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


# Supporting Information

## Developing effective electronic-only coupled-cluster and Møller-Plesset perturbation theories for the muonic molecules

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Table S1- The distance between hydrogen and central atoms computed at both HF and post-HF levels (in Angstroms) for hydrides.

| | HF | MP2 | CCSD | CCSD(T) |
|---|---|---|---|---|
| **LiH** | 1.607 | 1.604 | 1.610 | 1.610 |
| **$BeH_2$** | 1.331 | 1.329 | 1.333 | 1.333 |
| **$BH_3$** | 1.188 | 1.187 | 1.191 | 1.191 |
| **$CH_4$** | 1.082 | 1.086 | 1.088 | 1.090 |
| **$NH_3$** | 0.999 | 1.012 | 1.012 | 1.015 |
| **$H_2O$** | 0.941 | 0.961 | 0.959 | 0.962 |
| **FH** | 0.899 | 0.921 | 0.918 | 0.921 |
| **NaH** | 1.919 | 1.918 | 1.926 | 1.926 |
| **$MgH_2$** | 1.708 | 1.706 | 1.712 | 1.713 |
| **$AlH_3$** | 1.581 | 1.580 | 1.585 | 1.585 |
| **$SiH_4$** | 1.478 | 1.478 | 1.482 | 1.483 |
| **$PH_3$** | 1.408 | 1.412 | 1.417 | 1.419 |
| **$H_2S$** | 1.330 | 1.336 | 1.340 | 1.342 |
| **HCl** | 1.268 | 1.275 | 1.277 | 1.279 |

Table S2- The difference (in Angstroms) between the muonic bond lenghts (in Table 1) and the analog bond lengths in hydrides (in Table S1).

| | **EHF-HF** | **EMP2-MP2** | **ECCSD-CCSD** | **ECCSD(T)-CCSD(T)** |
|---|---|---|---|---|
| **LiMu-LiH** | 0.089 | 0.085 | 0.083 | 0.083 |
| **BeHMu-$BeH_2$** | 0.082 | 0.080 | 0.078 | 0.078 |
| **$BH_2$Mu-$BeH_3$** | 0.077 | 0.070 | 0.071 | 0.070 |
| **$CH_3$Mu-$CH_4$** | 0.069 | 0.062 | 0.061 | 0.060 |
| **$NH_2$Mu-$NH_3$** | 0.061 | 0.046 | 0.046 | 0.044 |
| **OHMu-$H_2O$** | 0.056 | 0.036 | 0.038 | 0.036 |
| **FMu-FH** | 0.055 | 0.033 | 0.036 | 0.034 |
| **NaMu-NaH** | 0.079 | 0.075 | 0.072 | 0.072 |
| **MgHMu-$MgH_2$** | 0.083 | 0.078 | 0.074 | 0.074 |
| **$AlH_2$Mu-$AlH_3$** | 0.083 | 0.078 | 0.075 | 0.074 |
| **$SiH_3$Mu-$SiH_4$** | 0.081 | 0.075 | 0.073 | 0.072 |
| **$PH_2$Mu-$PH_3$** | 0.081 | 0.072 | 0.068 | 0.067 |
| **SHMu-$H_2S$** | 0.076 | 0.064 | 0.062 | 0.059 |
| **MuCl-HCl** | 0.074 | 0.061 | 0.059 | 0.057 |

Table S3- The bond lengths of the vicinal clamped hydrogen to the central atoms computed at both HF and post-HF levels (in Angstroms) for the muonic species.

