Ca). Density isovalue: 0.05 a.u.

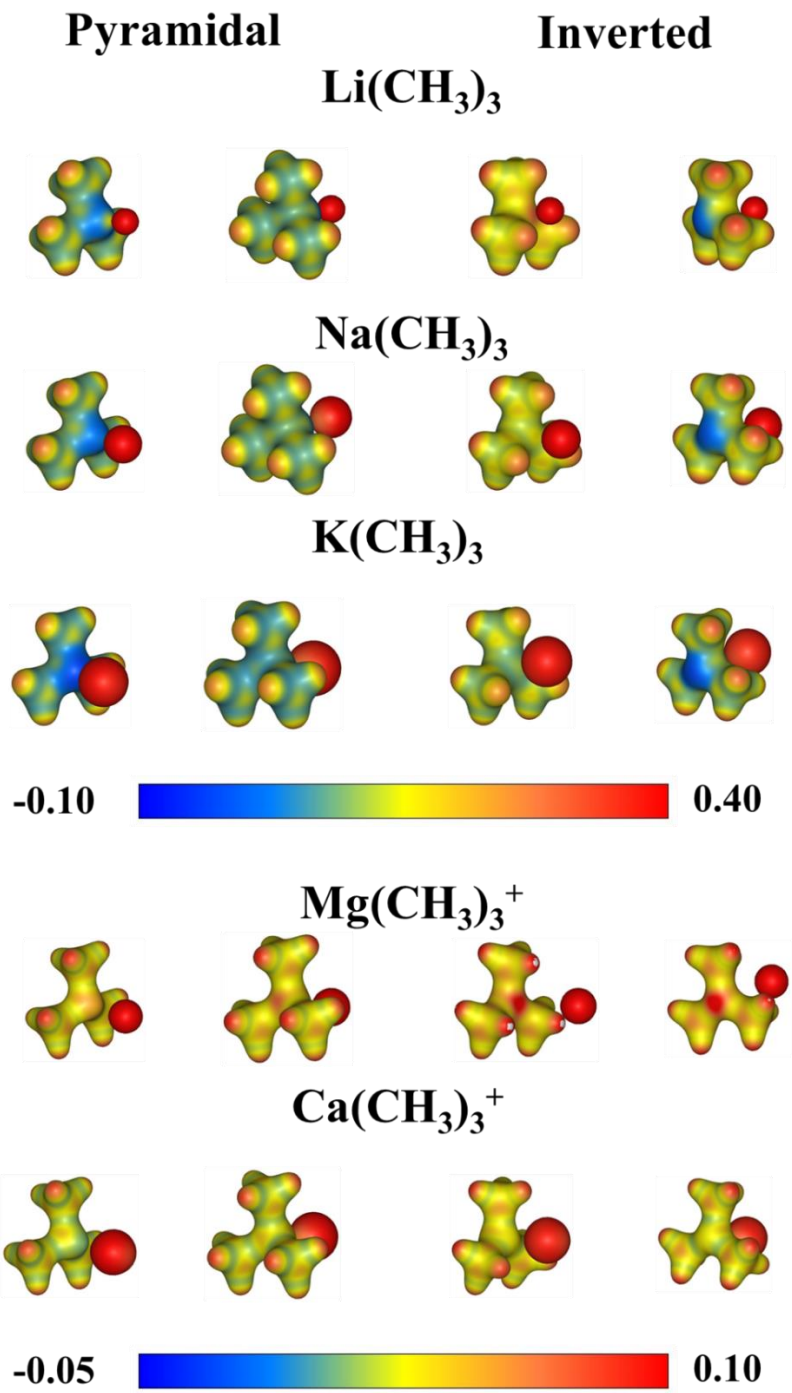
Pyramidal
Inverted
Li(CH3)3
Na(CH3)3
K(CH3)3
-0.10
0.40
Mg(CH3)3+
Ca(CH3)3+
-0.05
0.10

Figure S3. Electrostatic potential maps (in a.u) of pyramidal and inverted $(M^{n+}C(CH_3)_3)^{n-1}$ structures (M = Li, Na, K, Mg and Ca). Density isovalues: 0.05 a.u. (for M = Li, Na, K) and 0.10 (For M = Mg, Ca)

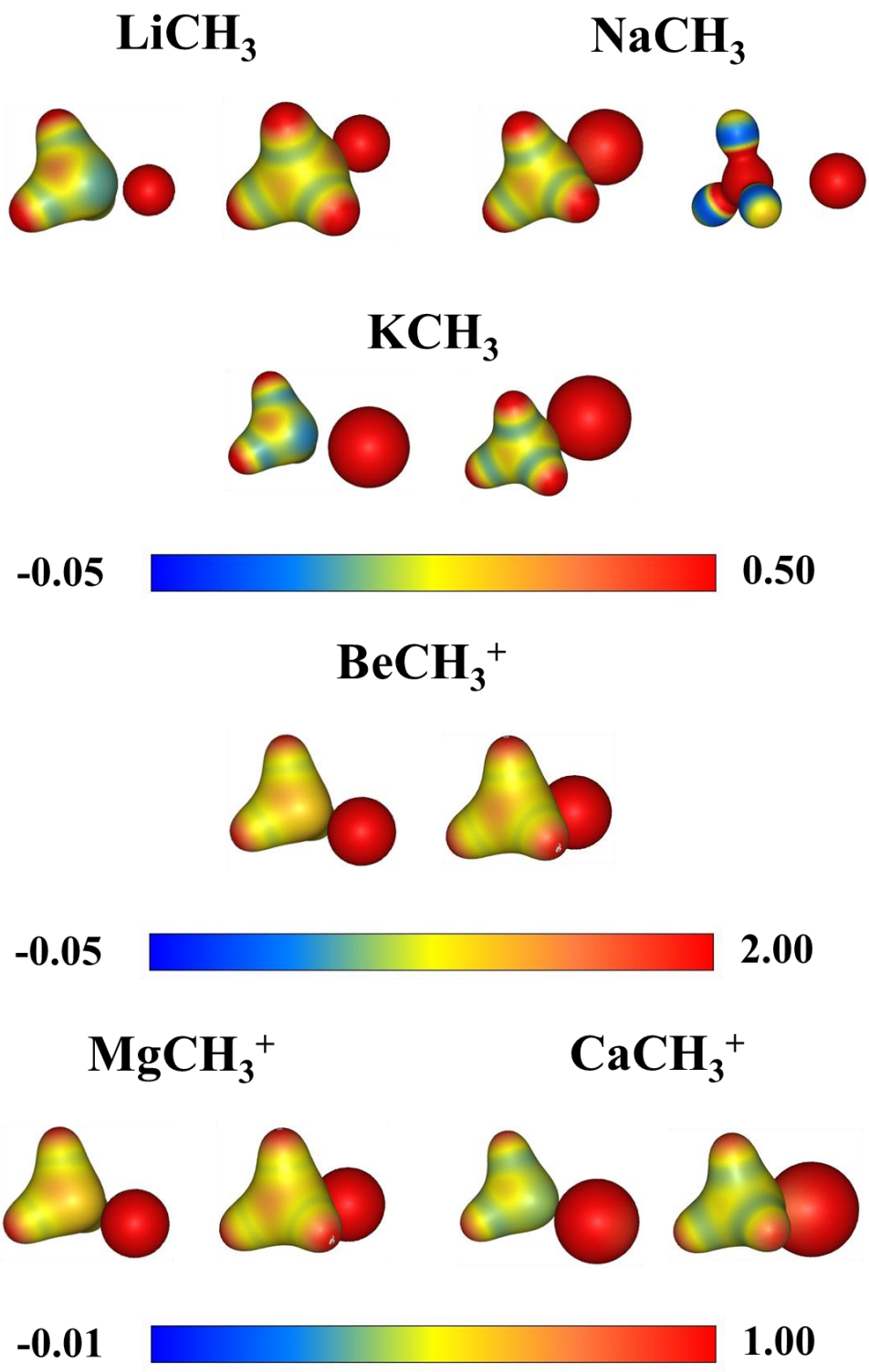

Figure S4. Electrostatic potential maps (in a.u) of $(M^{n+}CH_3)^{n-1}$ (M = Li, Na, K, Be, Mg, and Ca). Density isovalue: 0.10 a.u.

