Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Where to place the positive muon in the Periodic Table?

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Table S1- The optimized exponents of the electronic [4s1p] basis set for both protonic and muonic species.

Proton	**Li**	**Be**	**B**	**C**	**N**	**O**	**F**
S	6.863	8.531	10.158	10.554	10.490	7.889	8.161
S	1.449	1.884	2.351	2.487	2.460	1.633	1.732
S	0.372	0.492	0.630	0.707	0.717	0.469	0.534
S	0.106	0.134	0.178	0.213	0.242	0.140	0.151
P	0.345	0.742	0.981	1.105	0.772	0.687	0.829
μ^+							
S	3.537	4.406	5.165	3.604	4.016	4.455	3.858
S	0.967	1.310	1.653	0.894	1.047	1.214	1.011
S	0.286	0.412	0.533	0.271	0.340	0.399	0.350
S	0.090	0.121	0.164	0.068	0.099	0.121	0.099
P	0.308	0.727	0.878	0.950	0.691	0.652	0.787

Proton	**Na**	**Mg**	**Al**	**Si**	**P**	**S**	**Cl**
S	6.189	6.903	7.633	8.284	8.489	8.848	9.884
S	1.279	1.447	1.624	1.795	1.864	1.977	2.327
S	0.320	0.360	0.411	0.461	0.493	0.528	0.623
S	0.091	0.100	0.121	0.142	0.163	0.177	0.215
P	0.253	0.477	0.482	0.559	0.546	0.561	0.549
μ^+							
S	3.240	3.733	4.069	4.432	4.272	4.548	5.606
S	0.864	1.039	1.150	1.284	1.238	1.364	1.818
S	0.248	0.302	0.338	0.385	0.391	0.436	0.551
S	0.078	0.089	0.108	0.128	0.147	0.162	0.201
P	0.234	0.464	0.430	0.516	0.474	0.494	0.492

Table S2- The results of the ab initio NEO-CI/[6-311+g(d)/4s1p:1s] calculations on the muonic species. The symbol "K_X" stands for the total kinetic energy of muons, and "corr. Energy" is the electronic correlation energy computed as the energy difference between total energies of NEO-HF/[6-311+g(d)/4s1p:1s] and NEO-CI/[6-311+g(d)/4s1p:1s] computational levels. All results are offered in atomic units.

	Active space	**Number of the used determinants**	**Energy**	K_X	**virial ratio**	**corr. Energy**
Li	(2,5)	25	-7.8920	0.0385	2.0007	0.0002
Be	(4,6)	225	-15.5664	0.0845	2.0003	0.0003
B	(6,7)	1225	-26.0754	0.1339	2.0006	0.0012
C	(8,8)	4900	-39.7722	0.1810	2.0005	0.0006
N	(6,6)	400	-55.8881	0.1355	2.0005	0.0012
O	(8,8)	4900	-75.8512	0.0891	2.0021	0.0133
F	(8,8)	4900	-99.9603	0.0428	2.0018	0.0110
Na	(2,5)	25	-162.2887	0.0371	2.0008	0.0004
Mg	(4,6)	225	-200.5385	0.0791	2.0006	0.0001
Al	(6,7)	1225	-243.3367	0.1246	2.0002	0.0007
Si	(8,8)	4900	-290.8410	0.1701	2.0002	0.0006
P	(6,6)	400	-342.1709	0.1262	2.0000	0.0002
S	(8,8)	4900	-398.5028	0.0822	2.0001	0.0014
Cl	(8,8)	4900	-460.0010	0.0394	2.0000	0.0021

Table S3- The protonic/muonic contribution of selected topological indices computed at the LCPs derived from the topological analysis performed using NEO-HF/[6-311+g(d)/4s1p:1s] wavefunction. The symbol "ρ_x" stands for the one-particle protonic/muonic density, "Lap. ρ_x" for the Laplacian of the one-particle protonic/muonic density, "G_x" for the protonic/muonic Lagrangian kinetic energy density, and "H_x" for the protonic/muonic Hamiltonian energy density (see text for details). The mass-scaled quantities have been derived by dividing each quantity to the mass of proton/ μ^+. All results are offered in atomic units.