| | **EHF** | **EMP2** | **ECCSD** | **ECCSD(T)** |
|---|---|---|---|---|
| **LiMu** | -- | -- | -- | -- |
| **BeHMu** | 1.332 | 1.330 | 1.334 | 1.334 |
| **$BH_2Mu$** | 1.187 | 1.185 | 1.191 | 1.192 |
| **$CH_3Mu$** | 1.082 | 1.086 | 1.088 | 1.089 |
| **$NH_2Mu$** | 0.999 | 1.012 | 1.012 | 1.015 |
| **OHMu** | 0.941 | 0.962 | 0.959 | 0.962 |
| **FMu** | -- | -- | -- | -- |
| **NaMu** | -- | -- | -- | -- |
| **MgHMu** | 1.708 | 1.707 | 1.713 | 1.714 |
| **$AlH_2Mu$** | 1.582 | 1.581 | 1.585 | 1.586 |
| **$SiH_3Mu$** | 1.478 | 1.478 | 1.482 | 1.484 |
| **$PH_2Mu$** | 1.408 | 1.413 | 1.417 | 1.420 |
| **SHMu** | 1.330 | 1.337 | 1.340 | 1.343 |
| **MuCl** | -- | -- | -- | -- |

Table S4- The total energies at corresponding optimized geometries (in Hartrees) for the muonic species and the analog hydrides.*

| | EHF | EMP2 | ECCSD | ECCSD(T) |
|---|---|---|---|---|
| **LiMu** | -7.8917 | -7.9185 | -7.9265 | -7.9265 |
| **BeHMu** | -15.6687 | -15.7300 | -15.7452 | -15.7459 |
| **$BH_2Mu$** | -26.2914 | -26.4070 | -26.4284 | -26.4312 |
| **$CH_3Mu$** | -40.1034 | -40.3067 | -40.3258 | -40.3326 |
| **$NH_2Mu$** | -56.1117 | -56.3551 | -56.3655 | -56.3742 |
| **OHMu** | -75.9552 | -76.2281 | -76.2314 | -76.2405 |
| **FMu** | -99.9606 | -100.2464 | -100.2464 | -100.2543 |
| **NaMu** | -162.2992 | -162.3259 | -162.3344 | -162.3344 |
| **MgHMu** | -200.6408 | -200.6986 | -200.7143 | -200.7148 |
| **$AlH_2Mu$** | -243.5433 | -243.6393 | -243.6623 | -243.6641 |
| **$SiH_3Mu$** | -291.1569 | -291.3041 | -291.3332 | -291.3375 |
| **$PH_2Mu$** | -342.3847 | -342.5597 | -342.5869 | -342.5943 |
| **SHMu** | -398.6128 | -398.8097 | -398.8321 | -398.8410 |
| **MuCl** | -460.0102 | -460.2200 | -460.2384 | -460.2472 |

| | HF | MP2 | CCSD | CCSD(T) |
|---|---|---|---|---|
| **LiH** | -7.9870 | -8.0153 | -8.0234 | -8.0234 |
| **$BeH_2$** | -15.7721 | -15.8341 | -15.8492 | -15.8498 |
| **$BH_3$** | -26.4004 | -26.5157 | -26.5370 | -26.5397 |
| **$CH_4$** | -40.2139 | -40.4157 | -40.4354 | -40.4420 |
| **$NH_3$** | -56.2211 | -56.4620 | -56.4735 | -56.4819 |
| **$H_2O$** | -76.0617 | -76.3312 | -76.3358 | -76.3445 |
| **FH** | -100.0623 | -100.3446 | -100.3458 | -100.3534 |
| **NaH** | -162.3912 | -162.4197 | -162.4286 | -162.4286 |
| **$MgH_2$** | -200.7384 | -200.7972 | -200.8132 | -200.8136 |
| **$AlH_3$** | -243.6453 | -243.7418 | -243.7649 | -243.7666 |
| **$SiH_4$** | -291.2616 | -291.4085 | -291.4378 | -291.4419 |
| **$PH_3$** | -342.4885 | -342.6625 | -342.6903 | -342.6974 |
| **$H_2S$** | -398.7143 | -398.9101 | -398.9334 | -398.9420 |
| **HCl** | -460.1080 | -460.3171 | -460.3366 | -460.3452 |

* Note that the correlation energies reported in Table 2 of the main text is *not* the difference between the EHF/HF and post-EHF/HF total energies reported in this table, which are computed at different optimized geometries. The correlation energies in Table 2 are the difference between post-EHF/HF and the EHF/HF energies at the corresponding post-EHF/HF optimized geometries.