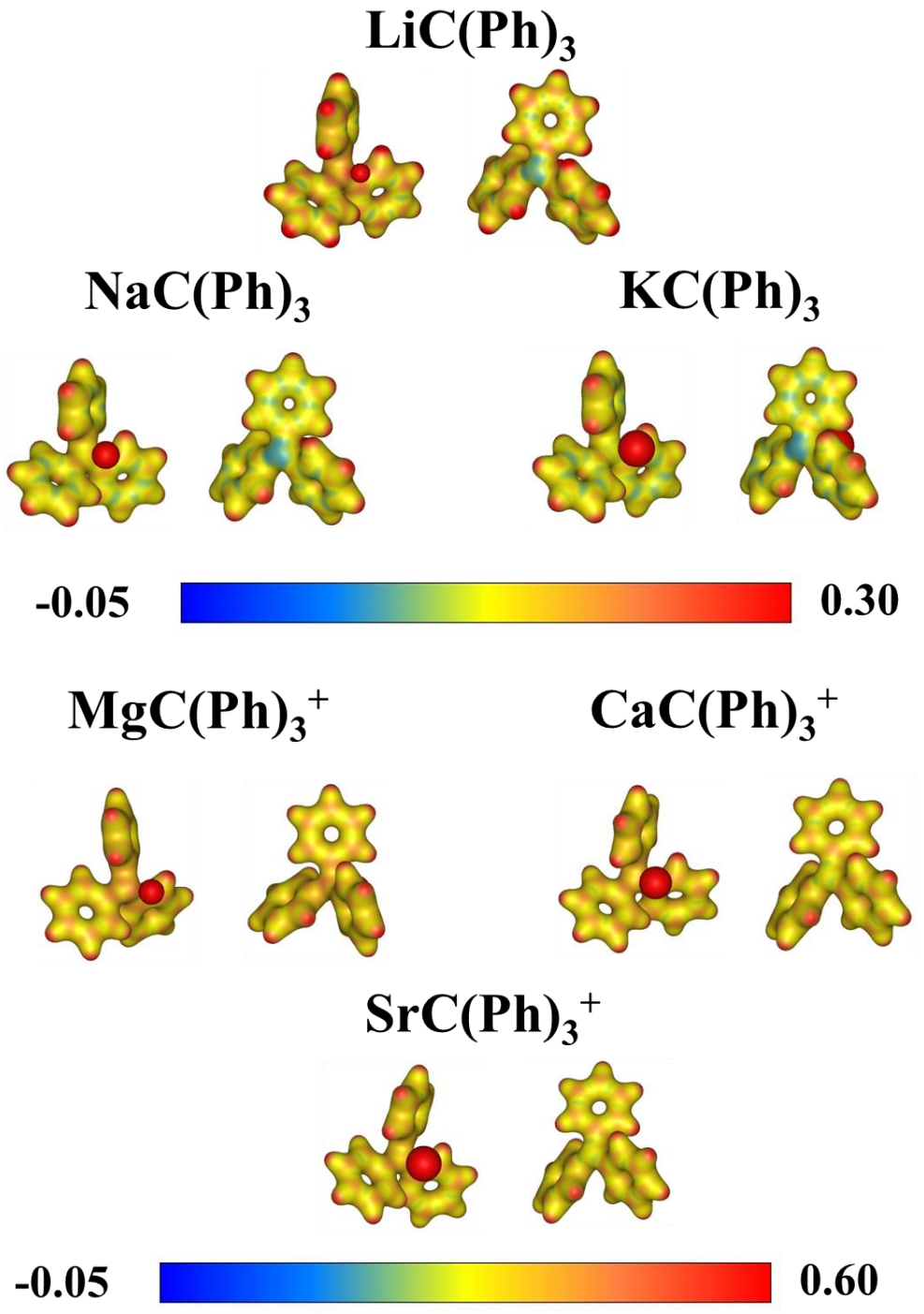

Figure S5. Electrostatic potential maps (in a.u) of $(M^{n+}C(Ph)_3)^{n-1}$ (M = Li, Na, K, Mg, Ca and Sr). Density isovalues: 0.05 a.u. (for M = Li, Na, K) and 0.06 (For M = Mg, Ca and Sr)

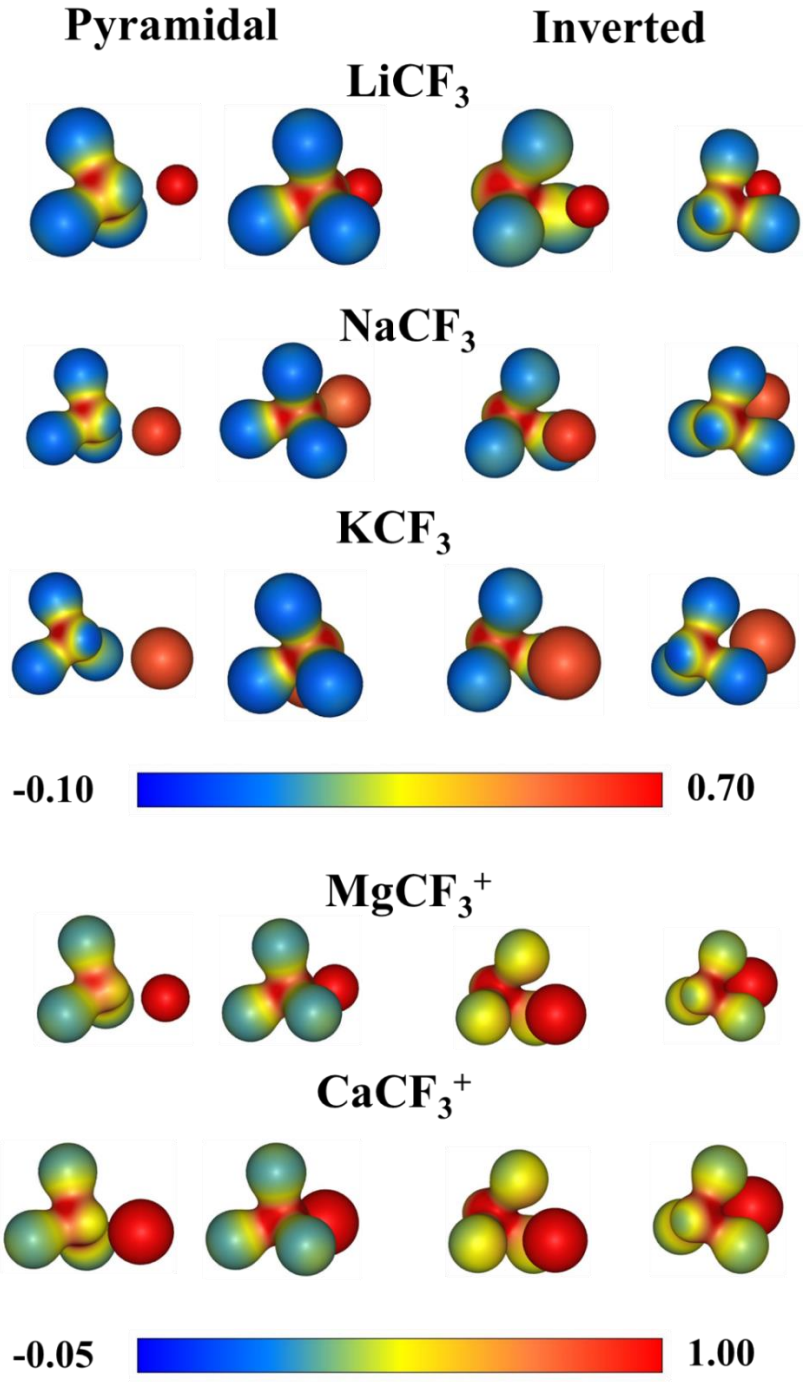

Figure S6. Electrostatic potential maps (in a.u) of pyramidal and inverted $(M^{n+}CF_3)^{n-1}$ structures (M = Li, Na, Mg and Ca). Density isovalue: 0.10 a.u.

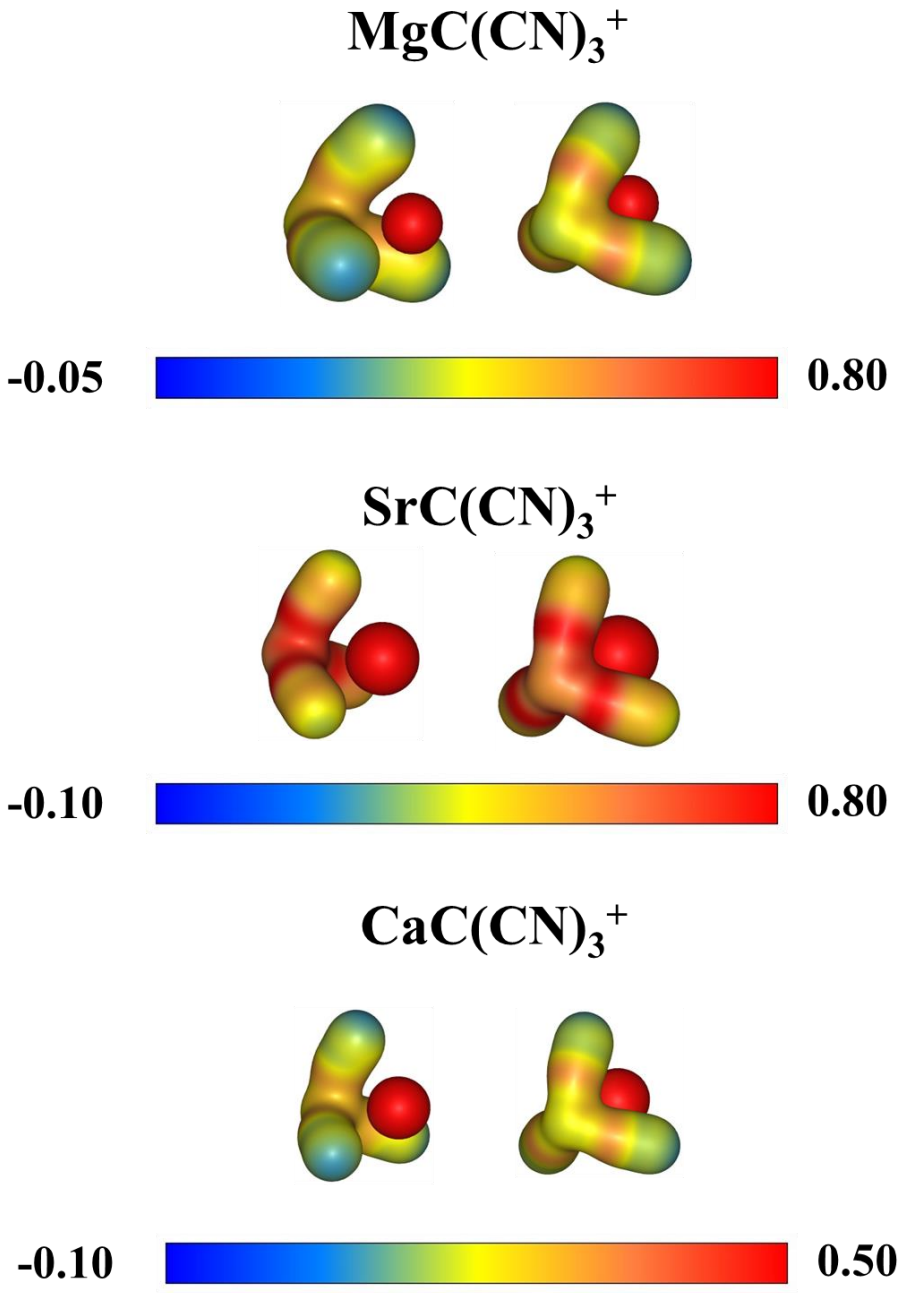

Figure S7. Electrostatic potential maps (in a.u) of $(MC(CN)_3)^+$ structures (M = Mg, Ca and Sr). Density isovalue: 0.05 a.u.