Proton

	ρ_x	Lap. ρ_x	mass-scaled ρ_x	mass-scaled Lap. ρ_x	G_x	H_x
Li	0.000	0.000	0.000	0.000	0.000	0.000
Be	0.000	0.000	0.000	0.000	0.000	0.000
B	0.000	0.000	0.000	0.000	0.000	0.000
C	0.000	0.000	0.000	0.000	0.000	0.000
N	0.007	10.351	0.000	0.006	0.001	0.001
O	2.316	723.883	0.001	0.394	0.093	0.006
F	--	--	--	--	--	--
Na	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000
Al	0.000	0.000	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000	0.000	0.000
P	0.000	0.000	0.000	0.000	0.000	0.000
S	0.000	0.000	0.000	0.000	0.000	0.000
Cl	0.000	0.021	0.000	0.000	0.000	0.000

μ^+

	ρ_x	Lap. ρ_x	mass-scaled ρ_x	mass-scaled Lap. ρ_x	G_x	H_x
Li	0.000	0.000	0.000	0.000	0.000	0.000
Be	0.000	0.000	0.000	0.000	0.000	0.000
B	0.000	0.000	0.000	0.000	0.000	0.000
C	0.058	9.817	0.000	0.048	0.009	0.003
N	1.554	9.176	0.008	0.045	0.076	-0.065
O	--	--	--	--	--	--
F	--	--	--	--	--	--
Na	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000
Al	0.000	0.000	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000	0.000	0.000
P	0.000	0.000	0.000	0.000	0.000	0.000
S	0.019	3.821	0.000	0.019	0.003	0.002
Cl	0.379	21.764	0.002	0.106	0.028	-0.002

Table S4- The protonic/muonic contribution of selected topological indices computed at the (3, -3) CPs in the hydrogen/μ^+ atomic basins derived from the topological analysis performed using NEO-HF/[6-311+g(d)/4s1p:1s] wavefunction. The symbol "ρ_x" stands for the one-particle protonic/muonic density, "Lap. ρ_x" for the Laplacian of the one-particle protonic/muonic density, "G_x" for the protonic/muonic Lagrangian kinetic energy density (see text for details). The mass-scaled quantities have been derived by dividing each quantity to the mass of proton/μ^+. All results are offered in atomic units.

Proton

	ρ_x	Lap. ρ_x	mass-scaled ρ_x	mass-scaled Lap. ρ_x	G_x
Li	45.865	-11077.238	0.025	-6.033	0.002
Be	51.142	-13280.651	0.028	-7.233	0.012
B	53.973	-14523.018	0.029	-7.910	0.031
C	53.189	-14156.223	0.029	-7.710	0.058
N	49.438	-12481.559	0.027	-6.798	0.098
O	40.599	-8789.329	0.022	-4.787	0.167
F	--	--	--	--	--
Na	43.594	-10178.548	0.024	-5.544	0.001
Mg	47.237	-11635.055	0.026	-6.337	0.004
Al	50.201	-12876.353	0.027	-7.013	0.009
Si	51.513	-13440.669	0.028	-7.321	0.018
P	50.480	-12991.807	0.027	-7.076	0.024
S	48.011	-11944.087	0.026	-6.505	0.035
Cl	44.354	-10454.663	0.024	-5.694	0.047

