

Noble Gas Bound Beryllium Chromate and Beryllium Hydrogen Phosphate: A Comparison with Noble Gas Bound Beryllium Oxide

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Supporting Information

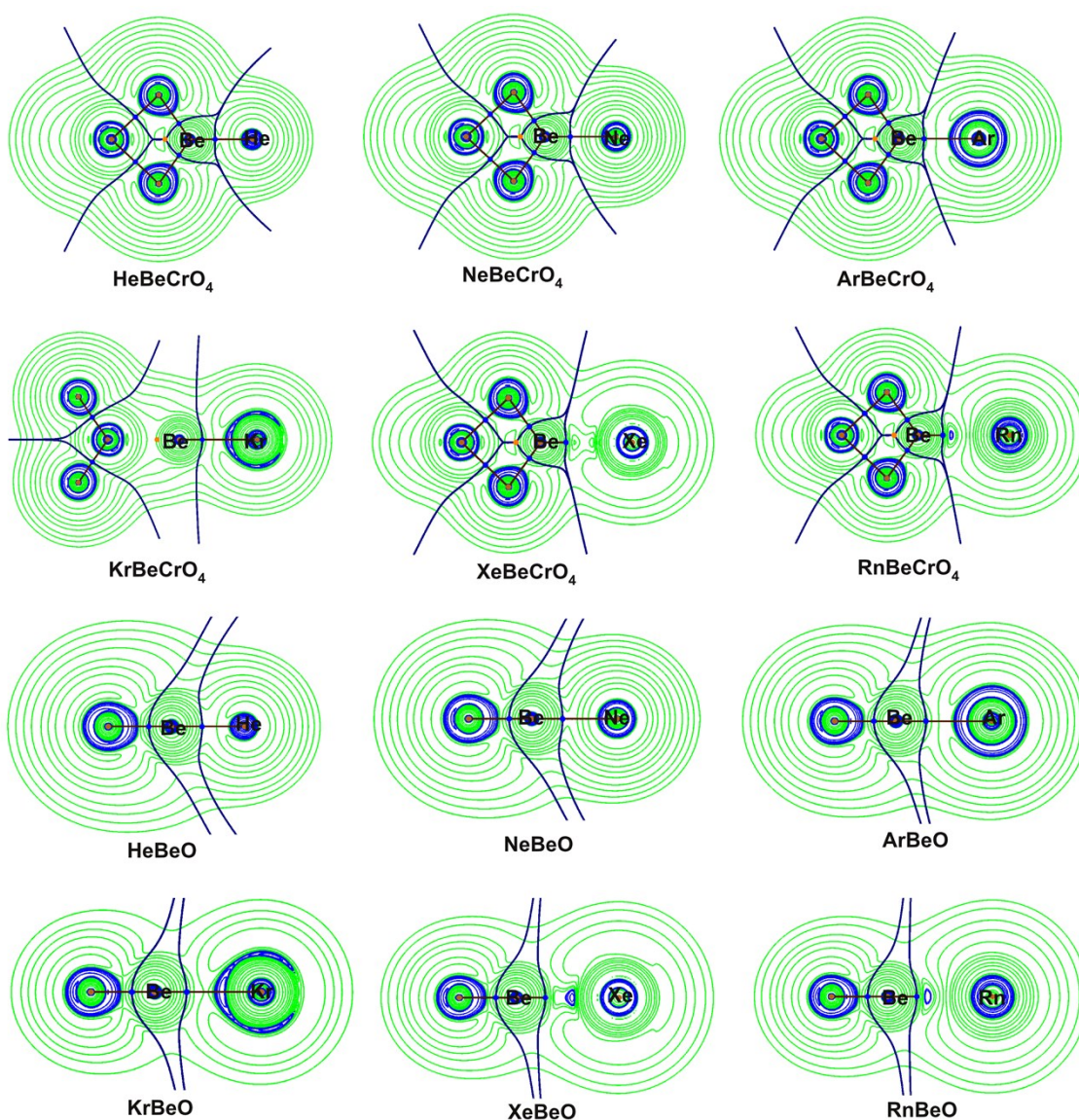


Fig. S1 The plots of Laplacian of electron density ($\nabla^2\rho(r)$) of NgBeCrO₄ and NgBeO (Ng = He–Rn) complexes at the MPW1B95/def2-QZVPPD/WTBS level. (Green solid lines show the region with $\nabla^2\rho(r)> 0$ and blue dashed lines show the region with $\nabla^2\rho(r)< 0$)

Table S1. ZPE corrected dissociation energy (D_0 , kcal/mol), dissociation enthalpy (ΔH , kcal/mol) and free energy change (ΔG , kcal/mol) at 298 K for the dissociation processes: NgBeHPO₄ $\rightarrow$ Ng + BeHPO₄ computed at the MP2/def2-QZVPPD level.

Complex	D_0	ΔH	ΔG
HeBeHPO ₄	2.2	2.6	-4.0
NeBeHPO ₄	3.9	4.1	-2.6
ArBeHPO ₄	9.4	9.5	2.7
KrBeHPO ₄	11.3	11.5	4.7
XeBeHPO ₄	13.7	13.8	7.2
RnBeHPO ₄	15.3	15.4	8.8