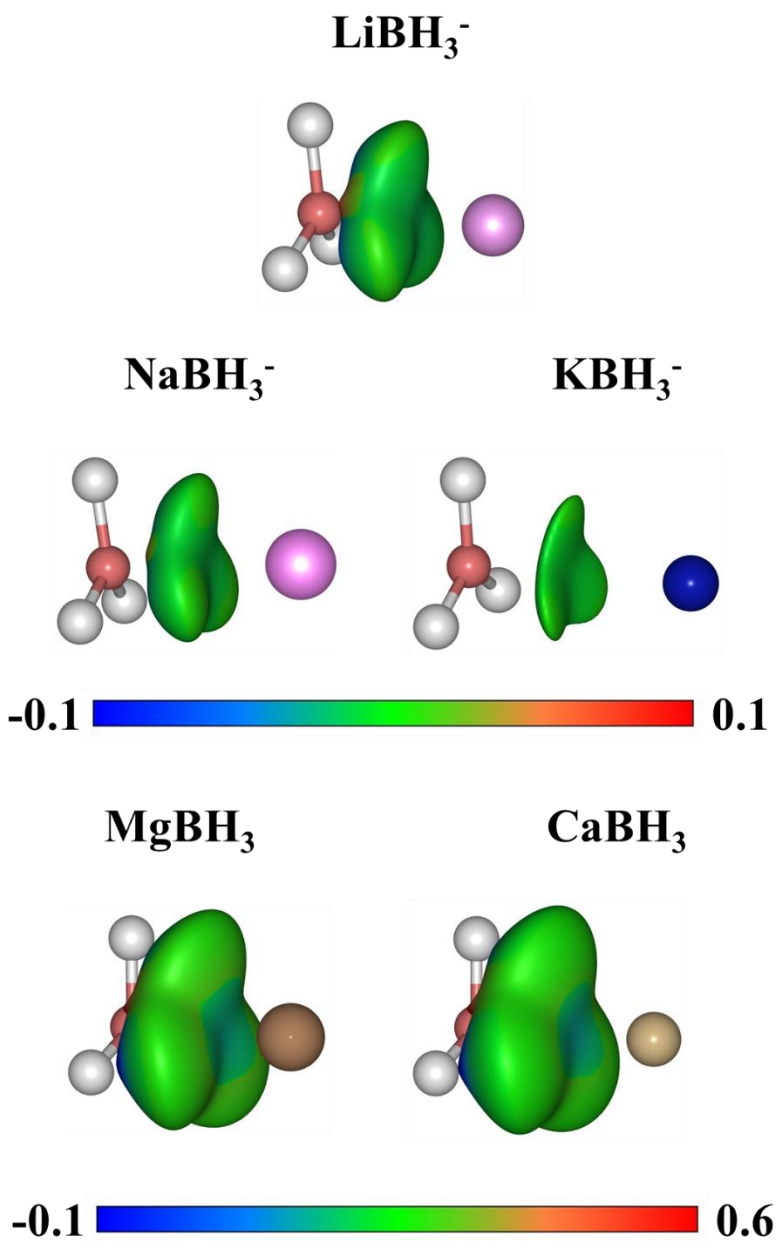

Figure S8. IGM plots (in a.u.) for $(M^{n+}BH_3)^{n-2}$ (M = Li, Na, K, Mg and Ca). Isovalue for δg^{inter} = 0.05.

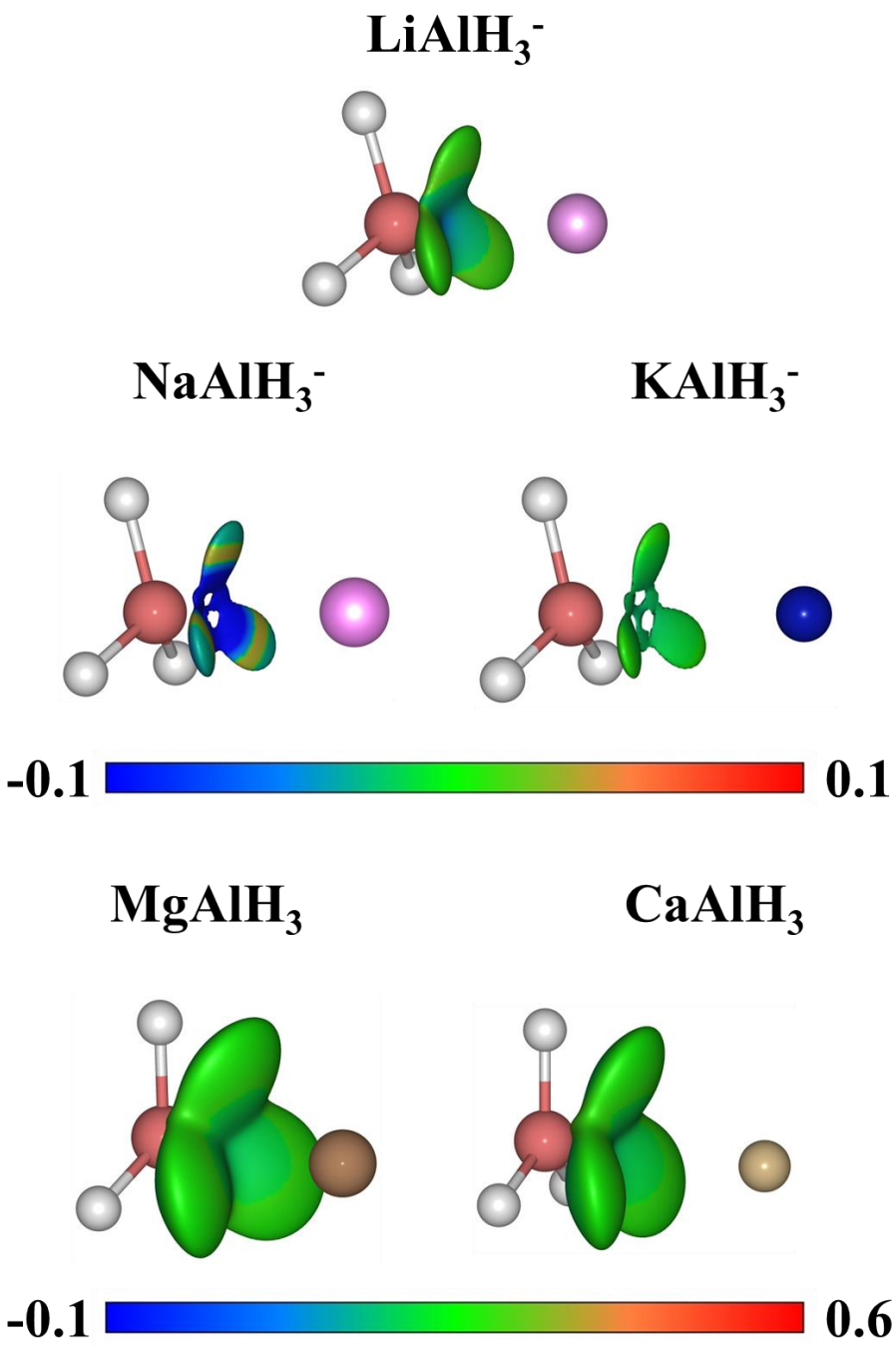

Figure S9. IGM plots (in a.u) for $(M^{n+}AlH_3)^{n-2}$ (M = Li, Na, K, Mg and Ca). Isovalue for δg^{inter} = 0.05.

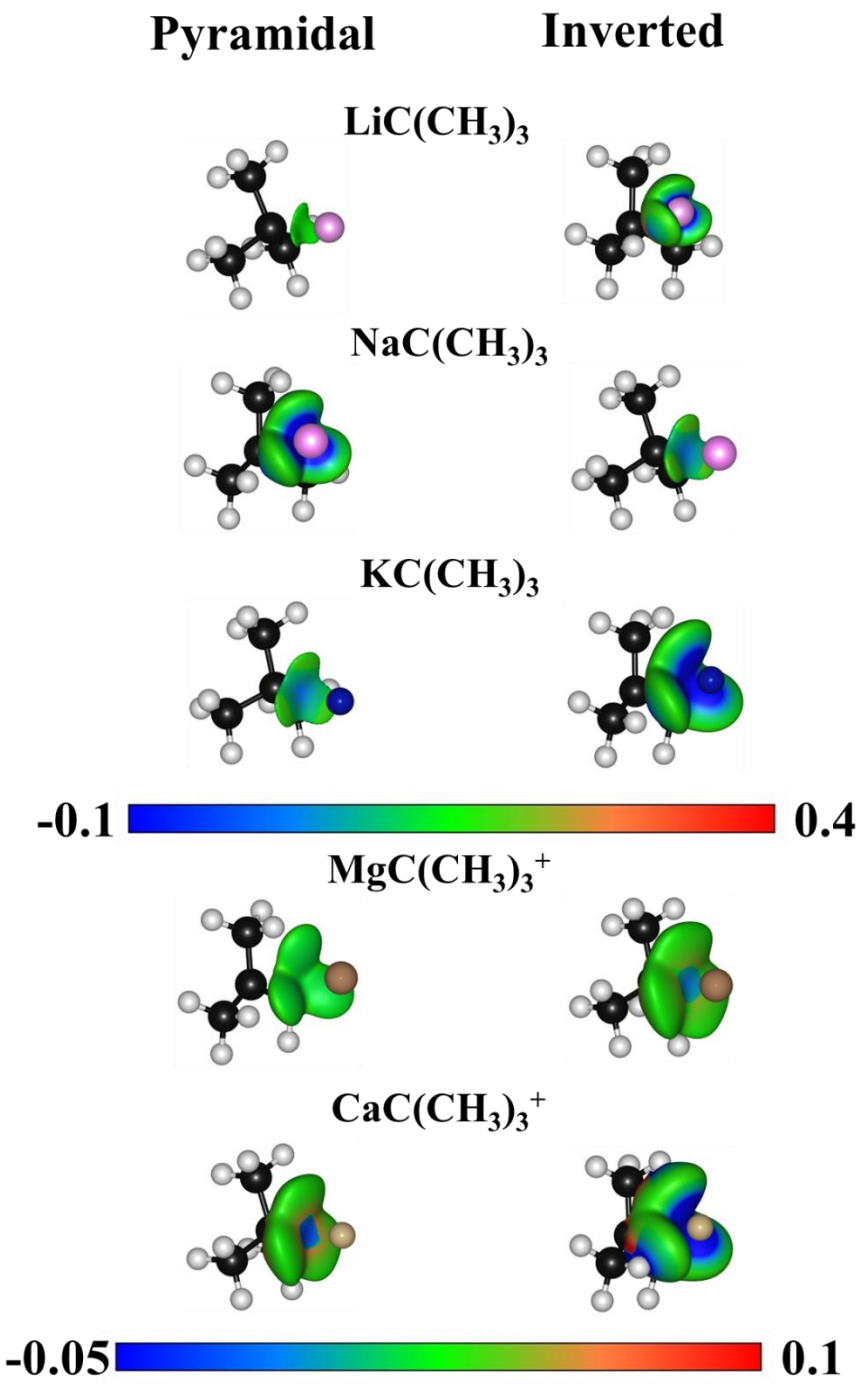

Figure S10. IGM plots (in a.u.) for pyramidal and inverted $(M^{n+}C(CH_3)_3)^{n-1}$ structures (M = Li, Na, K, Mg and Ca). Isovalue for $\delta g^{inter} = 0.1$.