Table S5- The total energies (in Hartrees) for the hydrogenated and the muoniated adducts (for details see the main text).

| | **B3LYP** | **MP2** | **CCSD** |
|---|---|---|---|
| **H-cC-NHC** | -226.84088 | -226.31437 | -226.33621 |
| **H-aC-NHC** | -226.81870 | -226.28751 | -226.31704 |
| **H-N-TAC** | -243.22921 | -242.69246 | -242.70513 |
| **H-C-TAC** | -243.22332 | -242.67744 | -242.70177 |
| **H-Si-NHSi** | -478.31277 | -477.40208 | -477.42712 |
| **H-C-NHSi** | -478.30383 | -477.39391 | -477.42554 |
| **H-Ge-NHGe** | -2265.87997 | -2263.85457 | -2263.87800 |
| **H-C-NHGe** | -2265.87359 | -2263.84930 | -2263.87687 |
| | **EB3LYP** | **EMP2** | **ECCSD** |
| **Mu-cC-NHC** | -226.73044 | -226.20609 | -226.22674 |
| **Mu-aC-NHC** | -226.70817 | -226.17889 | -226.20742 |
| **Mu-N-TAC** | -243.12379 | -242.59041 | -242.60056 |
| **Mu-C-TAC** | -243.11531 | -242.57072 | -242.59446 |
| **Mu-Si-NHSi** | -478.20860 | -477.29928 | -477.32386 |
| **Mu-C-NHSi** | -478.19280 | -477.28469 | -477.31536 |
| **Mu-Ge-NHGe** | -2265.77793 | -2263.75430 | -2263.77682 |
| **Mu-C-NHGe** | -2265.76280 | -2263.74025 | -2263.76676 |

## parent N-Heterocyclic carbene (NHC)

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.070944 | 0.000000 | -0.001735 |
| H | -0.075400 | 0.000000 | 1.062793 |
| C | 1.204366 | 0.000000 | -0.735965 |
| H | 2.235705 | 0.000000 | -0.434344 |
| N | 0.790425 | 0.000000 | -2.062069 |
| H | 1.413779 | 0.000000 | -2.848918 |
| N | -0.970072 | 0.000000 | -0.921622 |
| H | -1.942998 | 0.000000 | -0.674405 |
| C | -0.562129 | 0.000000 | -2.220938 |

## parent N-Heterocyclic silylene (NHSi)

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.048524 | 0.000000 | -0.035639 |
| H | -0.013346 | 0.000000 | 1.040245 |
| C | 1.182589 | 0.000000 | -0.770287 |
| H | 2.189757 | 0.000000 | -0.386927 |
| N | 0.921378 | 0.000000 | -2.132281 |
| H | 1.700681 | 0.000000 | -2.768784 |
| N | -1.087680 | 0.000000 | -0.830813 |
| H | -1.987148 | 0.000000 | -0.379807 |
| Si | -0.790134 | 0.000000 | -2.572907 |

## parent N-Heterocyclic germylene (NHGe)

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.040559 | 0.000000 | -0.043083 |
| H | 0.002864 | 0.000000 | 1.035062 |
| C | 1.179051 | 0.000000 | -0.780599 |
| H | 2.178401 | 0.000000 | -0.374251 |
| N | 0.958486 | 0.000000 | -2.139720 |
| H | 1.758559 | 0.000000 | -2.750829 |
| N | -1.109639 | 0.000000 | -0.799989 |
| H | -1.994423 | 0.000000 | -0.319647 |
| Ge | -0.849238 | 0.000000 | -2.664145 |