μ^+

	ρ_x	Lap. ρ_x	mass-scaled ρ_x	mass-scaled Lap. ρ_x	G_x
Li	6.154	-389.551	0.030	-1.891	0.001
Be	6.900	-471.295	0.033	-2.288	0.006
B	7.210	-506.642	0.035	-2.459	0.014
C	6.792	-456.767	0.033	-2.217	0.030
N	5.566	-319.477	0.027	-1.551	0.057
O	--	--	--	--	--
F	--	--	--	--	--
Na	5.822	-355.201	0.028	-1.724	0.000
Mg	6.358	-411.323	0.031	-1.997	0.002
Al	6.764	-455.903	0.033	-2.213	0.004
Si	6.887	-469.778	0.033	-2.280	0.008
P	6.659	-443.918	0.032	-2.155	0.011
S	6.184	-391.846	0.030	-1.902	0.016
Cl	5.420	-313.201	0.026	-1.520	0.024

Table S5- Selected topological indices computed at the LCPs and the (3, -3) CPs in μ^+ atomic basins derived from the topological analysis using NEO-CI/[6-311+g(d)/4s1p:1s] wavefunction. The symbol "Γ" stands for the Gamma density, "Lap. Γ" for the Laplacian of the Gamma density, "G" for the combined Lagrangian kinetic energy density, "H" for the combined Hamiltonian energy density, "M-LCP" and "LCP-X" for the lengths of the line paths linking each of (3, -3) CPs located in the M (central atoms) and X basins to the LCP, respectively, and "TF" for the topological floppiness index (see text for details). All results are offered in atomic units.

	LCP					**(3, -3)**					
	Γ	**Lap. Γ**	**G**	**H**	**G/ Γ**	**Γ**	**Lap. Γ**	**G**	**M-LCP**	**LCP-X**	**TF**
Li	0.034	0.120	0.031	-0.001	0.934	0.191	-3.678	0.001	1.396	1.791	0.177
Be	0.086	0.091	0.068	-0.046	0.792	0.228	-4.593	0.007	1.128	1.496	0.378
B	0.165	-0.384	0.077	-0.173	0.467	0.254	-5.106	0.018	1.040	1.280	0.650
C	0.231	-0.871	0.031	-0.248	0.133	0.262	-4.702	0.042	1.554	0.520	0.883
N	0.262	-1.640	0.107	-0.517	0.410	0.266	-3.915	0.082	1.657	0.196	0.987
O	--	--	--	--	--	--	--	--	--	--	--
F	--	--	--	--	--	--	--	--	--	--	--
Na	0.027	0.096	0.024	0.000	0.866	0.177	-3.326	0.000	1.951	1.812	0.155
Mg	0.047	0.164	0.046	-0.005	0.986	0.201	-3.919	0.002	1.693	1.664	0.234
Al	0.074	0.188	0.074	-0.027	0.999	0.220	-4.391	0.005	1.514	1.590	0.335
Si	0.109	0.130	0.105	-0.073	0.961	0.231	-4.607	0.010	1.387	1.505	0.472
P	0.150	-0.196	0.101	-0.150	0.671	0.227	-4.380	0.015	1.357	1.396	0.661
S	0.180	-0.513	0.024	-0.153	0.136	0.218	-3.979	0.025	1.947	0.629	0.824
Cl	0.189	-0.675	0.051	-0.220	0.270	0.204	-3.376	0.037	2.037	0.389	0.925