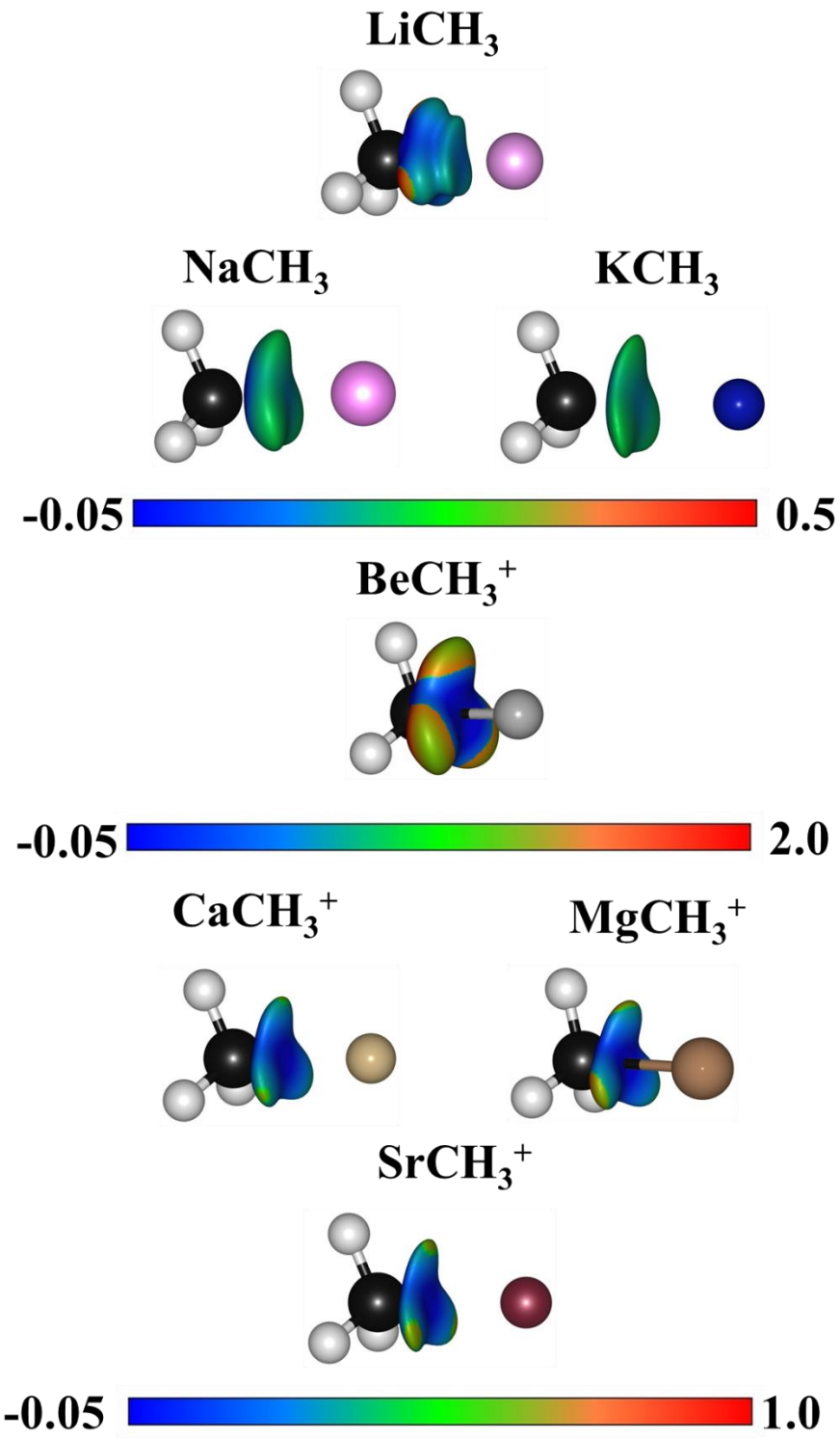

Figure S11. IGM plots (in a.u.) for $(M^{n+}CH_3)^{n-1}$ (M = Li, Na, K, Be, Mg, Ca and Sr). Isovalue for $\delta g^{inter} = 0.1$.

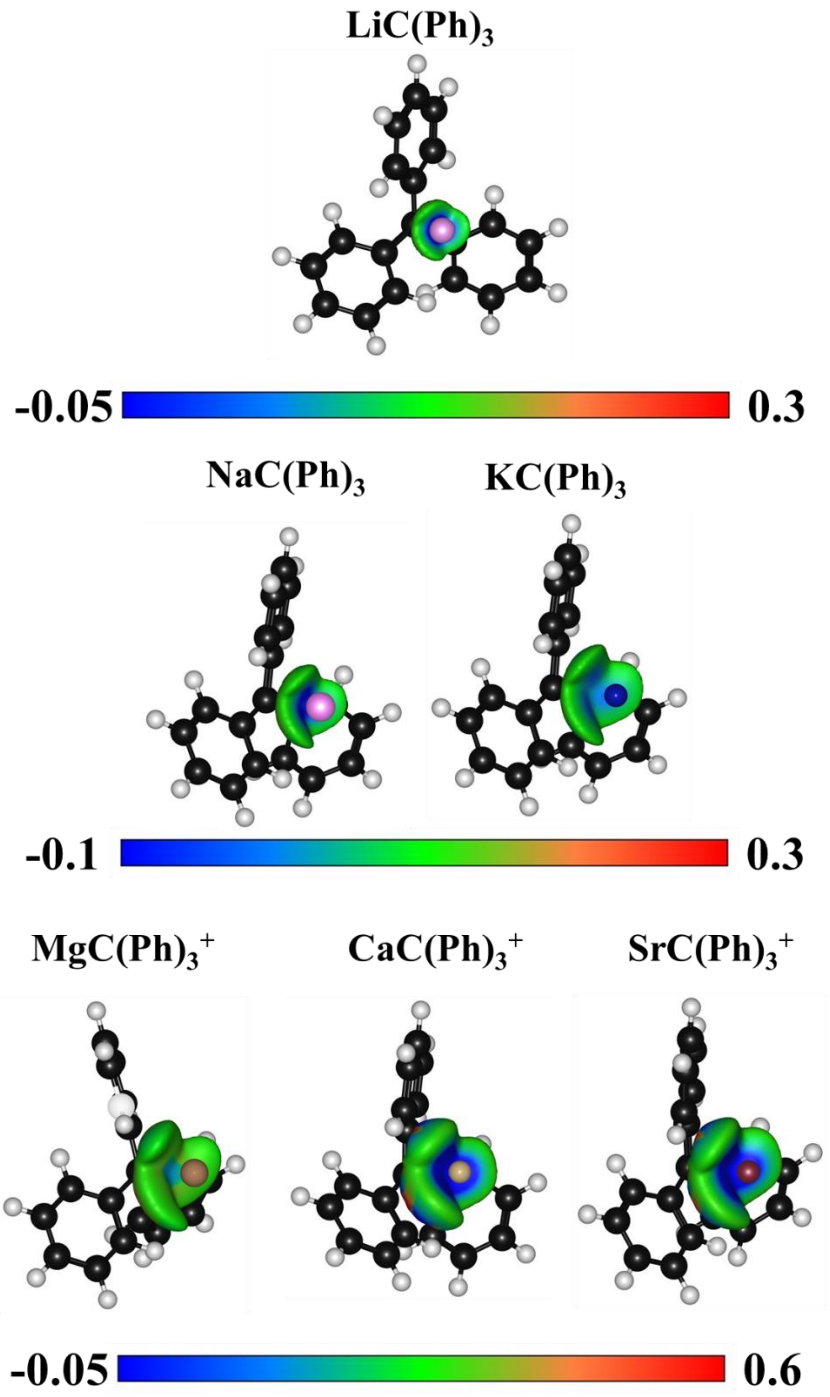

Figure S12. IGM plots (in a.u.) for $(M^{n+}C(Ph)_3)^{n-1}$ (M = Li, Na, K, Mg, Ca and Sr). Isovalues for δg^{inter} = 0.05 (M = Li), 0.04 (M = Na, K) and 0.06 (M = Mg, Ca, Sr).