## triazolium cation (TAC)

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.064639 | 0.000000 | 0.004819 |
| H | -0.104264 | 0.000000 | 1.066989 |
| C | 1.212923 | 0.000000 | -0.739038 |
| H | 2.251332 | 0.000000 | -0.458973 |
| N | 0.786060 | 0.000000 | -2.027153 |
| H | 1.342821 | 0.000000 | -2.874602 |
| N | -0.936424 | 0.000000 | -0.911334 |
| H | -1.937429 | 0.000000 | -0.749660 |
| N | -0.515037 | 0.000000 | -2.148248 |

## H-cC-NHC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.671566 | 0.978634 | -0.005403 |
| H | 1.353582 | 1.809759 | 0.009675 |
| C | -0.671567 | 0.978633 | -0.005404 |
| H | -1.353584 | 1.809757 | 0.009675 |
| N | -1.117536 | -0.343232 | 0.071695 |
| H | -2.006349 | -0.598628 | -0.326600 |
| N | 1.117536 | -0.343230 | 0.071695 |
| H | 2.006350 | -0.598625 | -0.326600 |
| C | 0.000001 | -1.201322 | -0.119089 |
| H | 0.000001 | -2.153033 | 0.406653 |

## H-aC-NHC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.486518 | -1.044784 | -0.197995 |
| H | 0.891583 | -1.967560 | -0.573209 |
| N | -0.875293 | -0.771218 | -0.178251 |
| H | -1.585672 | -1.475495 | -0.258924 |
| N | -0.004509 | 1.141233 | 0.106789 |
| H | 0.074829 | 2.131291 | 0.246710 |
| C | -1.201036 | 0.539529 | 0.030948 |
| C | 1.172540 | 0.271016 | -0.069760 |
| H | 1.854650 | 0.335280 | 0.787897 |
| H | 1.752871 | 0.555374 | -0.960374 |

## H-Si-NHSi

| atom | X | Y | Z |
|---|---|---|---|
| C | -1.284279 | 0.679186 | 0.010600 |
| H | -2.163743 | 1.299937 | -0.047200 |
| C | -1.284279 | -0.679188 | 0.010579 |
| H | -2.163742 | -1.299938 | -0.047231 |
| N | -0.020097 | -1.228519 | 0.055331 |
| H | 0.070784 | -2.225552 | -0.033477 |
| N | -0.020096 | 1.228518 | 0.055323 |
| H | 0.070787 | 2.225551 | -0.033494 |
| Si | 1.271695 | -0.000002 | -0.132177 |
| H | 2.042087 | 0.000006 | 1.174246 |

## H-C-NHSi

| atom | X | Y | Z |
|---|---|---|---|
| C | 1.143943 | -0.861844 | 0.000000 |
| H | 1.935578 | -1.592377 | 0.000000 |
| N | -0.180305 | -1.220611 | 0.000000 |
| H | -0.404105 | -2.202422 | 0.000000 |
| N | -0.000019 | 1.186920 | 0.000000 |
| H | -0.061640 | 2.190918 | 0.000000 |
| Si | -1.358639 | 0.101079 | 0.000000 |
| C | 1.350083 | 0.616694 | 0.000000 |
| H | 1.926760 | 0.949178 | 0.878447 |
| H | 1.926760 | 0.949178 | -0.878447 |

## H-Ge-NHGe

| atom | X | Y | Z |
|---|---|---|---|
| C | -1.712638 | 0.691910 | -0.008819 |
| H | -2.617521 | 1.277233 | -0.092619 |
| C | -1.712636 | -0.691912 | -0.008823 |
| H | -2.617515 | -1.277240 | -0.092626 |
| N | -0.501294 | -1.270568 | 0.071946 |
| H | -0.452687 | -2.273328 | -0.010462 |
| N | -0.501297 | 1.270569 | 0.071943 |
| H | -0.452691 | 2.273332 | -0.010465 |
| Ge | 1.010729 | 0.000000 | -0.068399 |
| H | 1.366874 | 0.000003 | 1.493561 |

