Leading Interaction Components in Structure and Reactivity of Noble Gases Compounds

Francesca Nunzi,[a,b] Giacomo Pannacci,[a] Francesco Tarantelli,[a,b] Leonardo Belpassi,[b] David Cappelletti,[a] Stefano Falcinelli,[c] Fernando Pirani[a,b]**

[a] Dipartimento di Chimica, Biologia e Biotecnologie, via Elce di Sotto 8, I-06123 Perugia, Italy

[b] Istituto CNR di Scienze e Tecnologie Chimiche "Giulio Natta" (CNR-SCITEC), via Elce di Sotto, I-06123 Perugia, Italy

[c] Dipartimento di Ingegneria Civile ed Ambientale, Università degli Studi di Perugia, via G. Duranti 93, 06215 Perugia, Italy

Corresponding Author **E-mail: francesca.nunzi@unipg.it; fernando.pirani@unipg.it*

Supporting Information

Table S1. Potential parameters (equilibrium distances, R_m, Å, potential well depth, D_m, meV, and long range dipole-dipole dispersion coefficient, C_6, eV·Å^6) predicted for NgRn systems.

system	R_m	D_m	C_6
HeRn	4.09	3.03	14.2
NeRn	4.08	6.77	31.3
ArRn	4.21	18.35	101.5
KrRn	4.29	24.22	150.0
XeRn	4.41	30.35	222.1
RnRn	4.49	36.77	300.6