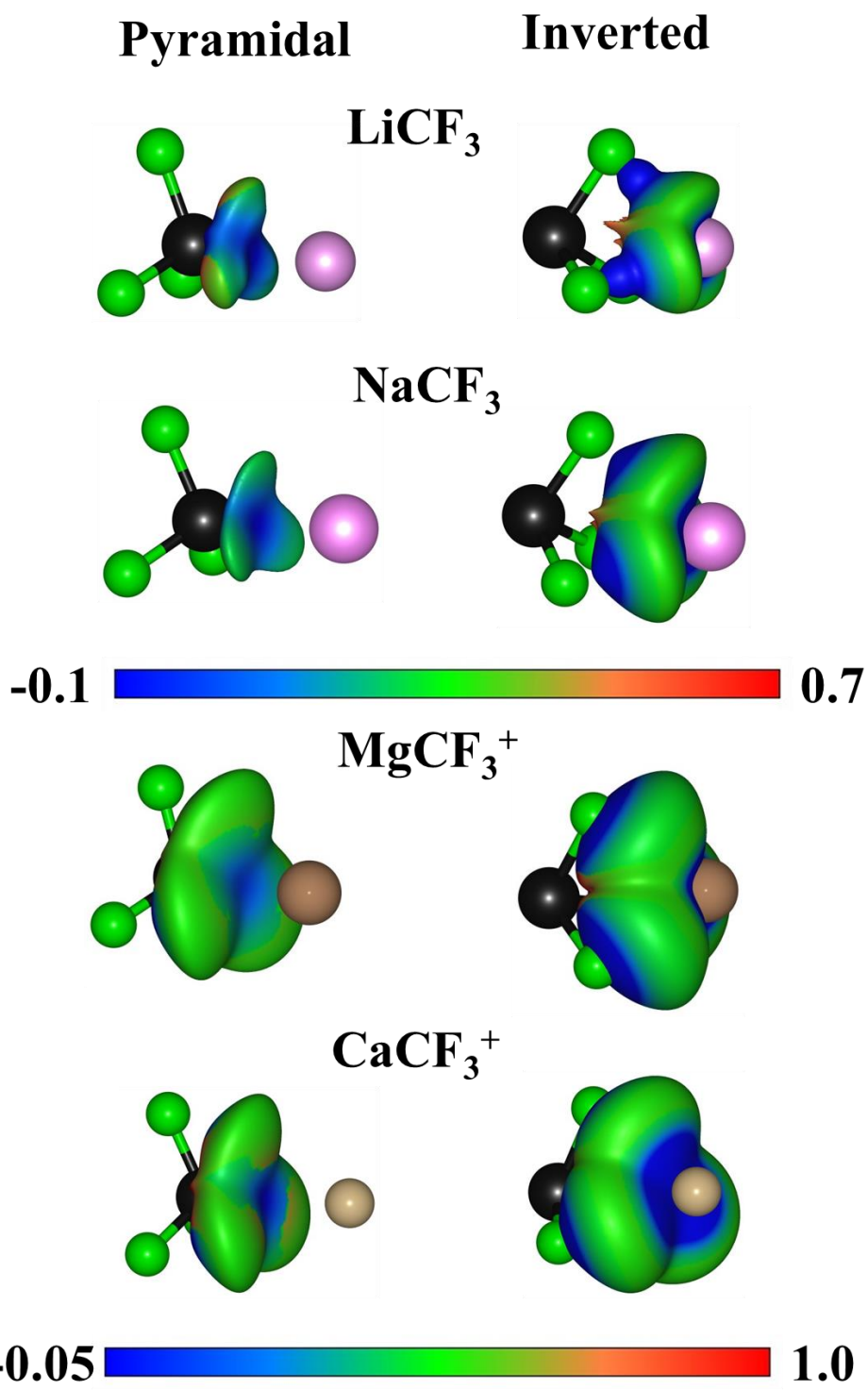

Figure S13. IGM plots (in.a.u.) for pyramidal and inverted $(M^{n+}CF_3)^{n-1}$ structures (M = Li, Na, Mg and Ca). Isovalue for $\delta g^{inter} = 0.05$.

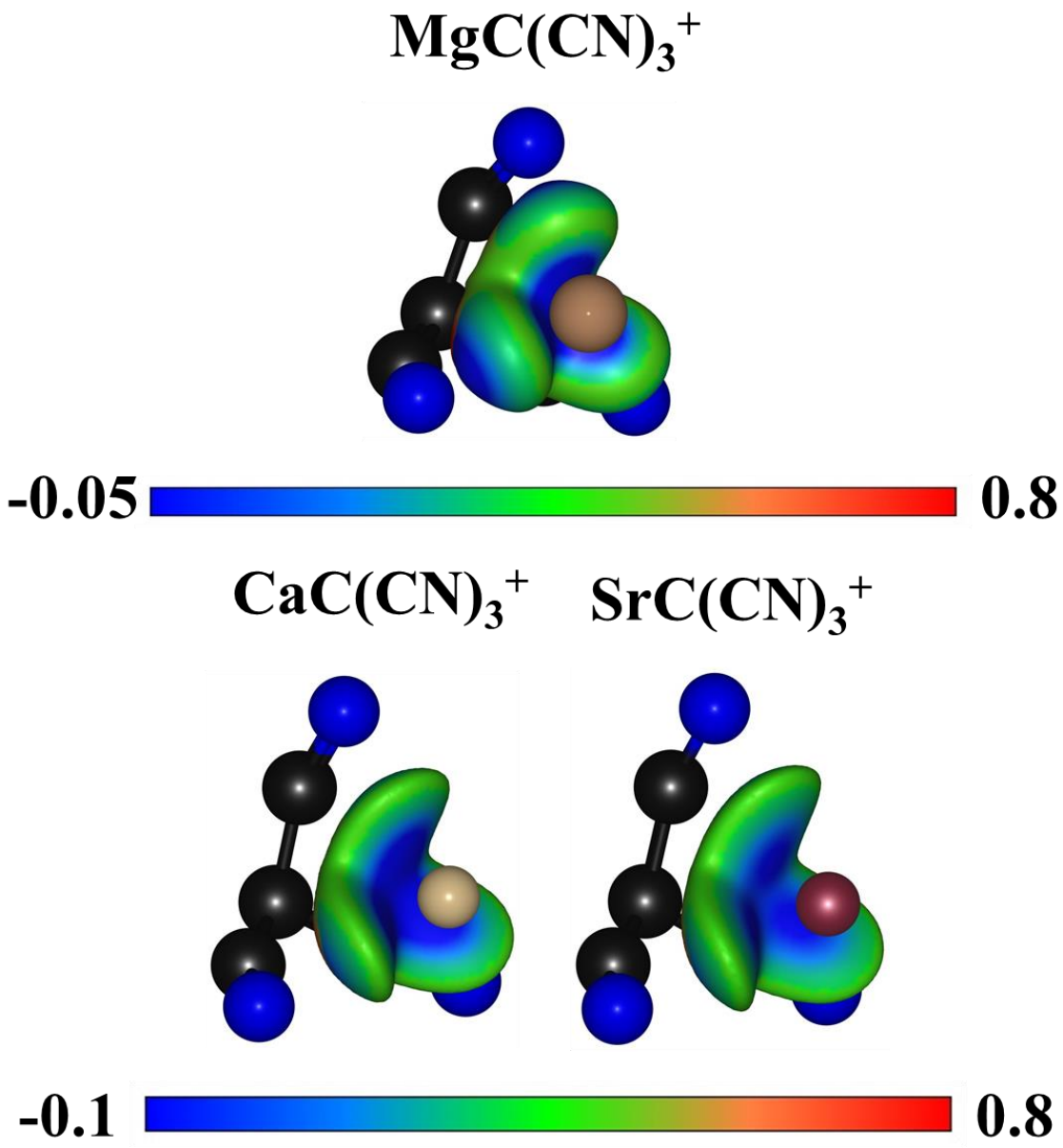

Figure S14. IGM plots (in a.u.) of inverted $(MC(CN)_3)^+$ structures (M = Mg, Ca and Sr). Isovalue for $\delta g^{inter} = 0.05$.

Table S1. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $LiC(CH_3)_3$.

IBSI		(*p*)$LiC(CH_3)_3$	(*i*)$LiC(CH_3)_3$
1(Li)	2(C)	0.12978	0.15967
1(Li)	3(C)	0.03792	0.10543
1(Li)	4(H)	0.01862	0.10378
1(Li)	5(H)	0.00624	0.02539
1(Li)	6(C)	0.03795	0.10545
1(Li)	7(H)	0.00625	0.02539
1(Li)	8(H)	0.01865	0.1038
1(Li)	9(C)	0.03799	0.10545
1(Li)	10(H)	0.00625	0.0254
1(Li)	11(H)	0.01867	0.02539
1(Li)	12(H)	0.01866	0.10381
1(Li)	13(H)	0.01862	0.02539
1(Li)	14(H)	0.01863	0.0254

Table S2. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $NaC(CH_3)_3$.

IBSI		(*p*)$NaC(CH_3)_3$	(*i*)$NaC(CH_3)_3$
1(Na)	2(C)	0.11278	0.08549
1(Na)	3(C)	0.02876	0.06658
1(Na)	4(H)	0.01434	0.09514
1(Na)	5(H)	0.0044	0.01441
1(Na)	6(C)	0.02878	0.06644
1(Na)	7(H)	0.0044	0.01438
1(Na)	8(H)	0.01437	0.09488
1(Na)	9(C)	0.02881	0.06654
1(Na)	10(H)	0.00441	0.01443
1(Na)	11(H)	0.01438	0.01437
1(Na)	12(H)	0.01438	0.09511
1(Na)	13(H)	0.01434	0.01441
1(Na)	14(H)	0.01435	0.01438

Table S3. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $KC(CH_3)_3$.

IBSI		(*p*)$KC(CH_3)_3$	(*i*)$KC(CH_3)_3$
1(K)	2(C)	0.08371	0.0856
1(K)	3(C)	0.02028	0.05666
1(K)	4(H)	0.01057	0.07744
1(K)	5(H)	0.00342	0.01087
1(K)	6(C)	0.02031	0.05659
1(K)	7(H)	0.00342	0.01082
1(K)	8(H)	0.01059	0.07735
1(K)	9(C)	0.02038	0.05657
1(K)	10(H)	0.00343	0.01087
1(K)	11(H)	0.01062	0.01083
1(K)	12(H)	0.01061	0.0773
1(K)	13(H)	0.01055	0.01085
1(K)	14(H)	0.01056	0.01089

Table S4. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $BeC(CH_3)_3^+$.

IBSI		(*p*)$BeC(CH_3)_3^+$	(*i*)$BeC(CH_3)_3^+$
1(Be)	2(C)	0.40635	0.47065
1(Be)	3(C)	0.09929	0.34214
1(Be)	4(H)	0.03352	0.33257
1(Be)	5(H)	0.00945	0.0546
1(Be)	6(C)	0.09929	0.3421
1(Be)	7(H)	0.00945	0.0546
1(Be)	8(H)	0.03354	0.33241
1(Be)	9(C)	0.09929	0.34215
1(Be)	10(H)	0.00945	0.05458
1(Be)	11(H)	0.03352	0.05461
1(Be)	12(H)	0.03354	0.33245
1(Be)	13(H)	0.03355	0.05462
1(Be)	14(H)	0.03352	0.05458

Table S5. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $MgC(CH_3)_3^+$.

IBSI		(*p*)$MgC(CH_3)_3^+$	(*i*)$MgC(CH_3)_3^+$
1(Mg)	2(C)	0.21368	0.01662
1(Mg)	3(C)	0.06246	0.01346
1(Mg)	4(H)	0.02596	0.03551
1(Mg)	5(H)	0.00664	0.00275
1(Mg)	6(C)	0.06246	0.01346
1(Mg)	7(H)	0.00664	0.00274
1(Mg)	8(H)	0.02598	0.03553
1(Mg)	9(C)	0.06247	0.01355
1(Mg)	10(H)	0.00664	0.00275
1(Mg)	11(H)	0.02597	0.00277
1(Mg)	12(H)	0.026	0.03588
1(Mg)	13(H)	0.026	0.00272
1(Mg)	14(H)	0.02598	0.00273

Table S6. IBSI values for M···C and M···H interactions in inverted and pyramidal conformers of $MgC(CH_3)_3^+$.