## H-C-NHGe

| atom | X | Y | Z |
|---|---|---|---|
| C | -0.775185 | -1.638381 | 0.000000 |
| H | -1.425510 | -2.499697 | 0.000000 |
| N | -1.263398 | -0.379850 | 0.000000 |
| H | -2.265202 | -0.265742 | 0.000000 |
| N | 1.218351 | -0.370197 | 0.000000 |
| H | 2.219021 | -0.264855 | 0.000000 |
| Ge | 0.000850 | 1.036347 | 0.000000 |
| C | 0.715228 | -1.738472 | 0.000000 |
| H | 1.071160 | -2.306866 | 0.877407 |
| H | 1.071160 | -2.306866 | -0.877407 |

## H-N-TAC

| atom | X | Y | Z |
|---|---|---|---|
| C | -0.680487 | 0.992095 | 0.008361 |
| H | -1.375698 | 1.812736 | -0.009311 |
| C | 0.680492 | 0.992092 | 0.008362 |
| H | 1.375708 | 1.812729 | -0.009308 |
| N | 1.097529 | -0.304909 | 0.048048 |
| H | 1.990096 | -0.648849 | -0.283385 |
| N | -1.097530 | -0.304904 | 0.048049 |
| H | -1.990100 | -0.648839 | -0.283383 |
| N | -0.000003 | -1.151603 | -0.107844 |
| H | -0.000005 | -1.916289 | 0.569785 |

## H-C-TAC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.523599 | -1.054702 | 0.000008 |
| H | 0.944408 | -2.045400 | 0.000328 |
| N | -0.778609 | -0.819784 | -0.000175 |
| H | -1.527564 | -1.504503 | -0.000051 |
| N | -0.000131 | 1.112835 | 0.000116 |
| H | -0.041099 | 2.122330 | 0.000408 |
| N | -1.132251 | 0.456859 | -0.000161 |
| C | 1.199589 | 0.270335 | -0.000007 |
| H | 1.827688 | 0.444663 | 0.884052 |
| H | 1.827179 | 0.444014 | -0.884519 |

## Mu-cC-NHC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.671609 | 0.985203 | -0.006768 |
| H | 1.353921 | 1.816064 | 0.013696 |
| C | -0.671495 | 0.985210 | -0.007292 |
| H | -1.353850 | 1.816065 | 0.013113 |
| N | -1.115712 | -0.337112 | 0.063533 |
| H | -2.005644 | -0.594382 | -0.331208 |
| N | 1.115895 | -0.337254 | 0.064172 |
| H | 2.005225 | -0.594116 | -0.332052 |
| C | 0.000041 | -1.199165 | -0.117447 |
| Bq | 0.000011 | -2.201800 | 0.426548 |

## Mu-aC-NHC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.483972 | -1.045086 | -0.182049 |
| H | 0.890641 | -1.970403 | -0.549491 |
| N | -0.878317 | -0.769807 | -0.186302 |
| H | -1.587997 | -1.473553 | -0.277234 |
| N | -0.007864 | 1.137098 | 0.125869 |
| H | 0.071330 | 2.128157 | 0.258516 |
| C | -1.205114 | 0.539353 | 0.027770 |
| C | 1.167097 | 0.268116 | -0.061458 |
| H | 1.863361 | 0.335704 | 0.782592 |
| Bq | 1.769370 | 0.565087 | -1.004384 |

## Mu-Si-NHSi

| atom | X | Y | Z |
|---|---|---|---|
| C | -1.289712 | 0.678870 | 0.008953 |
| H | -2.169042 | 1.300999 | -0.033849 |
| C | -1.289771 | -0.678978 | 0.008890 |
| H | -2.169252 | -1.300932 | -0.033626 |
| N | -0.023904 | -1.226537 | 0.033410 |
| H | 0.068124 | -2.224311 | -0.045004 |
| N | -0.023810 | 1.226315 | 0.033545 |
| H | 0.068428 | 2.224089 | -0.044579 |
| Si | 1.270107 | -0.000157 | -0.148462 |
| Bq | 2.077949 | 0.000643 | 1.233223 |