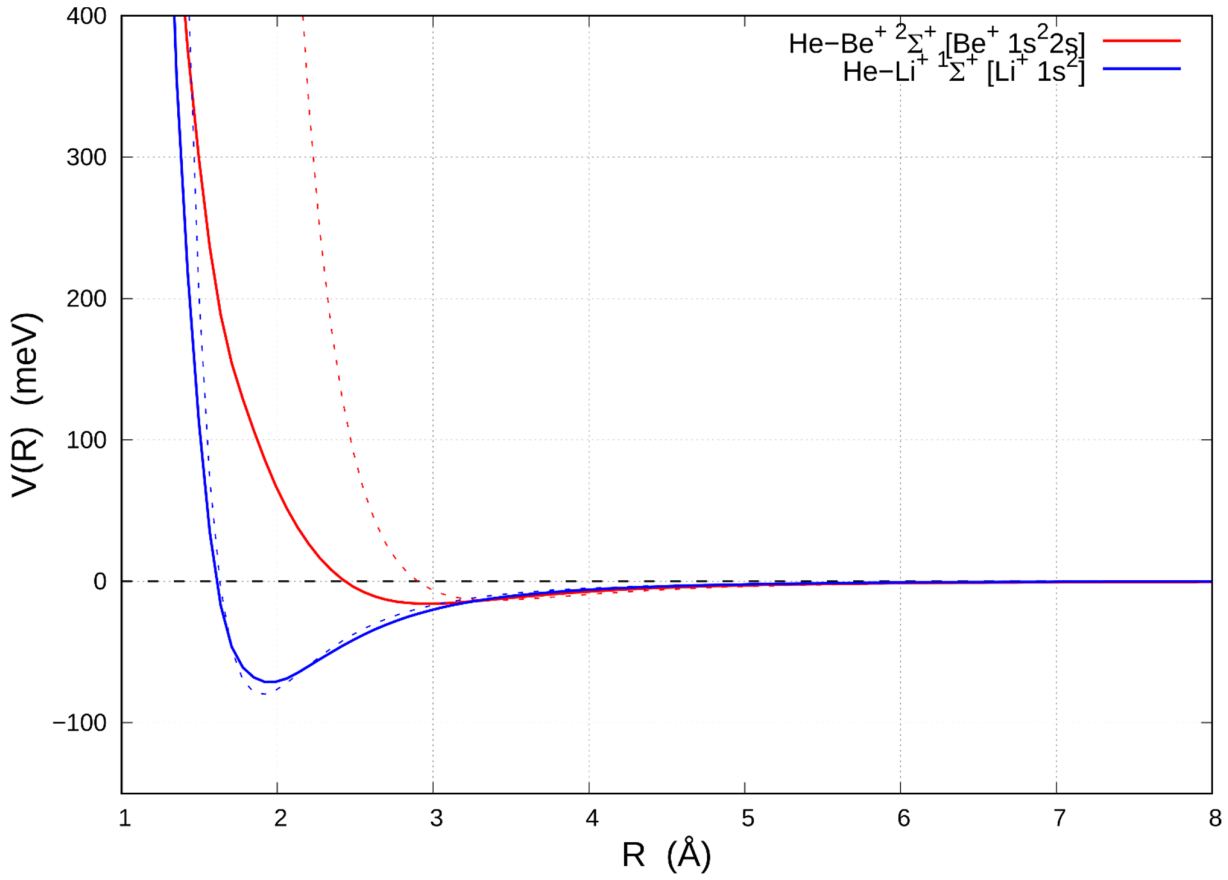

Figure S1. Potential energy curves for the ionic adducts $HeBe^+$ and $HeLi^+$ in the excited $^2\Sigma^+$ [Be^+ *1s*^{2} *2s*] and $^1\Sigma^+$ [Li^+ *1s*^{2}] electronic state, computed at FCI/AVTZ level of theory (solid lines) compared to the parametrized energy functions (dashed lines). The curves are shifted to a unique relative energy scale for an easy comparison of their character.

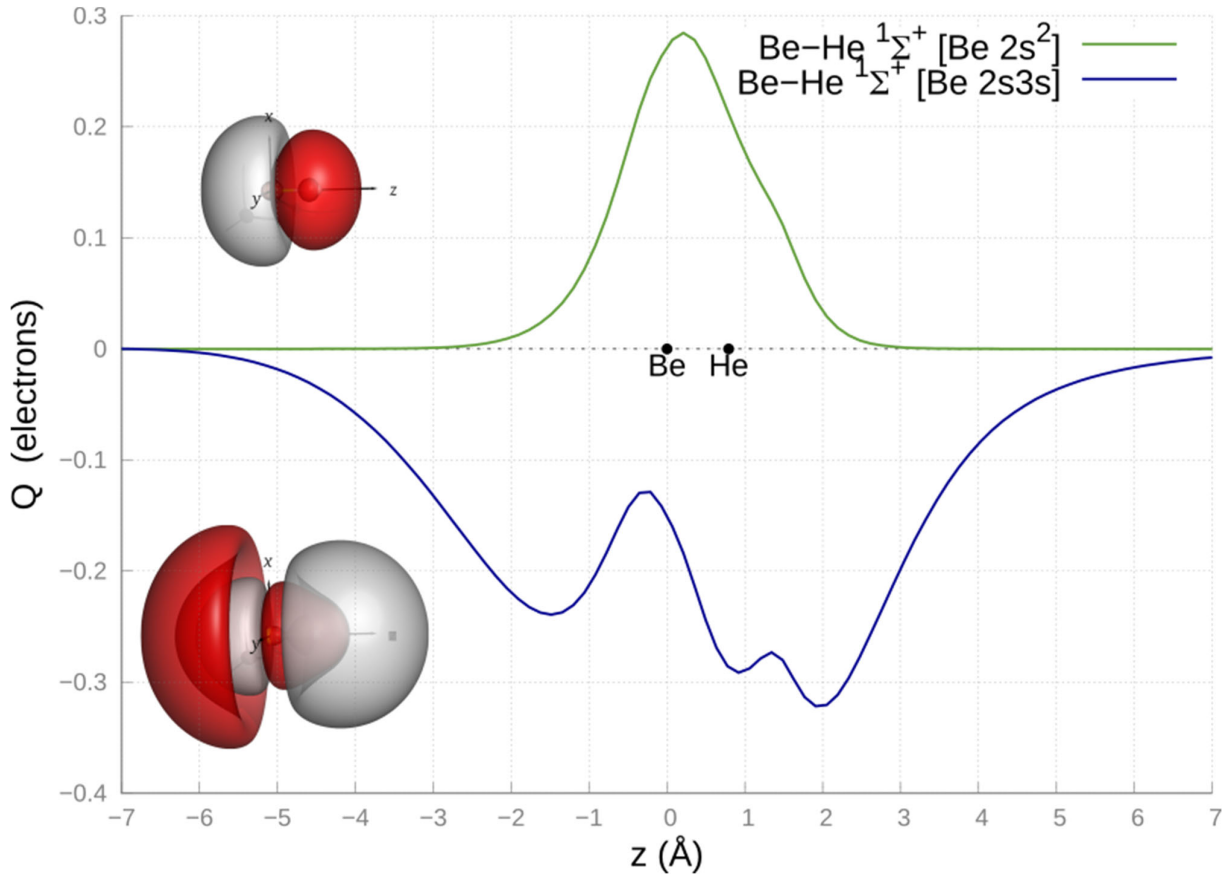

Figure S2. CDF curves (CCSD/AVTZ) for the ground and excited $^1\Sigma^+$ (Be *2s3s*) states of Be–He at a separation of 1.5 Å. The function gives, at each point along the *z* axis joining the atoms, the amount of electronic charge *Q* that, upon formation of the adduct, shifts from left to right (if positive) or from right to left (if negative) across a perpendicular plane through *z*. Dots correspond to the nuclei position projection on the *z* axis. 3D contour plot of the electron density difference between the adduct and its fragments is also shown (cutoff $=\pm 2\times10^{-4}$ e/bohr^3, with grey/red colors corresponding to positive/negative isodensity values).