IBSI		(*p*)$CaC(CH_3)_3^+$	(*i*)$CaC(CH_3)_3^+$
1(Ca)	2(C)	0.23046	0.24104
1(Ca)	3(C)	0.0566	0.12325
1(Ca)	4(H)	0.02592	0.12646
1(Ca)	5(H)	0.00781	0.02375
1(Ca)	6(C)	0.05656	0.12316
1(Ca)	7(H)	0.0078	0.02358
1(Ca)	8(H)	0.02591	0.12638
1(Ca)	9(C)	0.05657	0.12315
1(Ca)	10(H)	0.0078	0.02368
1(Ca)	11(H)	0.0259	0.02368
1(Ca)	12(H)	0.02592	0.12635
1(Ca)	13(H)	0.02594	0.02364
1(Ca)	14(H)	0.02591	0.02379

Cartesian Coordinates of all species

$LiBH_3^-$

5	0.000000000	0.629209212	0.000000000
1	1.193759843	0.777298936	0.000000000
1	-0.596880186	0.777298936	1.033830308
1	-0.596880186	0.777298936	-1.033830308
3	0.000000000	-1.825981132	0.000000000

$NaBH_3^-$

5	0.000000000	-1.555240822	0.000000000
1	-1.194240336	-1.672850466	0.000000000
1	0.597119904	-1.672850466	1.034239891
1	0.597119904	-1.672850466	-1.034239891
11	0.000000000	1.163159640	0.000000000

KBH_3^-

5	0.000000000	0.000000000	-2.301160076
1	0.000000000	1.193879967	-2.346009965
1	-1.033930322	-0.596939983	-2.346009965
1	1.033930322	-0.596939983	-2.346009965
19	0.000000000	0.000000000	0.975990176

$MgBH_3$

5	0.000000529	-1.428261037	0.000000000
1	-1.191969637	-1.498001307	0.000000000
1	0.595980585	-1.498001307	1.032270293
1	0.595980585	-1.498001307	-1.032270293
12	0.000000529	0.969608827	0.000000000

$CaBH_3$

5	-0.000000529	-1.911028912	0.000000000
1	-1.194890695	-1.967628652	0.000000000
1	0.597449581	-1.967628652	1.034809815
1	0.597449581	-1.967628652	-1.034809815
20	-0.000000529	0.772901473	0.000000000

$LiAlH_3^-$

13	0.000000529	0.380234491	0.000000000
1	1.548190594	0.831644381	0.000000000
1	-0.774099530	0.831644381	1.340770046
1	-0.774099530	0.831644381	-1.340770046
3	0.000000529	-2.479326118	0.000000000

$NaAlH_3^-$

13	0.000000529	1.213252087	0.000000000
1	1.554850289	1.611772298	0.000000000
1	-0.777429643	1.611772298	1.346540194
1	-0.777429643	1.611772298	-1.346540194
11	0.000000529	-1.873418168	0.000000000

$KAlH_3^-$

13	0.000000000	-1.952399989	0.000000000
1	-1.561440134	-2.287520003	0.000000000
1	0.780720067	-2.287520003	1.352250017
1	0.780720067	-2.287520003	-1.352250017
19	0.000000000	1.697040216	0.000000000

$MgAlH_3$

13	-0.000000529	1.282941556	0.000000000
1	1.575849630	1.361101565	0.000000000
1	-0.787920582	1.361101565	1.364730133
1	-0.787920582	1.361101565	-1.364730133
12	-0.000000529	-1.730128611	0.000000000

$CaAlH_3$

13	0.000000529	-1.859670672	0.000000000
1	-1.577209616	-1.962360164	0.000000000
1	0.788600574	-1.962360164	1.365900144
1	0.788600574	-1.962360164	-1.365900144
20	0.000000529	1.503139618	0.000000000

(*p*)$LiC(CH_3)_3$

6	-0.000020109	-0.000089960	0.291141151
3	-0.003414781	-0.001669554	2.303741403
6	1.392631533	-0.295210524	-0.264988683
1	1.767059891	-1.276696206	0.041801298
1	1.385229931	-0.292467270	-1.371058564
6	-0.439954261	1.353520571	-0.265848596
1	-0.436268012	1.345889306	-1.371928531
1	-1.455474506	1.622671233	0.040581545
6	-0.951614684	-1.057784574	-0.267318650
1	-0.944803644	-1.051065611	-1.373378477
1	-1.989044456	-0.891646202	0.038921516
1	-0.677988242	-2.071877629	0.039881443
1	2.133392367	0.448846026	0.043651302
1	0.221886666	2.168742466	0.042391331

(*i*)$LiC(CH_3)_3$

6	-0.000036513	-0.000008996	-0.440371252
6	0.473093457	1.370038310	-0.107945809

1	0.562507478	1.629139367	1.020941137
1	1.478724438	1.570906585	-0.476770709
6	-1.423063987	-0.275304464	-0.107991318
1	-1.763624473	-1.242526702	-0.477040590
1	-1.692124689	-0.327712591	1.020888749
6	0.949989581	-1.094678283	-0.108011427
1	1.957976988	-0.905656169	-0.476677045
1	0.621364159	-2.066037629	-0.477017306
1	1.129538363	-1.301854351	1.020858586
1	-0.194387441	2.148579754	-0.476810398
1	-2.099758390	0.495316784	-0.476663286
3	-0.000036513	-0.000144465	1.461403408

(*p*)NaC(CH$_3$)$_3$

6	-0.225049559	-0.000049743	-0.000251359
11	2.121510750	-0.000347140	-0.001058884
6	-0.762006243	-1.166177538	-0.818607570
1	-0.449587932	-2.135812824	-0.421100734
1	-1.869895964	-1.165634602	-0.817603721
6	-0.760867453	1.292605391	-0.600093350
1	-1.868757175	1.293018149	-0.598959324
1	-0.447442648	2.176631440	-0.037898087
6	-0.759115347	-0.126033087	1.419942900
1	-1.867015653	-0.125860046	1.421316644
1	-0.445750868	0.703110931	2.060398716
1	-0.446186910	-1.055195310	1.904241685
1	-0.450399161	-1.121584300	-1.865835058
1	-0.449350332	1.433073904	-1.638858765

(*i*)NaC(CH$_3$)$_3$

6	-0.823151615	0.001006495	-0.001821957
6	-0.534043034	1.403722559	-0.353104103
1	0.584517018	1.702303413	-0.425651658
1	-0.915342230	1.683621339	-1.335966704
6	-0.540990602	-0.396128859	1.390034860
1	-0.926839135	-1.386182450	1.636397033
1	0.576116859	-0.482150854	1.690071481
6	-0.535608340	-1.005891336	-1.040153447
1	-0.915343817	-0.723827162	-2.023001760
1	-0.922950211	-1.995070197	-0.792657776
1	0.582654843	-1.223899663	-1.257999845
1	-0.918808870	2.113813338	0.380059334
1	-0.926272915	0.315032975	2.121879058
11	1.671366123	-0.001808728	0.003376151

(*p*)KC(CH$_3$)$_3$

6	-0.682791583	-0.000101602	-0.000483668

19	2.044298498	-0.000223842	-0.000950402
6	-1.234073095	-1.170146896	-0.802451789
1	-0.925423056	-2.139713389	-0.397817464
1	-2.345213553	-1.171992137	-0.802017864
6	-1.232542186	1.280834372	-0.611272749
1	-2.343682114	1.284025840	-0.610299063
1	-0.922630588	2.175588961	-0.061346460
6	-1.229149630	-0.110224975	1.415702602
1	-2.340279504	-0.110072572	1.420895419
1	-0.919248616	0.725309917	2.052082695
1	-0.920109588	-1.034570627	1.914906194
1	-0.927584745	-1.141060669	-1.853303612
1	-0.926163375	1.414572280	-1.654002760

(*i*)$KC(CH_3)_3$

6	-1.096887069	0.000753548	0.000026988
6	-0.915957134	1.466209396	-0.046329997
1	0.158069478	1.883390513	-0.058559813
1	-1.354588980	1.910554769	-0.942903898
6	-0.917763216	-0.692452772	1.292184166
1	-1.361188879	-1.691004420	1.292858867
1	0.155901968	-0.894317488	1.658386993
6	-0.918006108	-0.772779762	-1.245774263
1	-1.355864827	-0.271843645	-2.112401493
1	-1.360119941	-1.769909511	-1.182398408
1	0.155563294	-0.996187284	-1.599624505
1	-1.356132590	1.966735930	0.819364294
1	-1.353946559	-0.136842062	2.125678550
19	1.619157496	-0.000576803	-0.000054505

(*p*)$BeC(CH_3)_3^+$

6	-0.000003175	0.000010584	0.170920547
6	1.427492672	0.323416201	-0.272657519
1	2.151208707	-0.424259393	0.048846235
1	1.422684567	0.322600739	-1.368628582
6	-0.993837737	1.074560551	-0.272595605
1	-0.990838360	1.070749417	-1.368565081
1	-2.013553300	0.868098872	0.049433093
6	-0.433685098	-1.397941826	-0.272659107
1	-0.431829802	-1.393448582	-1.368634932
1	-1.443099167	-1.650788008	0.048729816
1	0.254927435	-2.177834789	0.049410338
1	1.758548075	1.309783013	0.049257406
1	-0.708143936	2.075151648	0.048862110
4	0.000073556	-0.000081493	1.923310058

(*i*)$BeC(CH_3)_3^+$

6	-0.000001058	-0.000050801	-0.558369841
6	-0.120859321	1.409351946	-0.126578669
1	-0.127925954	1.493903358	1.113056609
1	0.730960472	2.044024913	-0.349336890
6	-1.160272978	-0.809364431	-0.126362235
1	-1.102278326	-1.870053659	-0.349124690
1	-1.230194755	-0.857528028	1.112720581
6	1.281097902	-0.600076417	-0.126407745
1	2.170652266	-0.019665814	-0.349725306
1	1.404524262	-1.655196583	-0.348959587
1	1.358384769	-0.635425457	1.112688301
1	-1.068543277	1.889400909	-0.349056426
1	-2.135663596	-0.388781233	-0.349501993
4	0.000074085	0.000040217	1.095888511

(*p*)$MgC(CH_3)_3^+$

6	0.313579854	0.000010054	0.000001058
6	0.718902110	-0.230555648	1.441078768
1	0.389240030	-1.193728093	1.828515891
1	1.817242299	-0.234110132	1.468399131
6	0.719003183	1.363268546	-0.520941663
1	1.817343372	1.388988677	-0.530739909
1	0.388768533	1.545528303	-1.542823678
6	0.718724835	-1.132853659	-0.920184731
1	1.817054970	-1.154753130	-0.937182962
1	0.388870135	-0.987024051	-1.948009406
1	0.387842473	-2.108778217	-0.567246260
1	0.387919203	0.562819163	2.110031837
1	0.388739957	2.180505018	0.118992384
12	-1.883690028	0.000111127	0.000028046

