Using SCPC at 0D system - $C_4H_5N_2^+$

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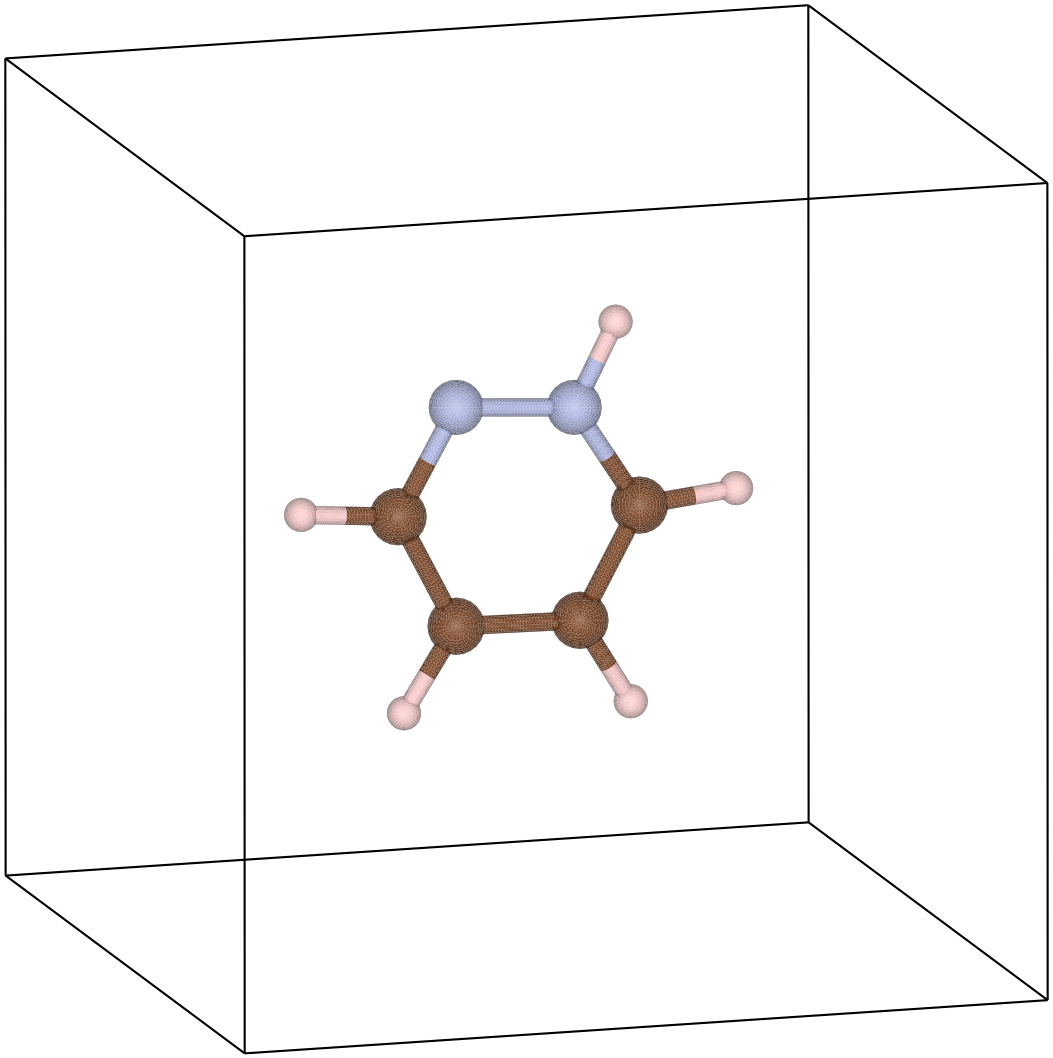
0D System: charged molecule $C_4H_5N_2^+$



Formation Energy (ΔE)

- Default calculation

$$\Delta E_{Def}(X^q) = [E(X^q) + qE_{fermi}(X)] - E(X) \quad (1)$$

- SCPC method

$$\Delta E_{SCPC}(X^q) = [E(X^q)_{SCPC} + qE_{PotAlig} + qE_{fermi}(X)] - E(X) \quad (2)$$

Plain Results

Table: Lateral unit cell size (L), electronic energy for the charged ($E(X^q)$) and neutral ($E(X)$) systems, the Fermi energy of the neutral system ($E_{fermi}(X)$), the defaulft formation energy ($\Delta E_{Def}(X^q)$) the corrected electronic energy for the charged system ($E(X^q)_{SCPC}$), the potential alignment ($E_{PotAlig}$) and the corrected formation energy ($\Delta E_{SCPC}(X^q)$). All energies are expressed in eV.

L(Å)	$E(X^q)$	$E(X)$	$E_{fermi}(X)$	$\Delta E_{Def}(X^q)$	$E(X^q)_{SCPC}$	$E_{PotAlig}$	$\Delta E_{SCPC}(X^q)$
7	-66.69	-68.57	-0.95	0.93	-64.41	0.02	3.23
9	-65.64	-68.68	-1.75	1.29	-63.74	0.03	3.22
11	-65.05	-68.69	-2.10	1.54	-63.42	0.03	3.19
13	-64.67	-68.69	-2.19	1.83	-63.26	0.02	3.26
15	-64.41	-68.69	-2.33	1.95	-63.17	0.02	3.21
17	-64.22	-68.69	-2.31	2.15	-63.12	0.02	3.27
19	-64.07	-68.69	-2.38	2.23	-63.08	0.02	3.24
NWChem PBE/Def2-TZVP 3.05 eV							

Formation Energy vs. 1/L