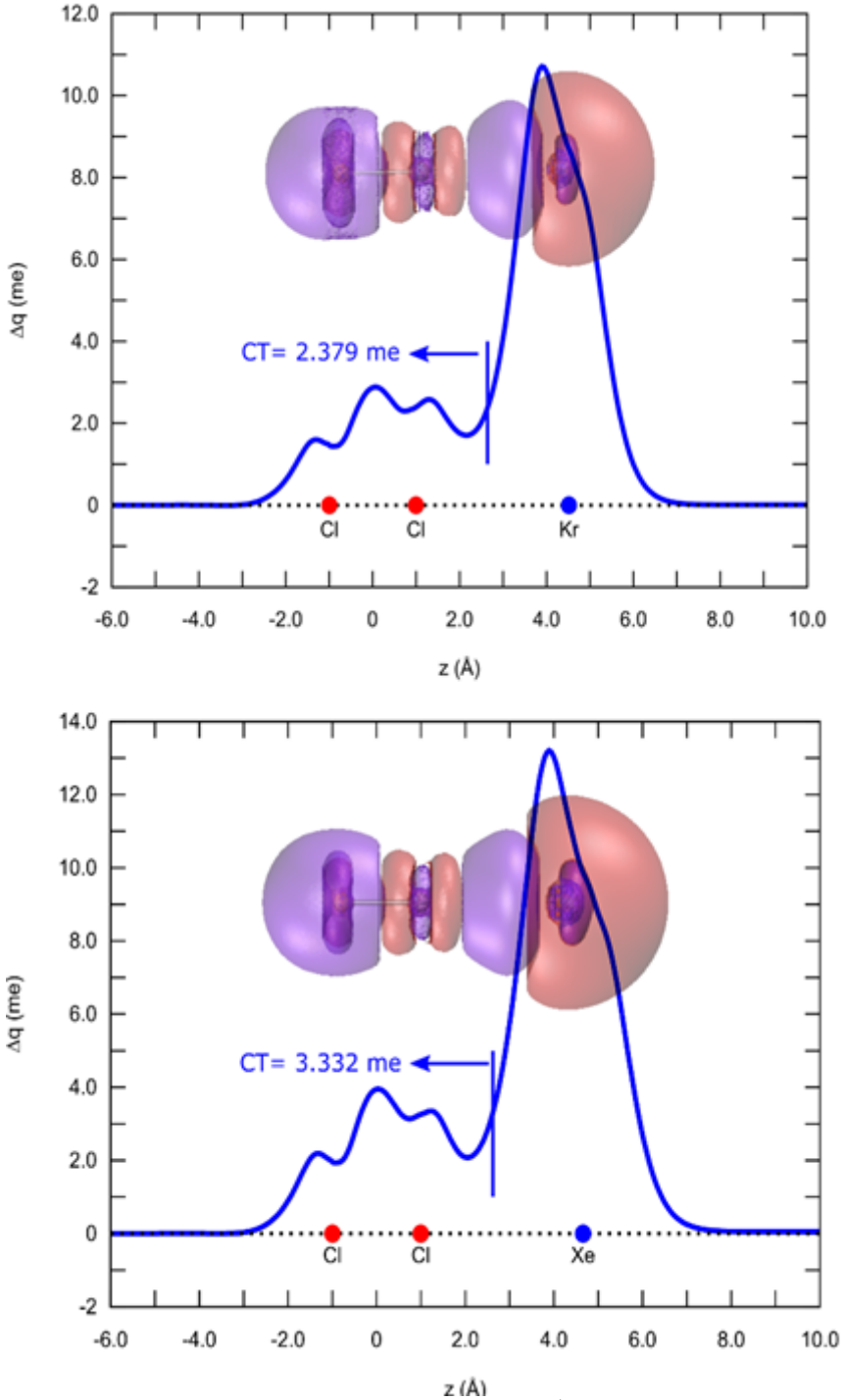

Figure S3. CDF curves (CCSD/AVQZ) for the $(X^1\Sigma_g)$ $Kr\text{-}Cl_2$ (top) and $Xe\text{-}Cl_2$ (bottom) in the linear configuration. Dots correspond to the nuclei position projection on the z axis. 3D contour plot of the electron density difference between the adduct and its fragments is also shown (cutoff $=\pm 8\times10^{-5}$ e/bohr^3, with blue/red colors corresponding to positive/negative isodensity values).