(*i*)$MgC(CH_3)_3^+$

6	-1.131000480	-0.000203204	0.001259442
6	-0.984514692	-0.973715243	-1.062428104
1	0.137793522	-1.031786625	-1.132842546
1	-1.326834692	-1.973514162	-0.811380597
6	-0.983896084	1.407446379	-0.310665146
1	-1.327929560	2.082104508	0.468002771
1	0.138525374	1.495303032	-0.332194193
6	-0.978140752	-0.434209512	1.375407342
1	-1.323879237	-1.444951817	1.572185607
1	-1.319215069	0.282039832	2.117315433
1	0.144871268	-0.462827418	1.456055543
1	-1.334300325	-0.638168183	-2.034501840
1	-1.331316294	1.690637701	-1.300076844
12	2.667299932	0.000437630	-0.002000290

(*i*)$CaC(CH_3)_3^+$

6	-0.909372581	0.000440275	-0.000421225
6	-0.816881923	1.354575751	-0.575694046
1	0.264878614	1.754940674	-0.741671548
1	-1.241901214	1.437898413	-1.574447840
6	-0.818623446	-0.178242244	1.460089990
1	-1.251484085	-1.111078544	1.817211607
1	0.262686232	-0.237185710	1.890479372
6	-0.818362032	-1.175421206	-0.884947876
1	-1.245871631	-1.016616701	-1.873427693
1	-1.247102498	-2.080528618	-0.458279140
1	0.263068298	-1.522931376	-1.145318958
1	-1.247132131	2.130625299	0.054967758
1	-1.242053617	0.646528125	2.030655779
20	1.343217490	-0.000488431	0.000283110

(*p*)$SrC(CH_3)_3^+$

6	1.068402516	-0.000163516	0.000321211
6	1.551569920	0.669614541	-1.283577098
1	1.223248775	1.711668792	-1.366263160
1	2.649130102	0.694693838	-1.331507327
6	1.556847933	-1.445084111	0.061127910
1	2.654607086	-1.495443793	0.061572419
1	1.231716669	-1.963017931	0.970195156
6	1.556603454	0.776851781	1.220096466
1	2.654345143	0.805083917	1.261814683
1	1.231191725	0.327929024	2.165054629
1	1.228986644	1.822338805	1.214046382
1	1.223474733	0.140947419	-2.185443300
1	1.229104121	-2.038597142	-0.799555073
38	-1.308588131	-0.000339732	0.000586328

$LiCH_3$

6	0.000000000	0.384660001	0.000000000
1	1.010060195	0.806160263	0.000000000
1	-0.505029833	0.806160263	0.874740047
1	-0.505029833	0.806160263	-0.874740047
3	0.000000000	-1.575480264	0.000000000

$NaCH_3$

6	0.000000529	-1.199601431	0.000000000
1	-1.020149488	-1.590601504	0.000000000
1	0.510070775	-1.590601504	0.883469884
1	0.510070775	-1.590601504	-0.883469884
11	0.000000529	1.088128656	0.000000000

KCH_3

6	0.000000529	-1.773516912	0.000000000
1	-1.015289524	-2.186427040	0.000000000
1	0.507640264	-2.186427040	0.879260279
1	0.507640264	-2.186427040	-0.879260279
19	0.000000529	0.905283099	0.000000000

$BeCH_3^+$

6	0.000000000	0.425841633	0.000000000
1	1.031780275	0.783061676	0.000000000
1	-0.515890137	0.783061676	0.893550181
1	-0.515890137	0.783061676	-0.893550181
4	0.000000000	-1.226058706	0.000000000

$MgCH_3^+$

6	0.000000000	-1.133990331	0.000000000
1	1.041000130	-1.444899957	0.000000000
1	-0.520499800	-1.444899957	0.901530174
1	-0.520499800	-1.444899957	-0.901530174
12	0.000000000	0.928220287	0.000000000

$CaCH_3^+$

6	-0.000000529	-1.520726824	0.000000000
1	1.013849633	-1.931636662	0.000000000
1	-0.506920583	-1.931636662	0.878019888
1	-0.506920583	-1.931636662	-0.878019888
20	-0.000000529	0.745963705	0.000000000

$SrCH_3^+$

6	-1.907349543	0.000189445	0.000540819
1	-2.318188471	-0.693846625	-0.740037449
1	-2.323940098	0.985246015	-0.233189363
1	-2.328600033	-0.293302840	0.967341832
38	0.484600416	0.000020109	0.000069322

$LiC(Ph)_3$

6	0.000330736	-0.000049743	-0.436760676
6	-0.889682425	-1.145322662	-0.266570922
6	-0.541117075	-2.270666237	0.517039510
6	-2.203123641	-1.143734601	-0.791810564
6	-1.434257144	-3.315210797	0.743319406
1	0.466636965	-2.365247145	0.908759265
6	-3.081398592	-2.180091201	-0.562540816
1	-2.509337877	-0.304217650	-1.402510743
6	-2.708745623	-3.282510818	0.209879105
1	-1.116189338	-4.161051416	1.339509545
1	-4.070570573	-2.141830098	-1.000880557

1	-3.400056431	-4.096071625	0.378439522
6	-0.546878228	1.343151343	-0.266640774
6	-1.696325298	1.603072095	0.516439423
6	0.111099705	2.480373360	-0.790890854
6	-2.155227279	2.898473129	0.742809279
1	-2.281799068	0.777031172	0.907389225
6	-0.348002834	3.758824318	-0.561330588
1	0.991776592	2.326400773	-1.401010525
6	-1.489791651	3.986419219	0.210319381
1	-3.047340215	3.045249436	1.338329480
1	0.179693777	4.596762733	-0.998890851
1	-1.849299857	4.991656493	0.379009446
6	1.437002516	-0.197918112	-0.266630720
6	2.237683678	0.667974091	0.515279467
6	2.092146705	-1.337328277	-0.789840966
6	3.588995993	0.417147250	0.741179414
1	1.816023604	1.588766318	0.905519642
6	3.428803456	-1.579413639	-0.560700867
1	1.517953935	-2.023343079	-1.399090670
6	4.197678948	-0.703908931	0.209599171
1	4.162800876	1.116731745	1.335639672
1	3.889949148	-2.456052903	-0.997620825
1	5.248007415	-0.895445694	0.377839435
3	0.002199790	0.001661087	1.552229274

$NaC(Ph)_3$

6	-0.000061385	0.000191033	-0.479309173
6	-0.436637907	1.383805915	-0.343969445
6	-1.591811203	1.760419246	0.385460646
6	0.322151467	2.455854461	-0.871539054
6	-1.953375263	3.091417505	0.565070813
1	-2.254815791	0.993931931	0.773820654
6	-0.039684060	3.773621701	-0.686629177
1	1.204383606	2.221475508	-1.452989490
6	-1.183472638	4.113336561	0.037100617
1	-2.853944981	3.322389615	1.120560871
1	0.568709435	4.554059187	-1.126229418
1	-1.467272513	5.147646833	0.170390841
6	1.416433925	-0.313437506	-0.344259434
6	2.320383498	0.498769666	0.384920885
6	1.965456380	-1.506769774	-0.871579271
6	3.653869948	0.146318039	0.564431037
1	1.988333770	1.456353470	0.773070810
6	3.287577161	-1.852312992	-0.686729191
1	1.321345007	-2.153657210	-1.452979435
6	4.153865189	-1.031493461	0.036670925
1	4.304226671	0.810918096	1.119660741

1	3.659109861	-2.769542268	-1.126209309
1	5.191523035	-1.302825391	0.169800808
6	-0.979960064	-1.069695296	-0.344468989
6	-0.728464872	-2.258884635	0.384271055
6	-2.288042301	-0.948252292	-0.871429514
6	-1.700447059	-3.237431266	0.563920910
1	0.267021252	-2.450299688	0.771951071
6	-3.248397936	-1.920406462	-0.686449257
1	-2.526293245	-0.066806511	-1.452499472
6	-2.970646027	-3.081199621	0.036670925
1	-1.450023980	-4.133072756	1.118920951
1	-4.228645342	-1.783355905	-1.125569534
1	-3.724534690	-3.844068423	0.169960620
11	0.000768365	-0.002386060	1.901401061

$KC(Ph)_3$

6	0.000049213	0.000019050	-0.557830080
6	-0.450023974	1.380465748	-0.459730144
6	-1.629240439	1.760321348	0.228229914
6	0.306521688	2.451952308	-0.991969741
6	-2.012861665	3.088631916	0.368050185
1	-2.289238771	0.993959977	0.620650299
6	-0.076603699	3.769602071	-0.846749746
1	1.204799539	2.219242380	-1.548739880
6	-1.242150457	4.110869537	-0.161290050
1	-2.932102344	3.319289166	0.892670160
1	0.533079402	4.547149191	-1.289929871
1	-1.543205744	5.143892320	-0.059019668
6	1.420499594	-0.300480601	-0.459799995
6	2.339272480	0.531014023	0.227690153
6	1.969989312	-1.491667055	-0.991669698
6	3.681481888	0.199106644	0.367260124
1	2.005755344	1.485959349	0.619840129
6	3.302734914	-1.818642502	-0.846720112
1	1.319197077	-2.153460356	-1.548029724
6	4.181278158	-0.979565297	-0.161899663
1	4.341028831	0.880058278	0.891410189
1	3.671171398	-2.735562738	-1.289659990
1	5.226466197	-1.235306078	-0.059860001
6	-0.970477207	-1.079858674	-0.459949752
6	-0.710054266	-2.291249116	0.227640411
6	-2.276732725	-0.959988385	-0.992009959
6	-1.668811785	-3.287481909	0.367280232
1	0.283671285	-2.479812961	0.619930089
6	-3.226552440	-1.950332494	-0.846820126
1	-2.524118327	-0.065545482	-1.548610231
6	-2.939479075	-3.130667640	-0.161790123

1	-1.409138688	-4.199140536	0.891570000
1	-4.204811728	-1.810758819	-1.289770059
1	-3.683721366	-3.907789301	-0.059629809
19	0.000428104	-0.000761486	2.161560472