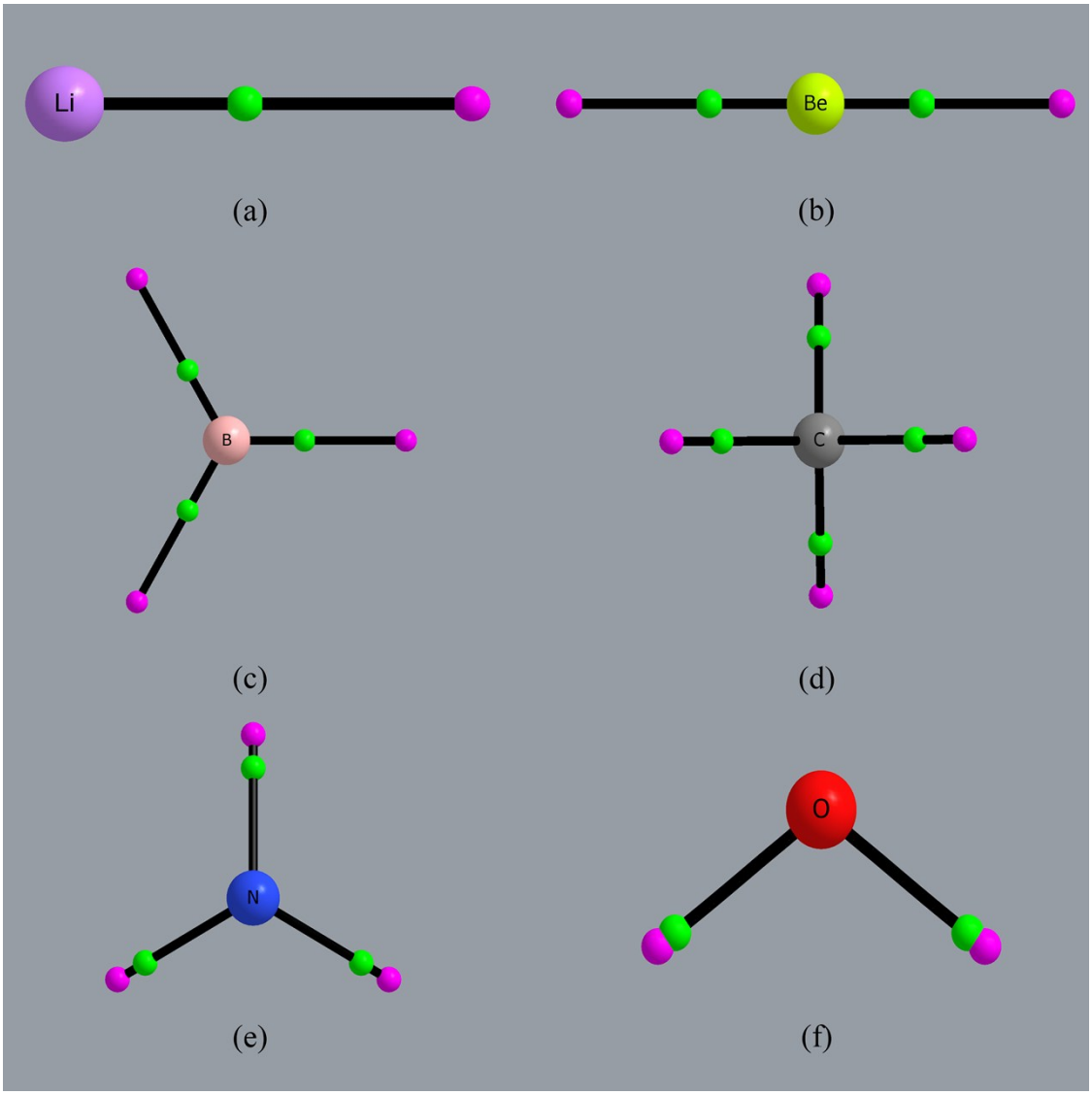

Figure S1- The MGs of the protonic species: a) LiH, (b) BeH_2, (c) BH_3, (d) CH_4, (e) NH_3 and (f) H_2O. The FH molecule has just a single (3, -3) CP very near to the fluorine nucleus thus it has no MG at the considered computational level. The purple and green spheres are the (3,-3) CPs and LCPs, respectively, while the black line are the line paths, i.e. gradient paths, connection the (3, -3) CPs and LCPs. The (3, -3) CPs at (or very near) to the central nuclei have not been depicted for clarity of the shapes. Except from HCl molecule that has a MG similar to LiH molecule, the congener species containing central atoms from the third row of the PT have exactly the same MG depicted in this figure.