## Mu-C-NHSi

| atom | X | Y | Z |
|---|---|---|---|
| C | 1.139992 | -0.860289 | 0.059105 |
| H | 1.932048 | -1.589876 | 0.023282 |
| N | -0.182138 | -1.221086 | -0.016394 |
| H | -0.404259 | -2.203137 | -0.031161 |
| N | -0.003534 | 1.184604 | 0.035850 |
| H | -0.065399 | 2.188502 | 0.027486 |
| Si | -1.361759 | 0.099034 | -0.028738 |
| C | 1.344693 | 0.612792 | 0.013394 |
| H | 1.952455 | 0.969817 | 0.856777 |
| Bq | 1.926316 | 0.936352 | -0.939601 |

## Mu-Ge-NHGe

| atom | X | Y | Z |
|---|---|---|---|
| C | -1.718225 | 0.690833 | -0.011272 |
| H | -2.622440 | 1.278367 | -0.083779 |
| C | -1.718249 | -0.690733 | -0.010428 |
| H | -2.622495 | -1.278487 | -0.080928 |
| N | -0.502970 | -1.268065 | 0.055538 |
| H | -0.452245 | -2.270997 | -0.021511 |
| N | -0.502846 | 1.267953 | 0.054289 |
| H | -0.452311 | 2.271192 | -0.018854 |
| Ge | 1.002727 | -0.000138 | -0.085374 |
| Bq | 1.394116 | 0.000073 | 1.553497 |

## Mu-C-NHGe

| atom | X | Y | Z |
|---|---|---|---|
| C | -0.772806 | -1.633089 | 0.060746 |
| H | -1.421981 | -2.495241 | 0.083493 |
| N | -1.262712 | -0.380362 | -0.036875 |
| H | -2.264817 | -0.268648 | -0.049083 |
| N | 1.215789 | -0.367904 | 0.085998 |
| H | 2.215268 | -0.262505 | 0.033980 |
| Ge | 0.001070 | 1.038577 | -0.054143 |
| C | 0.710182 | -1.731481 | 0.013141 |
| H | 1.092013 | -2.363305 | 0.828301 |
| Bq | 1.054469 | -2.270622 | -0.965557 |

## Mu-N-TAC

| atom | X | Y | Z |
|---|---|---|---|
| C | -0.679135 | 0.998900 | 0.006222 |
| H | -1.375781 | 1.818190 | -0.010165 |
| C | 0.679177 | 0.998870 | 0.006124 |
| H | 1.375732 | 1.818224 | -0.010577 |
| N | 1.096153 | -0.300885 | 0.048452 |
| H | 1.985632 | -0.643870 | -0.291657 |
| N | -1.096255 | -0.300853 | 0.048729 |
| H | -1.985453 | -0.643815 | -0.292129 |
| N | -0.000060 | -1.147538 | -0.096295 |
| Bq | -0.000007 | -1.962965 | 0.580669 |

## Mu-C-TAC

| atom | X | Y | Z |
|---|---|---|---|
| C | 0.519816 | -1.052118 | 0.012546 |
| H | 0.940987 | -2.042548 | 0.016560 |
| N | -0.782688 | -0.820130 | -0.003537 |
| H | -1.529556 | -1.506783 | -0.013073 |
| N | -0.004098 | 1.111149 | 0.016891 |
| H | -0.045134 | 2.120307 | 0.010394 |
| N | -1.139098 | 0.455349 | -0.004343 |
| C | 1.192371 | 0.268721 | 0.008073 |
| H | 1.833921 | 0.444832 | 0.881352 |
| Bq | 1.856288 | 0.447870 | -0.924863 |