$MgC(Ph)_3^+$

6	-0.000310098	-0.000269880	0.327519441
6	0.938330748	-1.131762495	0.049859610
6	2.235600836	-1.132528215	0.583839671
6	0.576463999	-2.181141089	-0.797220343
6	3.129881811	-2.142735521	0.296779535
1	2.549653246	-0.314645088	1.229349659
6	1.479456290	-3.196465539	-1.092310744
1	-0.404861342	-2.195122481	-1.249630377
6	2.750543746	-3.186999616	-0.545470616
1	4.121285862	-2.124520711	0.727689627
1	1.180288049	-3.995203562	-1.756760515
1	3.446754206	-3.983442068	-0.767940436
6	-1.449529200	-0.247253836	0.049519349
6	-2.099441942	-1.370176955	0.583019447
6	-2.176613448	0.591048124	-0.797680727
6	-3.421483876	-1.638759809	0.296269408
1	-1.548458886	-2.050906863	1.228919438
6	-3.507514338	0.317722254	-1.092280581
1	-1.696964015	1.447135202	-1.250580780
6	-4.135602753	-0.787333195	-0.545550522
1	-3.902300145	-2.505656920	0.727719790
1	-4.049690297	0.976405051	-1.756560486
1	-5.173686058	-0.990773272	-0.767820313
6	0.510149093	1.378217803	0.049119820
6	-0.139319140	2.502725278	0.579399874
6	1.602230174	1.588445107	-0.794830578
6	0.290092322	3.781885862	0.293219760
1	-1.006784588	2.366231415	1.222139619
6	2.031768639	2.877475905	-1.089350526
1	2.106086292	0.744910113	-1.244730725
6	1.387039188	3.974444996	-0.545400236
1	-0.222205760	4.631728120	0.722499457
1	2.875542821	3.017142186	-1.750800391
1	1.730851996	4.975047735	-0.766840277
12	-0.001330352	0.001870112	2.550219994

$CaC(Ph)_3^+$

6	0.000159812	0.000079906	-0.695410344
6	-0.404042176	1.396851721	-0.531750109
6	-1.501858480	1.765271272	0.289919810
6	0.377079537	2.459044342	-1.037570003

6	-1.804123995	3.104920520	0.558400004
1	-2.224019263	1.015525537	0.607319795
6	0.072068650	3.774613909	-0.766489961
1	1.219935067	2.220592311	-1.673110292
6	-1.019724559	4.112371871	0.039579812
1	-2.675779997	3.342908463	1.153530201
1	0.680186973	4.558045480	-1.198649970
1	-1.256699127	5.148586122	0.232949646
6	1.411770816	-0.347931395	-0.532660294
6	2.281095792	0.420140806	0.286479629
6	1.939986020	-1.557321547	-1.035600405
6	3.592502850	0.011832932	0.554510022
1	1.993823455	1.421116615	0.602169842
6	3.231846330	-1.951025716	-0.764820407
1	1.311126595	-2.169348903	-1.668960484
6	4.071693487	-1.172756269	0.038279624
1	4.235357956	0.648856505	1.147470063
1	3.605047526	-2.870890295	-1.194830369
1	5.087542352	-1.485777312	0.231570081
6	-1.007608517	-1.048011199	-0.532850268
6	-0.778076826	-2.185263379	0.285929814
6	-2.318915031	-0.899753197	-1.035950192
6	-1.788178826	-3.115913649	0.554120019
1	0.232235786	-2.438043414	0.601430052
6	-3.306604258	-1.820768207	-0.765080233
1	-2.533901226	-0.048883807	-1.669160513
6	-3.053558577	-2.937396233	0.038029852
1	-1.558628086	-3.991376023	1.147010208
1	-4.289663183	-1.683284783	-1.195260061
1	-3.833222935	-3.659929028	0.231319780
20	0.001679079	-0.003100450	1.648140005

$SrC(Ph)_3^+$

6	0.000149757	0.000040217	-0.814169890
6	-0.043884140	1.458698783	-0.701729779
6	-1.040425973	2.121430845	0.060590266
6	0.984876649	2.276514704	-1.217789782
6	-1.014214765	3.503022682	0.267690132
1	-1.926439612	1.582305592	0.388000167
6	1.003706363	3.638837081	-1.007749807
1	1.759277811	1.815511889	-1.816649620
6	0.007080921	4.267568975	-0.257419860
1	-1.817524350	3.971577385	0.820850223
1	1.796148236	4.229867742	-1.447189707
1	0.024558587	5.337874941	-0.111109759
6	1.285454089	-0.691130888	-0.701589547
6	2.357416910	-0.159610442	0.061140610

6	1.479590701	-1.990771690	-1.218079771
6	3.540917064	-0.872961482	0.268110299
1	2.333212342	0.877111290	0.388990258
6	2.650097967	-2.688098185	-1.008169974
1	0.693356078	-2.430917513	-1.817199965
6	3.692713146	-2.139463618	-0.257479657
1	4.348191246	-0.411614702	0.821550325
1	2.765976672	-3.669685998	-1.447989823
1	4.610979609	-2.689594169	-0.111199720
6	-1.241090515	-0.767438247	-0.701979550
6	-1.316931669	-1.961758489	0.060460617
6	-2.463647126	-0.285483717	-1.218359706
6	-2.526621864	-2.629779148	0.267430306
1	-0.407033615	-2.459323218	0.388150454
6	-3.652933304	-0.950180614	-1.008309676
1	-2.451483987	0.615622586	-1.817279871
6	-3.699282881	-2.127525379	-0.257799810
1	-2.530907142	-3.559709207	0.820660249
1	-4.560942725	-0.559484818	-1.447919972
1	-4.634985735	-2.647440968	-0.111419857
38	-0.000531823	-0.000357195	1.652920592

(*p*)$LiCF_3$

6	0.063823539	0.264609262	0.000000000
9	-1.285521824	-0.011807532	0.000000000
9	0.532702628	-0.450379582	1.079860261
9	0.532702628	-0.450379582	-1.079860261
3	0.532702628	2.208479973	0.000000000

(*i*)$LiCF_3$

6	0.000000000	0.000000000	0.745795000
3	0.000000000	0.000000000	-1.400930000
9	0.000000000	1.241703000	-0.010073000
9	-1.075346000	-0.620851000	-0.010073000
9	1.075346000	-0.620851000	-0.010073000

(*p*)$NaCF_3$

6	-0.218520041	0.000002117	0.000000000
9	-0.807659951	1.246672276	0.000000000
9	-0.807659951	-0.623337990	1.079650178
9	-0.807659951	-0.623337990	-1.079650178
11	2.101630619	0.000002117	0.000000000

(*i*)$NaCF_3$

6	0.000000000	0.000000000	-1.076992000
11	0.000000000	0.000000000	1.451401000
9	0.000000000	1.246857000	-0.351980000

9	1.079810000	-0.623429000	-0.351980000
9	-1.079810000	-0.623429000	-0.351980000

(C_{2v})KCF_3

6	0.759100001	0.000000000	-0.304649988
9	1.603080033	1.068860254	-0.255990023
9	1.603140359	-1.068809982	-0.256069929
9	0.244659809	-0.000059797	1.092749961
19	-1.874339995	0.000000000	-0.178850268

(*i*)KCF_3

6	-0.493248000	0.003258000	0.000000000
19	-3.405309000	-0.001167000	0.000000000
9	-1.206620000	-0.622018000	1.083893000
9	-1.206620000	-0.622018000	-1.083893000
9	-1.205357000	1.254805000	0.000000000

(*p*)$BeCF_3^+$

6	-0.000080964	0.000077789	0.121429774
9	1.243219395	-0.091616457	-0.314030184
9	-0.543215792	1.122649534	-0.311120238
9	-0.701792222	-1.031273323	-0.310430191
4	0.004146104	0.000424400	1.922910000

(*p*)$MgCF_3^+$

6	0.309342732	0.000000000	0.000000000
9	0.756762625	1.246180142	0.000000000
9	0.756762625	-0.623089806	1.079219957
9	0.756762625	-0.623089806	-1.079219957
12	-1.857387273	0.000000000	0.000000000

(*i*)$MgCF_3^+$

6	0.000000000	0.000000000	-1.102112000
12	0.000000000	0.000000000	1.193217000
9	0.000000000	1.242710000	-0.285405000
9	1.076219000	-0.621355000	-0.285405000
9	-1.076219000	-0.621355000	-0.285405000

(*p*)$CaCF_3^+$

6	0.617267269	0.001474817	0.000000000
9	1.137446388	1.251841809	0.000000000
9	1.137446388	-0.624103181	1.083039558
9	1.137446388	-0.624103181	-1.083039558
20	-1.720733069	-0.002078608	0.000000000

(*i*)$CaCF_3^+$

6	0.000000000	0.000000000	-1.383799000

20	0.000000000	0.000000000	1.220483000
9	0.000000000	1.254201000	-0.596550000
9	1.086170000	-0.627100000	-0.596550000
9	-1.086170000	-0.627100000	-0.596550000

$(C_{2v})SrCF_3^+$

6	0.365070388	1.173208186	0.000000000
9	0.964263608	2.310159265	0.000000000
9	0.964263608	0.401136463	1.093861762
9	0.964263608	0.401136463	-1.093861762
38	-0.742777000	-0.922398279	0.000000000

$MgC(CN)_3^+$

6	-0.000012171	-0.000889547	-1.315542049
6	0.013371780	1.280802092	-0.682811692
6	1.103050925	-0.652500419	-0.681861819
6	-1.116433289	-0.629341506	-0.681861819
7	0.020913614	2.002731096	0.228478098
7	1.724398680	-1.019293279	0.229638055
7	-1.745298535	-0.983086972	0.229638055
12	0.000003704	0.000760428	1.279848515

$CaC(CN)_3^+$

6	0.000327032	0.002630011	-1.335998454
6	-0.679470467	-1.151220872	-0.863518314
6	-0.658461601	1.166979770	-0.859378561
6	1.338666037	-0.010459188	-0.860908412
7	-1.128496413	-1.913732479	-0.114298052
7	-1.093563835	1.934725469	-0.107308150
7	2.222174022	-0.019680631	-0.110138190
20	-0.000358253	-0.002838507	1.292051871

$SrC(CN)_3^+$

6	-1.643730371	0.001134556	0.003199935
6	-1.211688898	-1.053660696	-0.840405969
6	-1.205970079	-0.202068978	1.336565203
6	-1.209152022	1.257881838	-0.489359307
7	-0.522294770	-1.781340798	-1.421738398
7	-0.511849340	-0.342234273	2.253742620
7	-0.518096277	2.123638043	-0.829326055
38	1.118129831	-0.000530236	-0.002072258