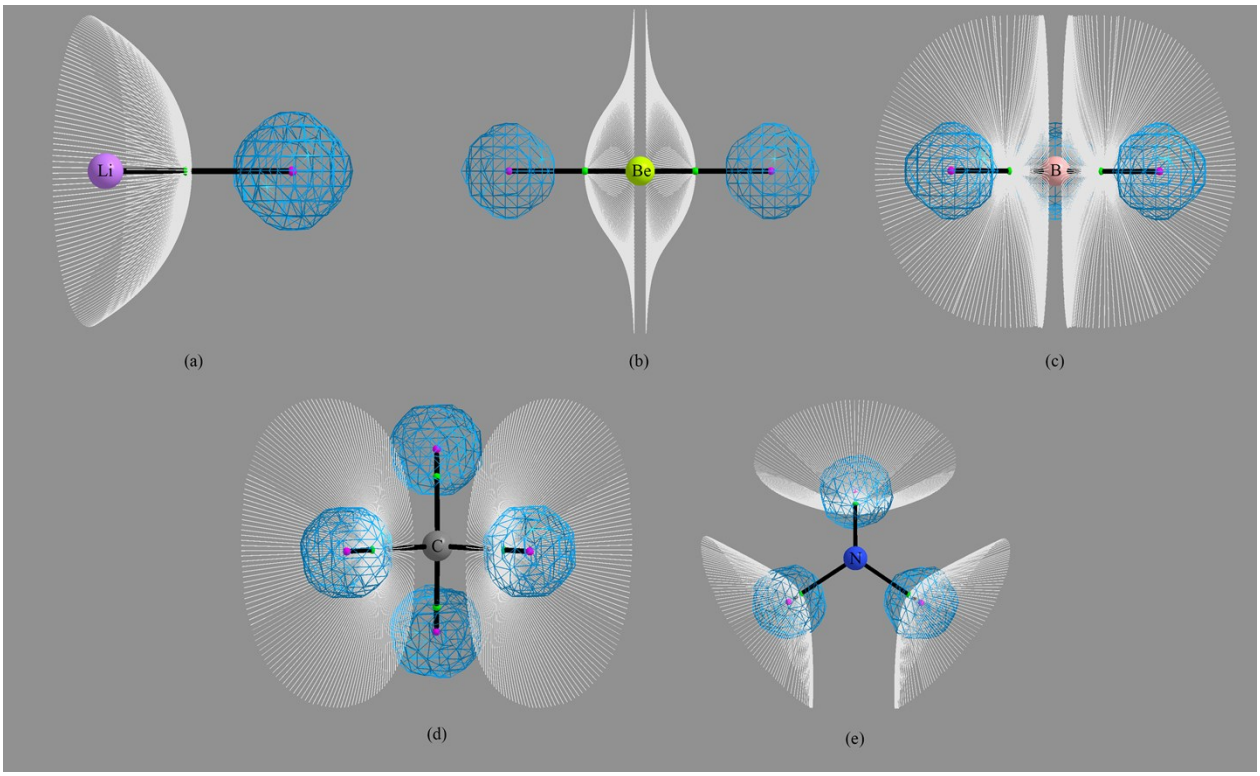

Figure S2- The MGs of the muonic species: (a) $Li\mu$, (b) $Be\mu_2$, (c) $B\mu_3$, (d) $C\mu_4$, (e) $N\mu_3$. The purple and green spheres are the (3,-3) CPs and LCPs, respectively. The (F^-,μ^+) and ($O^{2-},2\mu^+$) species have just a single (3, -3) CP very near to the fluorine and oxygen nuclei thus they have no MG at the considered computational level. The purple and green spheres are the (3,-3) CPs and LCPs, respectively, while each white line is one of the gradient paths on the inter-atomic surface. The blue spherical mesh is an iso-density surface of the muonic one-particle density, $\rho_\mu(\vec{r})=10^{-3}au$.